APS March Meeting 2011

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Sunday, March 20, 2011 1:00PM - 3:00PM –

Session 1A FIAP: Industrial Physics Forum: History, Current Status, Future Prospects Ballroom C1

1:00PM 1A.00001 Room-Temperature Superconductivity: Prospects but Challenges[1] J.C. SEAMUS DAVIS, Brookhaven National Laboratory, Cornell University and St. Andrews University — Why do we not have ambient temperature superconductivity and all the benefits it would bring? If the challenge were less than profound, our celebrated industrial research/development approach should have succeeded in achieving this objective already. In fact, however, the unknowns we face with this issue are believed to involve entangled-many-body quantum mechanics beyond the limits of present understanding. We shall review these issues.

[1]This work was supported by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Basic Energy Sciences.

1:40PM 1A.00002 Confirmation of BCS Theory and Its Impact on Applications Past and Future , MALCOLM BEASLEY, Stanford University — The experimental confirmation of BCS theory established it as the correct microscopic theory of superconductivity. It also led to applications of superconductivity distinct from those based on the Josephson effect and the magnetic properties of superconductors. The most prominent of these are SIS mixers for astronomy and high-Q filters for the cellular phone industry. In this talk we trace these historical developments and consider where today's more novel (beyond simple BCS) superconductors might be useful looking forward.

2:20PM 1A.00003 From BCS to Vortices: A 40 Year Personal Journey through Superconductivity from Basic Research to Power Applications , PAUL M. GRANT, IBM Research Staff Member Emeritus, San Jose, CA 95120 USA — A century has passed since the discovery of superconductivity in Leiden followed 75 years later by the Great Leap Forward in Zuerich.[1] This talk will chronicle the author's trajectory through the science and technology of superconductivity first taking off with his IBM career in fundamental research on organic and layered copper oxide perovskite superconductors to a final landing at EPRI to explore applications of the latter to the electric power industry. Although many fundamental mysteries remain with respect to the copper and iron compounds, especially regarding the BCS pairing mechanism, nonetheless a significant number of successful demonstrations of cables, rotating machinery, storage and power conditioning equipment employing both low-and high-T_C superconducting materials[2] have been undertaken worldwide since the decade of the 1960s to the present. However, massive application to the power industry has yet to take place or be inserted into utility long-range planning cycles.[3] Although there will certainly be a relatively small number of opportunistic deployments in those situations where superconductivity has a compelling advantage over conventional technology, its time will more likely await a future revolution in energy and electricity infrastructure such as a symbiosis[4] of nuclear and hydrogen with superconductivity. Perhaps the distant future will even deliver the dream[5] of a room temperature superconductor.

[1] "20th Anniversary of the Woodstock of Physics," APS March Meeting 2007, Denver, CO.
[2]P. M. Grant, IEEE Trans. Appl. Supercon. **7**, 112 (1997).
[3]P. M. Grant, "Superconductivity in Power Applications," submitted to the ICEC-ICMC 2010 Conference Proceedings.
[4]P. M. Grant, C. Starr and T. J. Overbye, "A Power Grid for the Hydrogen Economy," Scientific American, July 2006, p.76.
[5]P. M. Grant, Physics Today, May 1998.

Sunday, March 20, 2011 3:30PM - 5:30PM –

Session 1B FIAP: Industrial Physics Forum: Large-Scale Applications Ballroom C1

3:30PM 1B.00001 Superconducting Materials, Magnets and Electric Power Applications , GEORGE CRABTREE, Argonne National Laboratory and University of Illinois at Chicago — The surprising discovery of superconductivity a century ago launched a chain of convention-shattering innovations and discoveries in superconducting materials and applications that continues to this day. The range of large-scale applications grows with new materials discoveries - low temperature NbTi and Nb_3Sn for liquid helium cooled superconducting magnets, intermediate temperature MgB_2 for inexpensive cryocooled applications including MRI magnets, and high temperature YBCO and BSSCO for high current applications cooled with inexpensive liquid nitrogen. Applications based on YBCO address critical emerging challenges for the electricity grid, including high capacity superconducting cables to distribute power in urban areas; transmission of renewable electricity over long distances from source to load; high capacity DC interconnections among the three US grids; fast, self-healing fault current limiters to increase reliability; low-weight, high capacity generators enabling off-shore wind turbines; and superconducting magnetic energy storage for smoothing the variability of renewable sources. In addition to these grid applications, coated conductors based on YBCO deposited on strong Hastelloy substrates enable a new generation of all superconducting high field magnets capable of producing fields above 30 T, approximately 50% higher than the existing all superconducting limit based on Nb_3Sn. The high fields, low power cost and the quiet electromagnetic and mechanical operation of such magnets could change the character of high field basic research on materials, enable a new generation of high-energy colliding beam experiments and extend the reach of high density superconducting magnetic energy storage.

4:10PM 1B.00002 High Temperature Superconductors for the Electric Power Grid , ALEXIS P. MALOZEMOFF, American Superconductor Corp. — High Temperature Superconductor power equipment is positioned to play a key role in addressing our national and global energy challenges. While the most obvious benefit is efficiency by using the superconductor's lossless current flow to cut the 10% power lost in the grid, other benefits are likely to be even more impactful. These benefits arise from the high current density of superconductor wire which enables design of highly power-dense and compact equipment including high capacity cables and rotating machinery – generators and motors. Vast and dense urban areas are becoming home to an increasingly large proportion of world population, and high capacity ac superconductor cables offer a non-interfering and easily installed solution to increasing urban power needs. Longer term, the ultra-low loss of long-distance dc superconductor cables offers strengthened links and power sharing across wide geographical areas. Compact superconductor generators are the key to high power off-shore wind turbines, a major source of renewable energy. Some of these applications have reached a sophisticated level of demonstration, initiating commercial use.

4:50PM 1B.00003 Industrial Large Scale Applications of Superconductivity – Current and Future Trends , KATHLEEN AMM, GE Global Research — Since the initial development of NbTi and Nb3Sn superconducting wires in the early 1960's, superconductivity has developed a broad range of industrial applications in research, medicine and energy. Superconductivity has been used extensively in NMR low field and high field spectrometers and MRI systems, and has been demonstrated in many power applications, including power cables, transformers, fault current limiters, and motors and generators. To date, the most commercially successful application for superconductivity has been the high field magnets required for magnetic resonance imaging (MRI), with a global market well in excess of $4 billion excluding the service industry. The unique ability of superconductors to carry large currents with no losses enabled high field MRI and its unique clinical capabilities in imaging soft tissue. The rapid adoption of high field MRI with superconducting magnets was because superconductivity was a key enabler for high field magnets with their high field uniformity and image quality. With over 30 years of developing MRI systems and applications, MRI has become a robust clinical tool that is ever expanding into new and developing markets. Continued innovation in system design is continuing to address these market needs. One of the key questions that innovators in industrial superconducting magnet design must consider today is what application of superconductivity may lead to a market on the scale of MRI? What are the key considerations for where superconductivity can provide a unique solution as it did in the case of MRI? Many companies in the superconducting industry today are investigating possible technologies that may be the next large market like MRI.

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A1 DCMP: Silicon Qubits Ballroom A1

8:00AM A1.00001 Coherent control of donor states in Si[1] , THORNTON GREENLAND, London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, WC1H 0AH, England — The spin degrees of freedom of group V donors in Si satisfy many of the criteria required for qubits [1,2]. The orbital Rydberg states of group V donors can also be used to control these spins coherently [3,4]. Critical to such schemes are the population (T_1) and dephasing (T_2) lifetimes of these Rydberg states. We describe the use the free electron laser FELIX [5] to perform pump-probe experiments to measure T_1 [6] and photon echo experiments to measure T_2 [7]. The lifetimes we obtain from a theoretical analysis of the experiments are $\sim$ 200 ps, which is long enough for orbital excitation to be a practical control mechanism for 2-qubit quantum gates. The experimental and theoretical analysis of these gates is also described.

[1] DiVincenzo D P, "The Physical Implementation of Quantum Computation," arXiv:quant-ph/0002077
[2] Morley G W, *et al*, "Initializing, manipulating and storing quantum information with bismuth dopants in silicon" *Nature Materials* **9** 725 – 729 (2010) (doi:10.1038/nmat2828)
[3] Stoneham, A. M., Fisher, A. J. & Greenland, P.T. "Optically driven silicon-based quantum gates with potential for high-temperature operation" *J Phys Condens Matter* **15**, L447-451 (2003).
[4] http://arxiv.org/find/cond-mat/1/au:+Wu_W/0/1/0/all/0/1 Wu W, Greenland P T, Fisher A J, "Exchange in multi-defect semiconductor clusters: assessment of 'control-qubit' architectures" http://arxiv.org/abs/0711.0084
[5] Knippels G M H, *et al*, "Generation and Complete Electric-Field Characterization of Intense Ultrashort Tunable Far-Infrared Laser Pulses" *Phys. Rev. Lett.* **83**, 1578-1581 (1999)
[6] N Q Vinh N Q et al, "Silicon as a model ion trap: time domain measurements of donor Rydberg states" *PNAS* 105 10649-10653 (2008)
[7] Greenland P T et al *Nature*, 465, 1057-1061 (2010) (doi:10.1038/nature09112)

[1]Supported by EPSRC (COMPASSS, Grant Ref EP/H026622/1).

8:36AM A1.00002 Single-shot readout and microwave control of an electron spin in silicon , ANDREA MORELLO, Centre for Quantum Computation and Communication Technology, University of New South Wales — The electron spin of a donor in silicon is an excellent candidate for a solid-state qubit. It is known to have very long coherence and relaxation times in bulk [1], and several architectures have been proposed to integrate donor spin qubits with classical silicon microelectronics [2]. Here we show the first experimental proof of single-shot readout of an electron spin in silicon. The device consists of implanted phosphorus donors, tunnel-coupled to a silicon Single-Electron Transistor (SET), where the SET island is used as a reservoir for spin-to-charge conversion [3]. The large charge transfer signals allow readout fidelity $> 90\%$ with 3 μs response time. By measuring the occurrence of excited spin states as a function of wait time, we find spin lifetimes (T_1) up to $\sim$ 6 s at $B = 1.5$ T, and a magnetic-field dependence $T_1^{-1} \propto B^5$ consistent with that of phosphorus donors in silicon [4]. In a subsequent experiment we have integrated the single-shot spin readout device with an on-chip microwave transmission line for coherent control of the electron spin. We have detected the spin resonance of a single electron, and observed two hyperfine-split resonance lines, consistent with Stark-shifted coupling to the ^{31}P nuclear spin. Further experiments are underway to demonstrate coherent spin control and observe Rabi oscillations. This demonstrates the microwave control of a single spin, combined – for the first time in the same experiment – with electrically detected single-shot spin readout.

[1] A. M. Tyryshkin *et al.*, Phys. Rev. B **68**, 193207 (2003).
[2] L. C. L. Hollenberg *et al.*, Phys. Rev. B. **74**, 045311 (2006).
[3] A. Morello *et al.*, Phys. Rev. B **80**, 081307(R) (2009).
[4] A. Morello *et al.*, Nature **467**, 687 (2010).

9:12AM A1.00003 Integrated Quantum Photonics , JEREMY O'BRIEN, University of Bristol — Of the various approaches to quantum computing [1], photons are particularly appealing for their low-noise properties and ease of manipulation at the single qubit level [2]. Encoding quantum information in photons is also an appealing approach to quantum communication, metrology (eg. [3]), measurement (eg. [4]) and other quantum technologies [5]. However, the implementation of optical quantum circuits with bulk optics has reached practical limits. We have developed an integrated waveguide approach to photonic quantum circuits for high performance, miniaturisation and scalability [6]. Here we report high-fidelity silica-on-silicon integrated optical realisations of key quantum photonic circuits, including two-photon quantum interference and a controlled-NOT logic gate [7]. We have demonstrated controlled manipulation of up to four photons on-chip, including high-fidelity single qubit operations, using a lithographically patterned resistive phase shifter [8]. We have used this architecture to implement a small-scale compiled version of Shor's quantum factoring algorithm [9] and demonstrated heralded generation of tuneable four photon entangled states from a six photon input [10]. We have combined waveguide photonic circuits with superconducting single photon detectors [11]. Finally, we describe complex quantum interference behaviour in multi-mode inter- ference devices with up to eight inputs and outputs [12], and quantumwalks of correlated particles in arrays of coupled waveguides [13].

[1] T. D. Ladd, F. Jelezko, R. Laflamme, Y. Nakamura, C. Monroe, and J. L. OBrien, Nature 464, 45 (2010).
[2] J. L. O'Brien, Science 318, 1567 (2007).
[3] T. Nagata, R. Okamoto, J. L. O'Brien, K. Sasaki, and S. Takeuchi, Science 316, 726 (2007).
[4] R. Okamoto, J. L. O'Brien, H. F. Hofmann, T. Nagata, K. Sasaki, and S. Takeuchi, Science 323, 483 (2009).
[5] J.L.O'Brien,A.Furusawa, and J.Vuckovic, NaturePho- ton. 3, 687 (2009).
[6] A. Politi, M. J. Cryan, J. G. Rarity, S. Yu, and J. L. O'Brien, Science 320, 646 (2008).
[7] A. Laing, A. Peruzzo, A. Politi, M. R. Verde, M. Halder, T. C. Ralph, M. G. Thompson, and J. L. O'Brien, arXiv:1004.0326
[8] J. C. F. Matthews, A. Politi, A. Stefanov, and J. L. O'Brien, Nature Photon. 3, 346 (2009).
[9] A. Politi, J. C. F. Matthews, and J. L. O'Brien, Science 325, 1221 (2009).
[10] J. C. F. Matthews, A. Peruzzo, D. Bonneau, and J. L. O'Brien, arXiv:1005.5119
[11] C. M. Natarajan, A. Peruzzo, S. Miki, M. Sasaki, Z. Wang, B. Baek, S. Nam, R. H. Hadfield, and J. L. O'Brien, Appl. Phys. Lett. 96, 211101 (2010).
[12] A. Peruzzo, A. Laing, A. Politi, T. Rudolph, and J. L. O'Brien, arXiv:1005.5119
[13] A. Peruzzo, M. Lobino, J. C. F. Matthews, N. Matsuda, A. Politi, K. Poulios, X.-Q. Zhou, Y. Lahini, N. Ismail, K. Worhoff, Y. Bromberg, Y. Silberberg, M. G. Thompson, and J. L. O'Brien, Science 329, 1500 (2009)

9:48AM A1.00004 The initialization and manipulation of quantum information stored in silicon by bismuth dopants , JOHAN VAN TOL, National High Magnetic Field Laboratory and Florida State University, Tallahasse — This abstract not available.

10:24AM A1.00005 ABSTRACT WITHDRAWN –

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A2 DCMP: Compressibility and Transport in Bilayer Graphene Ballroom A2

8:00AM A2.00001 Electronic compressibility of bilayer graphene , ERIK HENRIKSEN, Caltech — We have recently measured the electronic compressibility of bilayer graphene [1], allowing exploration of the thermodynamic density of states as a function of applied electric and magnetic fields. Utilizing dual-gated field-effect devices, we can independently vary both the carrier density and the size of the tunable band gap. An oscillating voltage applied to a back gate generates corresponding signals in the top gate via electric fields lines which penetrate the graphene, thereby allowing a direct measurement of the inverse compressibility, K^{-1}, of the bilayer [2]. We have mapped K^{-1}, which is proportional to the inverse density of states, as a function of the top and back gate voltages in zero and finite magnetic field. A sharp increase in K^{-1} near zero density is observed with increasing electric field strength, signaling the controlled opening of a band gap. At high magnetic fields, broad Landau level (LL) oscillations are observed, directly revealing the doubled degeneracy of the lowest LL and allowing for a determination of the disorder broadening of the levels. We compare our results to tight-binding calculations of the bilayer band structure, and to recent theoretical studies of the compressibility of bilayer graphene. Together, these clearly illustrate the unusual hyperbolic nature of the low energy band structure, reveal a sizeable electron-hole asymmetry, and suggest that many-body interactions play only a small role in bilayer-on-substrate devices. This work is a collaboration with J. P. Eisenstein of Caltech, and is supported by the NSF under Grant No. DMR-0552270 and the DOE under Grant No. DE-FG03-99ER45766.

[1] E. A. Henriksen and J. P Eisenstein, Phys. Rev. B **82**, 041412(R) (2010).
[2] J. P. Eisenstein, L. N. Pfeiffer, and K. W. West, Phys. Rev. Lett. **68**, 674 (1992); Phys. Rev. B **50**, 1760 (1994).

8:36AM A2.00002 Electronic Structure and Carrier Transport in Graphene Bilayers[1] , SHAFFIQUE ADAM, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Gaithersburg, MD 20899 — Graphene bilayers come in different varieties ranging from the micro-mechanically exfoliated Bernal stacked sheets where the strongly coupled layers act like a single electronic material, to the essentially decoupled turbostratic graphene bilayers observed in both epitaxial and CVD grown graphene. In this talk I will first review the experimental evidence and early theoretical understanding for the band structure of bilayer graphene. I will then discuss electrical transport measurements and present the semi-classical theory for carrier transport in bilayer graphene. I will show that close to the Dirac point, the co-existence of electron and hole carriers gives rise to an interesting interplay between disorder and temperature [1-3]. For example, we predict that knowing the strength of the disorder potential from low temperature conductivity measurements completely determines the temperature dependence of the conductivity. Detailed comparison with recent experiments highlights both the successes and the shortcomings of this theoretical model. Finally, I will examine the different factors influencing the transport in twisted graphene bilayers. For example, the breaking of inversion symmetry results in a charge imbalance between the two layers giving rise to unexpected features in magneto-transport.

[1] S. Adam and S. Das Sarma, "Boltzmann transport and residual conductivity in bilayer graphene," *Phys. Rev. B*, **77**, 115436, (2008).
[2] S. Adam and M. D. Stiles, "Temperature dependence of the diffusive conductivity of bilayer graphene," *Phys. Rev. B*, **82**, 075423, (2010).
[3] S. Xiao, J. Chen, S. Adam, E. D. Williams, and M. S. Fuhrer, "Charged impurity scattering in bilayer graphene," *Phys. Rev. B*, **82**, 041406, (2010).

[1]This work was done in collaboration with Mark Stiles, Michael Fuhrer and Sankar Das Sarma.

9:12AM A2.00003 Probing layer imbalance in bilayer graphene with electrostatic capacitance measurements , ANDREA YOUNG, Columbia University — In bilayer graphene, application of an external electric field modulates both the charge carrier density and the band structure itself. In particular, application of an electric field perpendicular to the sample plane opens up a band gap in the bilayer graphene energy spectrum, leading to insulating behavior at charge neutrality. Using capacitance measurements, we extract the electronic compressibility as a function of density, applied bias, and temperature. We find that the compressibility remains high even in the region in which a gap is expected, confirming that the insulating behavior observed in transport is due to transport via localized states. Temperature dependent capacitance measurements allow us to estimate the gap in the spectrum, which we find to be in qualitative agreement with that measured by optics. Away from charge neutrality, the density dependence of the compressibility is consistent with hyperbolic electronic bands. Features identified with the $1/\sqrt{\epsilon}$ van Hove singularity—expected for the nearly quartic dispersion of gapped bilayer graphene—are observed near the band edge. These features show a polarization dependent asymmetry, appearing only where the near layer is at lower energy layer for the corresponding carrier type. Using a model of bilayer graphene that incorporates the finite interlayer separation, we show that capacitance measurements in bilayer graphene are sensitive to *layer indexed* compressibilities, in addition to the total charge compressibility. This allows an unambiguous determination of the layer polarization of the ground state, a particularly useful tool in the study of the broken symmetry states observed at high magnetic field.

9:48AM A2.00004 Compressibility of bilayer graphene: the role of disorder , DAVID ABERGEL, University of Maryland — We discuss the role of disorder caused by charged impurities on the compressibility of bilayer graphene. In doing so, we take into account the full hyperbolic dispersion relation and the presence of a gap between the valence and conduction bands to produce an exact calculation of $\frac{d\mu}{dn}$ for the non-disordered case. We then introduce two methods for including the disorder in a statistical way and evaluate the effectiveness of each by comparing their predictions with recent experiments. We find that averaging is best done at the level of the observable quantity: in this case the compressibility. This work is done in collaboration with Sankar Das Sarma and Euyheon Hwang, and supported by US-ONR, NRI-SWAN, and UMD-CNAM.

10:24AM A2.00005 Local Compressibility Measurements of Correlated States in Suspended Bilayer Graphene[1] , JENS MARTIN, Harvard University — Bilayer graphene has attracted considerable interest due to the important role played by many-body effects, particularly at low energies. The exceptional quality of suspended devices has enabled the observation of interaction-driven broken-symmetry states and the fractional quantum Hall effect. Here we report local compressibility measurements of a suspended graphene bilayer. We find that the energy gaps at filling factors +/- 4 do not vanish at low fields, but instead merge into an incompressible region near the charge neutrality point at zero electric and magnetic field. These results indicate the existence of a zero-field ordered state and are consistent with the formation of either an anomalous quantum Hall state or a nematic phase with broken rotational symmetry. At higher fields, we measure the intrinsic energy gaps of broken-symmetry states at filling factor 0, +/- 1 and +/-2, and find that they scale linearly with magnetic field, yet another manifestation of the strong Coulomb interactions in bilayers.

[1]U.S. DoE #DE-SC0001819, U.S. ONR MURI on Graphene, NSF PHY-0646094, the Alexander von Humbolt Foundation, CNS: NSF # ECS-0335765.

Monday, March 21, 2011 8:00AM - 11:00AM –
Session A3 DCMP: Experimental Studies of 5/2 Fractional Quantum Hall Effect Ballroom A3

8:00AM A3.00001 Observation of neutral modes via shot noise measurements , MOTY HEIBLUM, Weizmann Institute of Science — Current propagates in the quantum Hall regime along the edges of a two-dimensional-electron gas via chiral edge modes, with chirality dictated by the applied magnetic field. In the fractional regime, for some fractional states - the so called "holes-conjugate" states – e.g., between filling factor 1/2 and 1 - early predictions suggested the presence of counter propagating edge modes: a "downstream" mode with the expected chirality and an "upstream" mode with an opposite chirality. Since experiments in the ubiquitous 2/3 state did not find upstream propagating edge modes, it had suggested that in the presence of interactions and disorder edge reconstruction may take place with a resultant downstream charge mode accompanied by upstream neutral mode - with the latter carrying only energy - thus explaining why the upstream modes were not detected thus far. Moreover, a neutral upstream Majorana mode is also expected for selected wavefunctions proposed for the even denominator state 5/2. I will review some of our observations of neutral modes in selected quantum Hall states. Neutral mode detection was performed by allowing a chiral mode to impinge on a quantum point contact (QPC) constriction. The partitioning of the neutral mode led to current fluctuations propagating in the downstream chirality. The main following effects that were observed were: (a) Current noise, being proportional to the applied voltage on the injecting contact, without net current; (b) Similarly, partitioning charge current in a QPC led to generation of an upstream neutral mode; (c) The neutral mode decays fast with length and temperature; (d) Having a neutral mode impinge simultaneously with a charge mode affects strongly the Fano factor and the temperature of the partitioned charged quasiparticles; (e) For the 5/2 fractional state, our observation of an upstream neutral mode is likely to single out the proposed reconstructed Pfafian or anti-Pfafian wavefunctions for non-abelian quasiparticles.

8:36AM A3.00002 Competing Phases of 2D Electrons at $\nu = 5/2$ and $7/3$[1] , JING XIA, California Institute of Technology — The N=1 Landau level (LL) exhibits collective electronic phenomena characteristic of both fractional quantum Hall (FQHE) states seen in the lowest LL and anisotropic nematic states in the higher LLs. A modest in-plane magnetic field $B_{||}$ is sufficient to destroy the fractional quantized Hall states at $\nu = 5/2$ (and 7/2) and replace them with anisotropic compressible nematic phases, revealing the close competition between the two. We find that at larger $B_{||}$ these anisotropic phases $\nu = 5/2$ can themselves be replaced by a new isotropic state, dubbed re-entrant isotropic compressible (RIC) phase. We present strong evidence that this transition is a consequence of the mixing of Landau levels from different electric subbands in the confinement potential. In addition, we find that with $B_{||}$, the normally isotropic $\nu = 7/3$ FQHE state can transform into an anisotropic phase with an accurately quantized Hall plateau but an anisotropic longitudinal resistivities. As temperature is lowered towards zero, ρ_{xx} diminishes while ρ_{yy} tends to diverge, reminiscent of the anisotropic nematic states, while surprisingly ρ_{xy} and ρ_{yx} remain quantized at $3h/7e^2$, indicating a completely new quantum phase.

[1]This work represents a collaboration with J.P. Eisenstein (Caltech) and L.N. Pfeiffer and K.W West (Princeton), and is supported by Microsoft Project Q.

9:12AM A3.00003 Luminescence experiments measuring spin at 5/2 , ISRAEL BAR-JOSEPH, Wiezmann Institute — This abstract not available.

9:48AM A3.00004 Electrostatic Measurements of Fractional Charge in the Second Landau Level , VIVEK VENKATACHALAM, Harvard University — The fractional quantum Hall state at filling factor 5/2 is predicted to result from a BCS pairing instability in a Fermi sea of composite fermions. The resulting p-wave paired state would have the lucrative property of supporting non-Abelian braiding statistics which can be leveraged for decoherence-free quantum computation. A robust prediction of any theory involving pairing at half-integer filling in the quantum Hall regime is that quasiparticles should have charge e/4. Local compressibility measurements allow us to compare how quasiparticles charge disorder puddles at 7/3 and 5/2. From this comparison, we can extract the ratio of quasiparticle charges for these states. The value we obtain, 4/3, suggests a local charge of e/4 at 5/2 (assuming e/3 at 7/3). We additionally show that these e/4 quasiparticles can be pinned by disorder, a prerequisite for the interferometry measurements that may demonstrate non-Abelian braiding statistics.

10:24AM A3.00005 "Looking" at Competing Quantum Phases of the Second Landau Level[1] , ARON PINCZUK — Partially populated higher Landau levels of 2D electron systems support striking collective states in which quantum Hall phases overlap and compete with alternate phases emergent from remarkable interplays between fundamental interactions and quantization of 2D states in a magnetic field. Optical studies by light scattering methods are revealing previously unexpected roles of the spin degree of freedom in quantum phases of the second (N=1) Landau level [1,2]. Inelastic light scattering experiments uncover the collapse of the long wavelength ferromagnetic spin wave for filling factors that are below nu=3. This discovery, interpreted as loss of spin polarization in the N=1 Landau level, is made more intriguing by findings that a sharp spin wave does not recover at filling factors nu=8/3 and 5/2 that support well-known fractional quantum Hall states. Simultaneous resonant elastic (Rayleigh) scattering measurements indicate that below nu=3 the collective states of quasiparticles in the partially populated N=1 Landau level break into sub-micron size domains of fluid that seem to lack full spin polarization and that persist to temperatures that are above 1K. The determination of spin polarization in the quantum Hall state at nu=5/2 requires further consideration. While coexisting with spin unpolarized domains, quasiparticle condensation at nu=5/2 may still result in an incompressible fluid that has spin polarization. This work is in collaboration with T. D. Rhone, U. Wurstbauer, Y. Gallais, J. Yan, L.N. Pfeiffer and K.W. West.

[1] T.D. Rhone et al BAPS.2010.MAR.Y2.3
[2] T.D. Rhone et al., submitted for publication.

[1]Supported by NSF and DOE.

Monday, March 21, 2011 8:00AM - 11:00AM –
Session A4 DPOLY: Nanostructures in Polymer-base Photovoltaics Ballroom A4

8:00AM A4.00001 Multiscale simulation of solar cell morphologies guided by SANS and neutron reflectivity data , PHILLIP DUXBURY, Michigan State Univ — This abstract not available.

8:36AM A4.00002 Achievements, opportunities and challenges for organic solar cells , GILLES DENNLER, Konarka — This abstract not available.

9:12AM A4.00003 Impact of the interfacial nanostructures on the electronic processes in organic solar cells , JEAN-LUC BREDAS, Georgia Institute of Technology — After a brief description of the optical and electronic processes that take place in a solid-state organic solar cell [1], we turn our attention to recent theoretical advances regarding the determination of the energetics and dynamics at the organic-organic, donor-acceptor interfaces [2]. We underline the complexity of the processes taking place at the nanoscale [3] and highlight the balance that needs to be found for the optimization of materials parameters in terms of photovoltaic performance.

[1] J.L. Bredas, J. Norton, J. Cornil, and V. Coropceanu, *Acc. Chem. Res.* **42**, 1691 (2009).
[2] Y.Yi, V. Coropceanu, and J.L. Bredas, *J. Amer. Chem. Soc.* **131**, 5131 (2009); *ibid.*, *J. Mater. Chem.* (2010).
[3] M. Linares *et al.*, *J. Phys. Chem. C* **114**, 3215 (2010).

9:48AM A4.00004 Interfacial Aspects of Polymer Based Photovoltaic Structures[1] , THOMAS RUSSELL, University of Massachusetts Amherst — Controlling thin film morphology is key in optimizing the efficiency of polymer-based photovoltaic (PV) devices. Poly(3-hexylthiophene) and [6,6]-penyl-C61 butyric acid methyl ester (P3HT:PCBM) based solar cell performance is dictated by nanostructure of the active layer, the interfaces between the active layer and the electrodes, and the P3HT chain orientation in the thin film. The above parameters were systematically studied by scanning transmission electron microscopy, scanning force microscopy, optical microscopy, grazing incident angle x- ray diffraction., dynamic secondary ion mass spectroscopy and near edge x-ray absorption fine structure analysis. The influence of thermal annealing on the morphology, interfaces and crystal structure was investigated in films that were either initially confined by two electrodes or confined by only one electrode. While the bulk morphology in these films were identical, significant differences in the concentration of components at the electrode interfaces were found, giving rise to a marked difference in performance. In addition, a model was established, based on the crystallization of the P3HTand the diffusion of the PCBM to describe the origins of the nanoscale morphology found in the active layer. The device performance parameters were quantitatively studied.

[1]In collaboration with D. Chen, H. Liu, Y. Gu and F. Lu at UMass Amherst , A. Nakahara at Kuraray Co., D. Wei at Carl Zeiss NTS LLC, D. Nordlund at SSRL and supported by the DOE-supported EFRC at the UMass Amherst (DE-PS02-08ER15944).

10:24AM A4.00005 Morphology control in printable solar cells , JOACHIM LOOS, School of Physics and Astronomy, University of Glasgow Glasgow G12 8QQ, Scotland, United Kingdom — Nanostructured polymer-based solar cells (PSCs) have emerged as a promising low-cost alternative to conventional inorganic photovoltaic devices and are now a subject of intensive research both in academia and industry. For PSCs to become practical efficient devices, several issues should still be addressed, including further understanding of their operation and stability, which in turn are largely determined by the morphological organization in the photoactive layer. The latter is typically a few hundred nanometers thick film and is a blend composed of two materials: the bulk heterojunction consisting of the electron donor and the electron acceptor. The main requirements for morphology of efficient photoactive layers are nanoscale phase segregation for a high donor/acceptor interface area and hence efficient exciton dissociation, short and continuous percolation pathways of both components leading through the layer thickness to the corresponding electrodes for efficient charge transport and collection, and high crystallinity of both donor and acceptor materials for high charge mobility. In this contribution we review recent progress of our understanding on how the efficiency of a bulk-heterojunction PSC largely dependents on the local nanoscale volume organization of the photoactive layer.

Monday, March 21, 2011 8:00AM - 11:00AM –
Session A5 FIAP: Industrial Physics Forum: Small-Scale Applications Ballroom C1

8:00AM A5.00001 Prospects of superconducting qubits for quantum computation , MICHEL DEVORET, Yale University — Superconducting qubits are solid state electrical circuits fabricated using techniques adapted from those of conventional integrated microprocessor fabrication. They are based on the Josephson tunnel junction, the only non-dissipative, strongly non-linear circuit element compatible with low temperature operation. In contrast to microscopic entities such as spins, atoms or ions, superconducting qubits can be well coupled to each other, an appealing feature for 2-qubit gate implementation. Very recently, new circuit architectures have greatly improved the isolation of qubits from unwanted noise, yielding coherence quality factors well in excess of 100,000. Entanglement, the key property that distinguishes a quantum processor from a classical one, has been produced and measured for up to 3 qubits.[1,2] Current experiments are addressing the problem of whether the Preskill criterion of 10,000 coherent 1- and 2-qubit gate operations can be met to enable quantum error correction.

[1]DiCarlo, L. et al. Nature 467, 574-578 (2010);
[2]Neeley, M. et al. Nature 467, 570-573 (2010).

8:36AM A5.00002 Superconductor Digital Electronics: – Current Status, Future Prospects , OLEG MUKHANOV, HYPRES — Two major applications of superconductor electronics: communications and supercomputing will be presented. These areas hold a significant promise of a large impact on electronics state-of-the-art for the defense and commercial markets stemming from the fundamental advantages of superconductivity: simultaneous high speed and low power, lossless interconnect, natural quantization, and high sensitivity. The availability of relatively small cryocoolers lowered the foremost market barrier for cryogenically-cooled superconductor electronic systems. These fundamental advantages enabled a novel Digital-RF architecture - a disruptive technological approach changing wireless communications, radar, and surveillance system architectures dramatically. Practical results were achieved for Digital-RF systems in which wide-band, multi-band radio frequency signals are directly digitized and digital domain is expanded throughout the entire system. Digital-RF systems combine digital and mixed signal integrated circuits based on Rapid Single Flux Quantum (RSFQ) technology, superconductor analog filter circuits, and semiconductor post-processing circuits. The demonstrated cryocooled Digital-RF systems are the world's first and fastest directly digitizing receivers operating with live satellite signals, enabling multi-net data links, and performing signal acquisition from HF to L-band with 30 GHz clock frequencies. In supercomputing, superconductivity leads to the highest energy efficiencies per operation. Superconductor technology based on manipulation and ballistic transfer of magnetic flux quanta provides a superior low-power alternative to CMOS and other charge-transfer based device technologies. The fundamental energy consumption in SFQ circuits defined by flux quanta energy $2x10^{-19}$ J. Recently, a novel energy-efficient zero-static-power SFQ technology, eSFQ/ERSFQ was invented, which retains all advantages of standard RSFQ circuits: high-speed, dc power, internal memory. The voltage bias regulation, determined by SFQ clock, enables the *zero-power at zero-activity regimes*, indispensable for sensor and quantum bit readout.

9:12AM A5.00003 Superconducting Receivers for Millimeter and Submillimeter Astrophysics , PAUL L. RICHARDS, Department of Physics, U. C. Berkeley — Important information about the structure and evolution of the Universe can be obtained from astrophysical measurements at millimeter and submillimeter wavelengths. The noise in receiver systems used for such measurements should approach as closely as possible the fundamental limits such as photon noise and quantum fluctuations. Narrow line emissions are measured by such major projects as the recently launched 1.5B$HerschelSpacetelescopeandthe1B$ International Alma project, which is now under construction. These projects are enabled by heterodyne receivers with superconducting hot electron bolometer (HEB) mixers and Quasiparticle (SIS) mixers. The temperature and polarization of broad band thermal sources such as the Cosmic Microwave Background and dust emission are being measured from a variety of high altitude telescopes in Chile and at the South Pole using large format arrays of transition edge sensor (TES) bolomters. The status of international efforts in this field will be described with special reference to the rapidly developing technology of very large format arrays of TES bolometers with SQUID-based output multiplexers.

9:48AM A5.00004 The Ubiquitous SQUID: From Axions to Cancer[1] , JOHN CLARKE, UC Berkeley and LBNL — I briefly review the principles, practical implementation and applications of the dc SQUID (Superconducting QUantum Interference Device), an ultrasensitive detector of magnetic flux. Cosmological observations show that a major constituent of the universe is cold dark matter (CDM). A candidate particle for CDM is the axion which, in the presence of a magnetic field, is predicted to decay into a photon with energy given by the axion mass, ranging from 0.001 to 1 meV. The axion detector constructed at LLNL consists of a cooled, tunable cavity surrounded by a 7-T superconducting magnet. Photons from the axion decay would be detected by a cooled semiconductor amplifier. To search for the axion over an octave of frequency, however, would take two centuries. Now at the University of Washington, Seattle the axion detector will be upgraded by cooling it to 50 mK and installing a near-quantum limited SQUID amplifier. The scan time will be reduced by three orders of magnitude to a few months. In medical physics, we use an ultralow-field magnetic resonance imaging (ULFMRI) system with SQUID detection to obtain images in a magnetic field of 0.132 mT, four orders of magnitude lower than in conventional MRI. An advantage of low fields is that different types of tissue exhibit much greater contrast in the relaxation time T1 than in high fields. We have measured T1 in ex vivo specimens of surgically removed healthy and malignant prostate tissue. The percentage of tumor in each specimen is determined with pathology. The MRI contrast between two specimens from a given patient scales with the difference in the percentage of tumor; in healthy tissue T1 is typically 50 percent higher than in a tumor. These results suggest that ULFMRI with T1-weighted contrast may have clinical applications to imaging prostate cancer and potentially other types of cancer.

[1]Supported by DOE BES and HEP, and NIH

10:24AM A5.00005 Semiconductor Circuit Diagnostics By Magnetic Field Imaging , T. VENKATESAN, National University of Singapore and Neocera — At the forefront of IC technology development are 3D circuit technologies such as system-in-package (SiP), wafer-level-packaging (WLP), through-silicon-vias (TSV), stacked die approaches, flex packages, etc. They integrate multiple devices, many times stacking them in layers with complex, intricate and very long interconnections in significantly reduced area, in addition to an ever-increasing number of opaque layers. We could very well say that the near future looks like the perfect nightmare for the Failure Analysis (FA) engineer with localization of defects becoming a major challenge. Magnetic field imaging (MFI) allows the fields generated by the circuit currents to go through various packaging layers and be imaged. I will describe in this talk Magma, a scanning magnetic field imaging system based on a high temperature superconducting SQUID device based on YBa2Cu3O7-δ. The HTS SQUIDs used have a noise level of $\sim$ 20pT/$\sqrt{}$(Hz) and for typical scanning conditions, a field sensitivity of about 0.7 nT. While current shorts are imaged with spatial resolution, up to 3 micron (with peak localization) resistive opens can also be imaged and currently different strategies are being adapted for imaging opens with large working distances of 50-100s of microns. Higher spatial resolution ($\sim$250nm) is obtained by the use of magneto-resistive devices as sensors though the working distance requirement is sever

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A6 DCOMP: Great Advances in Computational Physics: Past, Present and Future

Ballroom C2

8:00AM A6.00001 The path integral picture of quantum systems , DAVID CEPERLEY, University of Illinois — The imaginary time path integral "formalism" was introduced in 1953 by Feynman to understand the superfluid transition in liquid helium. The equilibrium properties of quantum many body systems is isomorphic to the classical statistical mechanics of cross-linking polymer-like objects. With the Markov Chain Monte Carlo method, invented by Metropolis et al., also in 1953, a potential way of calculating properties of correlated quantum systems was in place. But calculations for many-body quantum systems did not become routine until computers and algorithms had become sufficiently powerful three decades later. Once such simulations could happen, it was realized that simulations provided a deeper insight into boson superfluids, in particular the relation of bose condensation to the polymer end-to-end distance, and the superfluid density to the polymer "winding number." Some recent developments and applications to supersolids, and helium droplets will be given. Finally, limitations of the methodology e.g. to fermion systems are discussed.

8:36AM A6.00002 Advances in Monte Carlo computer simulation , ROBERT H. SWENDSEN, Carnegie Mellon University — Since the invention of the Metropolis method in 1953, Monte Carlo methods have been shown to provide an efficient, practical approach to the calculation of physical properties in a wide variety of systems. In this talk, I will discuss some of the advances in the MC simulation of thermodynamics systems, with an emphasis on optimization to obtain a maximum of useful information.

9:12AM A6.00003 Computational Physics and Drug Discovery for Infectious Diseases[1] , J. ANDREW MCCAMMON, HHMI/UCSD — This lecture will provide a general introduction to some of the ways that modern computational physics is contributing to the discovery of new pharmaceuticals, with special emphasis on drugs for infectious diseases. The basic sciences and computing technologies involved have advanced to the point that physics-based simulations of drug targets are now yielding truly valuable suggestions for new compounds.

[1]Supported in part by NSF, NIH, HHMI, CTBP, NBCR, and SDSC.

9:48AM A6.00004 The need and potential for building a integrated knowledge-base of the Earth-Human system , CLIFFORD JACOBS[1], National Science Foundation — The pursuit of scientific understanding is increasingly based on interdisciplinary research. To understand more deeply the planet and its interactions requires a progressively more holistic approach, exploring knowledge coming from all scientific and engineering disciplines including but not limited to, biology, chemistry, computer sciences, geosciences, material sciences, mathematics, physics, cyberinfrastucture, and social sciences. Nowhere is such an approach more critical than in the study of global climate change in which one of the major challenges is the development of next-generation Earth System Models that include coupled and interactive representations of ecosystems, agricultural working lands and forests, urban environments, biogeochemistry, atmospheric chemistry, ocean and atmospheric currents, the water cycle, land ice, and human activities.

[1]In collaboration with Tim Killeen, National Science Foundation

10:24AM A6.00005 Simulating the First Cosmic Structures , EDMUND BERTSCHINGER, Massachusetts Institute of Technology — Understanding how the first stars and galaxies formed is one of the forefront challenges of modern astrophysics and cosmology. During the last three decades numerical simulations have proven to be a powerful tool in the development and testing of galaxy formation theories. The raw ingredients are the atomic and dark matter that comprise galaxies combined with a well-tested cosmological framework of small-amplitude seed perturbations generated in the early universe. This talk will briefly review progress in galaxy formation simulations and will highlight outstanding issues and prospects for the future.

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A7 DBP DPOLY DCMP: Prize Session: Single Molecule Biophysics I: Recent Advancements in Technology and Applications Ballroom C3

8:00AM A7.00001 Single Fluorescent Molecules as Nano-Illuminators for Biological Structure and Function , W.E. MOERNER, Stanford University — Since the first optical detection and spectroscopy of a single molecule in a solid (Phys. Rev. Lett. **62**, 2535 (1989)), much has been learned about the ability of single molecules to probe local nanoenvironments and individual behavior in biological and nonbiological materials in the absence of ensemble averaging that can obscure heterogeneity. Because each single fluorophore acts a light source roughly 1 nm in size, microscopic imaging of individual fluorophores leads naturally to superlocalization, or determination of the position of the molecule with precision beyond the optical diffraction limit, simply by digitization of the point-spread function from the single emitter. For example, the shape of single filaments in a living cell can be extracted simply by allowing a single molecule to move through the filament (PNAS **103**, 10929 (2006)). The addition of photoinduced control of single-molecule emission allows imaging beyond the diffraction limit (super-resolution) and a new array of acronyms (PALM, STORM, F-PALM etc.) and advances have appeared. We have used the native blinking and switching of a common yellow-emitting variant of green fluorescent protein (EYFP) reported more than a decade ago (Nature **388**, 355 (1997)) to achieve sub-40 nm super-resolution imaging of several protein structures in the bacterium *Caulobacter crescentus*: the quasi-helix of the actin-like protein MreB (Nat. Meth. **5**, 947 (2008)), the cellular distribution of the DNA binding protein HU (submitted), and the recently discovered division spindle composed of ParA filaments (Nat. Cell Biol. **12**, 791 (2010)). Even with these advances, better emitters would provide more photons and improved resolution, and a new photoactivatable small-molecule emitter has recently been synthesized and targeted to specific structures in living cells to provide super-resolution images (JACS **132**, 15099 (2010)). Finally, a new optical method for extracting three-dimensional position information based on a double-helix point spread function enables quantitative tracking of single mRNA particles in living yeast cells with 15 ms time resolution and 25-50 nm spatial precision (PNAS **107**, 17864 (2010)). These examples illustrate the power of single-molecule optical imaging in extracting new structural and functional information in living cells.

8:36AM A7.00002 Multiple Pathways of Single-Stranded DNA Stretching Observed Using Single-Molecule Manipulation[1] , CHING-HWA KIANG, Rice University — DNA has a double helix structure and contains the genetic code of life. When the information needed to be read, the DNA double helix has to be opened up to allow access to the bases that make up the DNA. During the reading process the DNA adopt a different conformation, and the energetics and mechanics of the dynamic process is important in gene regulation. We used an atomic force microscope to pull single DNA molecules and measured the force associated with the conformational changes of poly(dA), a single-stranded DNA composed of uniform A bases. We found that the DNA can be stretched in two different ways, and the DNA can hop between these two conformations. These results suggest that poly(dA) has a novel conformation when highly stretched, and the unique conformation makes poly(dA) more stable at large extensions. The unique property of poly(dA) may play a role in biological processes such as gene expression. Moreover, single molecule force measurement allows us to quantify the elastic and thermodynamic properties of single biological molecules, and may ultimately be developed into a tool for drug screening.

[1] W.-S. Chen, W.-H. Chen, Z. Chen, A. A. Gooding, K.-J. Lin, and C.-H. Kiang, "Direct Observation of Multiple Pathways of Single-Stranded DNA Stretching," *Phys. Rev. Lett.* **105** (2010) 218104.
[2] C. P. Calderon, W.-H. Chen, K.-J. Lin, N. C. Harris, and C.-H. Kiang, "Quantifying DNA Melting Transitions using Single-Molecule Force Spectroscopy," invited paper in special issue on DNA Melting, *J. Phys.: Condens. Matter* **21** (2009) 034114.

[1]We thank NSF DMR-0907676 and Welch Foundation No. C-1632 for support.

9:12AM A7.00003 Max Delbruck Prize in Biological Physics Talk: Zoom into life at the nanoscale with STORM , XIAOWEI ZHUANG, Howard Hughes Medical Institute, Harvard University — Powered by its molecule-specific contrast and live-cell compatibility, fluorescence microscopy is one of the most widely used imaging methods in biological research. The resolution of fluorescence microscopy is classically limited by the diffraction of light to several hundred nanometers. This resolution limit is substantially larger than the typical molecular length scales in cells, preventing detailed characterization of most sub-cellular structures. Here, I describe a new imaging method, stochastic optical reconstruction microscopy (STORM), which breaks the diffraction limit and allows for super-resolution imaging. STORM uses single-molecule imaging and photo-switchable fluorescent probes to temporally separate the spatially overlapping images of individual molecules, thereby allowing each molecule to be localized with high precision and a super-resolution image to be reconstructed from the numerous measured positions of the molecules. Using this approach, we have imaged cellular structures with nanometer-scale resolution. In this talk, I will discuss the general concept, recent technical advances, and various biological applications of STORM.

9:48AM A7.00004 DNA overstretching transition and the biophysical properties of S-DNA , JIE YAN, National University of Singapore — DNA double helix undergoes an "overstretching" transition in a narrow tensile force range slightly above 60 pN. Overstretched DNA is about 1.7 times longer than B-DNA. Despite numerous studies the basic question of whether the strands are separated or not remains controversial. Our recent experiments show that two distinct transitions are involved in DNA overstretching: a slow hysteretic strand-unpeeling transition to strand separation from free DNA ends or nicks, and a fast, non-hysteretic B-to-S transition to an elongated double helix called "S-DNA". We find that the relative fraction of these two overstretched forms is sensitive to factors that affect DNA base pair stability. Under conditions when S-DNA is stable, we characterize its force-extension curve and compare it with that of single-stranded DNA. We find that the S-DNA is 0.01 - 0.02 nm/bp shorter than that of a nucleotide of single-stranded DNA in the force range 75 - 110 pN. Under conditions when S-DNA is less stable than single-stranded DNA, a slow force increase leads to direct strand separation from B-DNA, while a quick force jump to greater than 70 pN leads to a quick formation of the S-DNA first, followed by a slow secondary transition which is a strand separation from S-DNA. From the secondary transition, the extension difference between S-DNA and single-stranded DNA can be directly calculated, which is found in perfect agreement with that computed from the force-extension curves. Finally, we show that DNA in between a pair of small GC-rich segments is biased toward B-to-S transition. This result also demonstrates that in the absence of nicks and free ends, torsion-unconstrained DNA still undergoes the overstretching transition but only through the B-S transition pathway.

10:24AM A7.00005 Ultra-high resolution optical trap with single fluorophore sensitivity , YANN CHEMLA, University of Illinois, Urbana-Champaign — We present a new single-molecule instrument that combines ultra- high resolution optical tweezers with single-fluorophore fluorescence microscopy. The new instrument will enable the simultaneous measurement of angstrom-scale mechanical motion of individual DNA-binding proteins (e.g., single base-pair stepping of DNA translocases) along with the detection of fluorescently labeled protein properties (e.g., internal configuration). The optical tweezers portion of the instrument is based on a timeshared dual optical trap design and is interlaced with a confocal fluorescence microscope. In a demonstration experiment, individual single-fluorophore labeled DNA oligonucleotides can be observed to bind and unbind to complementary DNA suspended between two trapped beads. Simultaneous with the single-fluorophore detection, coincident angstrom-scale changes in tether extension can be clearly observed.

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A8 DCMP GSNP: APS/GSNP/DCMP Prize Session: Heineman, Onsager, IUPAP/C10

Ballroom C4

8:00AM A8.00001 Dannie Heineman Prize for Mathematical Physics Talk: Shape fluctuations of growing droplets and random matrix theory , HERBERT SPOHN, TU Munchen — In 1986 Kardar, Parisi, and Zhang (KPZ) proposed a stochastic evolution equation for growing interfaces, thereby triggering an intense study of growth processes with local growth rules. Specifically we have in mind the recent spectacular experiment of Takeuchi and Sano [1] on droplet growth in a thin film of turbulent liquid crystal. Over the last ten years one has studied universal probability density functions on the basis of simplified lattice growth models. Surprisingly enough the one-point shape fluctuations are governed by the same statistical laws as the largest eigenvalue of a random matrix, Gaussian Unitary Ensemble (GUE) in case of a curved front and Gaussian Orthogonal Ensemble (GOE) for a flat front. Recently we obtained the first exact solution of the KPZ equation for initial conditions corresponding to droplet growth, thereby providing the probability density function for the height at any time [2]. For long times we recover the universal statistical properties as computed from lattice growth models.

[1] K.Takeuchi and M.Sano, Phys. Rev. Lett. **104**, 230601 (2010).
[2] T.Sasamoto and H.Spohn, Phys. Rev. Lett. **104**, 230602 (2010).

8:36AM A8.00002 Lars Onsager Prize Talk I , ALEXANDER BELAVIN, A.D. Landau Institute for Theoretical Physics — This abstract not available.

9:12AM A8.00003 Lars Onsager Prize Talk II , ALEXANDER POLYAKOV, Princeton University — This abstract not available.

9:48AM A8.00004 ABSTRACT WITHDRAWN –

10:24AM A8.00005 IUPAP C10 2011 Young Scientist Prize in the Structure and Dynamics of Condensed Matter Talk: Breakdown of thermalization in finite one-dimensional systems[1] , MARCOS RIGOL, Georgetown University — Little more than fifty years ago, Fermi, Pasta, and Ulam set up a numerical experiment to prove the ergodic hypothesis for a one-dimensional lattice of harmonic oscillators when nonlinear couplings were added. Much to their surprise, the system exhibited long-time periodic dynamics with no signals of ergodic behavior. Those results motivated intense research, which ultimately gave rise to the modern chaos theory and to a better understanding of the basic principles of classical statistical mechanics. More recently, experiments with ultracold gases in one-dimensional geometries have challenged our understanding of the quantum domain. After bringing a nearly isolated system out of equilibrium, no signals of relaxation to the expected thermal equilibrium distribution were observed. Some of those results can be understood in the framework of integrable quantum systems, but then it remains the question of why thermalization did not occur even when the system was supposed to be far from integrability. In the latter regime, thermalization is expected to occur and can be understood on the basis of the eigenstate thermalization hypothesis. In this talk, we utilize quantum quenches to study how thermalization breaks down in finite one-dimensional lattices as one approaches an integrable point. We establish a direct connection between the presence or absence of thermalization and the validity or failure of the eigenstate thermalization hypothesis, respectively. **References:**

[1] M. Rigol, V. Dunjko, and M. Olshanii, Nature **452**, 854 (2008).
[2] M. Rigol, Phys. Rev. Lett. **103**, 100403 (2009); Phys. Rev. A **80**, 053607 (2009).
[3] M. Rigol and L. F. Santos, Phys. Rev. A **82**, 011604(R) (2010).
[4] L. F. Santos and M. Rigol, Phys. Rev. E **81**, 036206 (2010); Phys. Rev. E **82**, 031130 (2010).

[1]This work was supported by the US Office of Naval Research.

Monday, March 21, 2011 8:00AM - 11:00AM –
Session A9 DFD: Micro-fluidics D220

8:00AM A9.00001 Hydrodynamic resistance of confined cells in rectangular microchannels , ZEINA S. KHAN, SIVA A. VANAPALLI, Texas Tech University, Department of Chemical Engineering — Several microfluidic approaches have been developed to screen suspended cells mechanically in microchannels by exploiting characteristics that are linked to their individual mechanical properties. Typically changes in cell shape due to shear-induced deformation and transit times are reported; while these measurements are qualitative compared to more precise techniques such as atomic force microscopy and micropipette aspiration their advantage lies in throughput, with the ability to screen hundreds to thousands of cells in a minute. We study the potential of a microfluidic cell squeezer to characterize the hydrodynamic resistance of LNCaP prostate cancer cells by measuring dynamical pressure-drop variations along a micrometer-sized channel. The hydrodynamic resistance of the cell introduces an excess pressure drop in the narrow channel which depends on the mechanical stiffness of the cell. We additionally visualize the cell size and assess the influence of cell size on the hydrodynamic resistance of each cell, demonstrating the capability of the microfluidic cell squeezer to yield the hydrodynamic resistance as a mechanical fingerprint of cells.

8:12AM A9.00002 Bio-inspired artificial iriodphores based on capillary origami , SUPONE MANAKASETTHARN, J. ASHLEY TAYLOR, TOM KRUPENKIN, University of Wisconsin - Madison — Many marine organisms have evolved complex optical mechanisms of dynamic skin color control that allow them to drastically change their visual appearance. In particular, cephalopods have developed especially effective dynamic color control mechanism based on the mechanical actuation of the micro-scale optical structures, which produce either variable degrees of area coverage by a given color (chromatophores) or variations in spatial orientation of the reflective and diffractive surfaces (iridophores). In this work we describe bio-inspired artificial iridophores based on electrowetting-controlled capillary origami. We describe the developed microfabrication approach, characterize mechanical and optical properties of the obtained microstructures and discuss their electrowetting-based actuation. The obtained experimental results are in good agreement with a simple theoretical model based on electrocapillarity and elasticity theory. The results of the work can enable a broad range of novel optical devices.

8:24AM A9.00003 Micropipette as Coulter counter for submicron particles[1] , YAUHENI RUDZEVICH, TONY ORDONEZ, GRANT EVANS, LEE CHOW, University of Central Florida — Coulter counter based on micropipette has been around for several decades. Typical commercial Coulter counter has a pore size of 20 μm, and is designed to detect micron-size blood cells. In recent years, there are a lot of interests in using nanometer pore size Coulter counter to detect single molecule and to sequence DNA. Here we describe a simple nanoparticle counter based on pulled micropipettes with a diameter of 50 – 500 nm. Borosilicate micropipettes with an initial outer diameter of 1.00 mm and inner diameter of 0.5 mm are used. After pulling, the micropipettes are fire polished and ultrasound cleaned. Chlorinated Ag/AgCl electrodes and 0.1 M of KCl solution are used. The ionic currents are measured using an Axopatch 200B amplifier in the voltage-clamp mode. Several types and sizes of nanoparticles are measured, including plain silica and polystyrene nanospheres. The results will be discussed in terms of pH values of the solution and concentrations of the nanoparticles.

[1]Financial support from National Science Foundation (NSF-0901361) is acknowledged.

8:36AM A9.00004 ABSTRACT WITHDRAWN –

8:48AM A9.00005 On demand fusion and triggering of confined chemical reactions in femtoliter volume aqueous droplets controlled by interfacial tension , PAT COLLIER, SEUNG-YONG JUNG, SCOTT RETTERER, ORNL — Droplet-based microfluidic platforms offer many opportunities to confine chemical and biochemical reactants in discrete ultrasmall reaction volumes, and investigate the effects of increased confinement on reaction dynamics. Current state-of-the-art microfluidic sampling strategies for creating ultrasmall reaction volumes are predominately steady-state approaches, which result in difficulty in trapping reacting species with a well-defined time-zero for initiation of biochemical reactions in the confined space. This talk describes stepwise, on-demand generation and fusion of femtoliter aqueous droplets based on interfacial tension. Sub-millisecond reaction times from droplet fusion were demonstrated, as well as a reversible chemical toggle switch based on alternating fusion of droplets containing acidic or basic solution, monitored with the pH-dependent emission of fluorescein.

9:00AM A9.00006 Acoustic actuation and sorting of droplets and cells at ultrahigh rates in microfluidics , THOMAS FRANKE, Harvard University/University of Augsburg, LOTHAR SCHMID, SUSANNE BRAUNMUELLER, ACHIM WIXFORTH, University of Augsburg, DAVID A. WEITZ, Harvard University, FRANKE TEAM, FRANKE/WEITZ TEAM — We direct the motion of droplets in microfluidic channels using a surface acoustic wave device. This method allows individual drops to be directed along separate microchannel paths at high volume flow rates, which is useful for droplet sorting. The same principle can be applied for biological cell sorting which operates in continuous flow at high sorting rates. The device is based on a surface acoustic wave cell-sorting scheme and combines many advantages of fluorescence activated cell sorting (FACS) and fluorescence activated droplet sorting (FADS) in microfluidic channels. It is fully integrated on a PDMS device, and allows fast electronic control of cell diversion. We direct cells (HaCaT, MV3 melanoma, fibroblasts) by acoustic streaming excited by a surface acoustic wave. The device underlying principle works without additional enhancement of the sorting by prior labeling of the cells with responsive markers such as magnetic or polarizable beads. We have combined the acoustic device successfully with a laser based fluorescence detection system and demonstrate sorting of fluorescent labeled drops at rates of several kHz without any false sorting.

9:12AM A9.00007 Microfluidic mixing using an array of superparamagnetic beads , WENBIN MAO, ZHENGCHUN PENG, PETER J. HESKETH, ALEXANDER ALEXEEV, Georgia Institute of Technology — We present a combined numerical and experimental study on the dynamics of superparamagnetic beads in a microfluidic channel, wall of which is decorated with an array of stationary magnetic disks. When exposed to a rotating magnetic field, the beads circulate around the magnetic disks. We conduct experiments with micrometer-sized supeparamagnetic beads and use a numerical method that is based on the lattice Boltzmann model to examine the dynamics of this microfluidic system. We isolate the conditions in which beads exhibit stable periodical motion around magnetic disks and probe the effect of microchannel flow on the bead dynamics. We demonstrate that the fluid circulations created by rotating beads can be exploited for microfluidic mixing, thereby offering a new approach for designing highly-efficient active microfluidic mixers.

9:24AM A9.00008 Separating Magnetically Labeled and Unlabeled Biological Cells within Microfluidic Channels , TOM BYVANK, GREG VIEIRA, The Ohio State University Department of Physics, BRANDON MILLER, BO YU, JEFFREY CHALMERS, L. JAMES LEE, The Ohio State University William G. Lowrie Department of Chemical and Biomolecular Engineering, R. SOORYAKUMAR, The Ohio State University Department of Physics — The transport of microscopic objects that rely on magnetic forces have numerous advantages including flexibility of controlling many design parameters and the long range magnetic interactions generally do not adversely affect biological or chemical interactions. We present results on the use of magnetic micro-arrays imprinted within polydimethylsiloxane (PDMS) microfluidic channels that benefit from these features and the ability to rapidly reprogram the magnetic energy landscape for cell manipulation and sorting applications. A central enabling feature is the very large, tunable, magnetic field gradients ($> 10^4$ T/m) that can be designed within the microfluidic architecture. Through use of antibody-conjugated magnetic microspheres to label biological cells, results on the transport and sorting of heterogeneous cell populations are presented. The effects of micro-array and fluid channel design parameters, competition between magnetic forces and hydrodynamic drag forces, and cell-labeling efficiency on cell separation are discussed.

9:36AM A9.00009 Coating microchannels to improve Field-Flow Fractionation , TYLER N. SHENDRUK, GARY W. SLATER, University of Ottawa — We propose a selective-steric-mode Field-Flow Fractionation (ssFFF) technique for size separation of particles. Grafting a dense polymer brush onto the accumulation wall of a microchannel adds two novel effects to FFF: the particles must pay an entropic cost to enter the brush and the brush has a hydrodynamic thickness that shifts the no-slip condition. For small particles, the brush acts as a low-velocity region, leading to chromatographic-like retention. We present an analytical retention theory for small but finite-sized particles in a microchannel with a dense Alexander brush coating that possesses a well-defined hydrodynamic thickness. This theory is compared to a numerical solution for the retention ratio given by a flow approximated by the Brinkman equation and particle-brush interaction that is both osmotic and compressional. Large performance improvements are predicted in several regimes. Multi-Particle Collision simulations of the system assess the impact of factors neglected by the theory such as the dynamics of particle impingement on the brush subject to a flow.

9:48AM A9.00010 Digital Flow Control of Electroosmotic Pump: Onsager Coefficients and Interfacial Parameters Determination , ZULI XU, Department of Physics, the Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong (PR China), JIANYING MIAO, Nano and Advanced Materials Institute Limited, Hong Kong (PR China), NING WANG, PING SHENG, Department of Physics, the Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong (PR China) — Electroosmosis (EO) and streaming potential (SP) are two complementary electrokinetic processes related by the Onsager relation. In particular, electroosmotic pump (EOP) is potentially useful for a variety of engineering and bio-related applications. By fabricating samples consisting of dry-etched cylindrical pores (50 μm in length and 3.5 μm in diameter) on silicon wafers, we demonstrate that the use of digital control via voltage pulses can resolve the flow regulation and stability issues associated with the EOP, so that the intrinsic characteristics of the porous sample medium may be revealed. Through the consistency of the measured electroosmosis and the streaming potential coefficients as required by the Onsager relation, we deduce the zeta potential and the surface conductivity, both physical parameters pertaining to the liquid-solid interface.

10:00AM A9.00011 AC electrophoretic effect in inhomogeneous electrical field: potentials for single molecule trapping[1] , WEIHUA GUAN, Department of Electrical Engineering, Yale University, JAE HYUN PARK, PREDRAG KRSTIC, Physics Division, Oak Ridge National Laboratory, MARK REED, Department of Electrical Engineering, Yale University — In micro-fabricated fluidic devices, we have experimentally observed trapping of objects in the supposed unallowed positive dielectrophoresis (pDEP) region. This 'anomalous' trapping behavior motivates us to investigate the missing contributions in the trapping dynamics. We present here a study on overlooked aspects of alternating current (AC) electrokinetics-AC electrophoretic (ACEP) phenomena. The dynamics of a particle with both polarizability and net charges in an *inhomogeneous* AC electric trapping field are investigated. It is found that either electrophoretic (EP) or dielectrophoretic (DEP) effects can dominate the trapping dynamics, depending on experimental conditions. A dimensionless parameter is developed to predict the relative strength of EP and DEP effect. Contrary to conventional thought, an ACEP trap is feasible for charged particles in 'salt-free' or low salt concentration solutions. In contrast to DEP traps, an ACEP trap favors the down scaling of particle size. We anticipate that this feature will allow the confinement of single nanometer-sized objects or macromolecules.

[1]Supported by NIH under grant No. 1R21HG004764-01

10:12AM A9.00012 Making robust electrowetting processes: dielectric breakdown and satellite droplets , GREG RANDALL, BRENT BLUE, General Atomics — For over ten years, charge-related wetting phenomena such as electrowetting or dielectrophoresis have been used to manipulate individual liquid droplets on grids of patterned electrodes. Many proof-of-principle droplet actuations have been shown, however some physics-based problems are complicating this technology's move to industry. These problems include: breakdown of a device's dielectric coating at field strengths lower than anticipated and generation of satellite droplets from the primary droplet's surface. We use atomic layer deposition (ALD) to fabricate high-quality dielectric layers required for robust droplet electrowetting and generate operating plots for several dielectric materials. Using scanning electron microscopy and X-ray spectroscopy, we study damage and ionic penetration into the device's dielectric layer. Using video and current measurements, we examine the physics of satellite droplet generation. We apply these findings to engineer a microfluidic process to mass produce inertial fusion energy targets.

10:24AM A9.00013 Introducing the Hybrid Free Surface Microfluidics for Gas Sensing , MEYSAM BARMI, CARL MEINHART, Department of Mechanical Engineering, University of California Santa Barbara — Free-Surface MicroFluidics (FSMF) have recently received much attention for their applications especially their ability for airborne chemical detection [Piorek, PNAS 2007]. Due to their sensitivity to the ambient condition and possibility of contamination, hybrid configuration is introduced to perform the measurement more accurately. The hybrid free surface microfluidics are combination of free surface and closed surface microfluidics. The gas is absorbed by the working fluid through a small opening on the microchannel and transported to the closed surface reaction chamber to carry out the measurements. The working fluid is transported by surface tension and regulated by temperature-controlled evaporator at the outlet. The microchannels are fabricated on Silicon substrates with built-in Ti/Pt electrodes to measure the conductivity of the working fluid before and after the gas absorption to find the concentration of the absorbed gas. It proves that the hybrid free surface microfluidics are appropriate for gas sensing and the minimum exposing time and required opening size are calculated. Numerical simulations are carried out by COMSOL multiphysics. Navier-Stokes equations along with the mass transport with reaction are solved simultaneously to find the correlation between vapor pressure of the surrounding gas and concentration of the absorbed gas.

10:36AM A9.00014 Motion-Reversal Transitions in Self-Assembled Colloidal Walkers , STEPHANIE MORAN, CHARLES SING, ALFREDO ALEXANDER-KATZ, MIT — Nature has created a variety of designs in order to move fluids and transport objects within living organisms. At microscopic scales (in the region of micrometers) two motifs are common: flagella and cilia. Within the cell, however, molecular motors with nanometer dimensions transport small sized vesicles. Here, we describe a novel approach that combines properties from two systems: cilia and molecular motors, to create self-assembled colloidal walkers. These walkers are assembled by superparamagnetic beads in the presence of a rotating homogeneous magnetic field, and are able move in a given direction due to the presence of surfaces which provide an effective friction. The motion is somewhat reminiscent of a person doing cartwheels on ice, where the friction is not high enough to avoid slip, but overall one can attain directed motion in one direction. Interestingly, the motion of the center of mass of these walkers is a non-monotonic function along one cycle of revolution. By exploiting this non-monotonicity, we show that motion reversal is possible in this systems if one carefully controls the friction properties of the surface as well as the confining "gravitational" field that maintains the beads near the surface. Our results our important in understanding the motion of micron scale organisms and may be useful in the development of virtual microfluidic platforms.

10:48AM A9.00015 Optimizing Nanopore Surface Properties for High-Efficiency Water Desalination , DAVID COHEN-TANUGI, JEFFREY GROSSMAN, Massachusetts Institute of Technology — As water resources worldwide become rapidly scarcer, it is becoming increasingly important to devise new techniques to obtain clean water from seawater. At present, water purification technologies are limited by costly energy requirements relative to the theoretical thermodynamic limit and by insufficient understanding of the physical processes underlying ion filtration and fluid transport at the molecular scale. New advances in computational materials science offer a promising way to deepen our understanding of these physical phenomena. In this presentation, we describe a new approach for high-efficiency water desalination based on surface-engineered porous materials. This approach is especially relevant for promising technologies such as nanofiltration and membrane distillation, which offers promising advantages over traditional desalination technologies using mesoporous membranes that are only permeable to pure water vapor. More accurate molecular modeling of mesoporous and nanoporous materials represents a key step towards efficient large-scale treatment of seawater. Results regarding the effect of pore properties (surface texture, morphology, density, tortuosity) on desired performance characteristics such as ion selectivity, maximal water flux and energy requirements will be presented.

Monday, March 21, 2011 8:00AM - 10:48AM –
Session A10 DCMP: Structure and Morphology of Oxide Surfaces and Interfaces D221

8:00AM A10.00001 The interactions of bridging oxygen vacancies on the rutile (110) surface , CRISTIAN CIOBANU, BRANDEN KAPPES, WILLIAM MADDOX, Colorado School of Mines, DANDA ACHARYA, PETER SUTTER, Brookhaven National Laboratory — Using density functional theory calculations at the level of Hubbard-corrected generalized gradient approximation (GGA+U), we calculate the formation and interaction energies of oxygen vacancies on the (110) surface of rutile for neutral and positively charged slabs for different values of the Hubbard parameter U. We find that the interaction of vacancies is elastically repulsive at long range, and that there is a short-range attraction between nearest neighbor vacancies (or oxygen vacancy pairs). With this physical description of the interactions, we derive a closed formula for the surface energy of reduced (110) rutile surface with two same-row vacancies within a given spatial periodicity along the bridge oxygen row, as well as a simple statistical mechanics description of the probability of finding two vacancies at a given distance d. The results of our theoretical model are consistent with our scanning tunneling microscopy determination of the distribution of inter-vacancy separations, and provide a framework for interpreting previous works in the literature.

8:12AM A10.00002 Revisiting Low-Temperature Reconstruction of TiO_2(001) , N.-H. YU, K.T. PARK, V.B. NASCIMENTO, Z. LIAO, G. LI, X. HE, J. TENG, J. ZHANG, E.W. PLUMMER, DEPARTMENT OF PHYSICS, BAYLOR UNIVERSITY TEAM, DEPARTMENT OF PHYSICS AND ASTRONOMY, LOUISIANA STATE UNIVERSITY TEAM — TiO_2(001) has been investigated by scanning tunneling microscopy (STM) and low energy electron diffraction (LEED). After cycles of Ar sputtering and surface annealing at moderate temperatures (up to 600 °C for 15 minutes), TiO_2(001) reveals the so-called latticework reconstruction: row-like linear structures running along [110] and [1-10] directions. Each row further consists of bright spots separated by 6.5 Å. In some areas, the rows are separated by 13 Å consistent with the lattice domains of $(2\sqrt{2}\times\sqrt{2})$ R45 observed by LEED. In other areas, the rows are distributed in a more random fashion. Thus various nearest neighbor distances and relative heights of the rows form different microfacets. From the LEED and STM data, the surface reconstruction is modeled by added rows of stoichiometric TiO_2, aligned along [110] and [1-10] directions.

8:24AM A10.00003 Cu/Cu oxide growth on ZnO and TiO2 for CO2 reduction , FEI WANG, ZIYU ZHANG, RICHARD KURTZ, PHILLIP SPRUNGER, Louisiana State University — Monolayer copper growth on ZnO(10-10) and TiO2(110) have been studied with STM, EELS and LEED. These systems are attractive due to their photochemical and electrochemical reduction of CO2. However, determination of the particular reaction pathway(s) has been elusive because final reduction products strongly depend on the coverage and size of Cu clusters. In order to detangle substrate effects, single crystal ZnO(10-10) and TiO2(110) have been chosen as supports for Cu growth. STM is employed to investigate the nucleation and growth of Cu on both substrates. Cu tends to grow nanoclusters on both substrates with preferred nucleation sites and directions. Upon annealing, Cu clusters ripening have been seen on ZnO substrate but not on TiO2. Subsequent oxidation of Cu clusters is also studied with STM. CO2 vibrational modes on both substrates will be studied with EELS.

8:36AM A10.00004 First-Principles Calculations of Palladium Nanostructures Formed on γ-Alumina[1] , XIN LIU, SANWU WANG, The University of Tulsa — Palladium clusters supported on the γ-alumina surface serve as a catalyst for a variety of important chemical reactions. We report results of our first-principles quantum mechanical calculations for the bonding configurations of palladium atoms and clusters that are supported on the γ-Al_2O_3(110) surface. In particular, our results show that while a single Pd atom prefers to be bonded on the bridge sites of two surface aluminum atoms, a chain nanostructure and a ring-like nanostructure may be formed when more Pd atoms are adsorbed on the surface.

[1]Supported in part by the Department of Energy (#DE-SC0004600), by the National Center for Supercomputing Applications (TG-DMR080005N), and by the National Center for Computational Sciences at Oak Ridge National Laboratory.

8:48AM A10.00005 Atomic structure and interfacial energy of copper and cuprous oxide forming heterojunctions with the ZnO(0001) surface[1] , OLIVER WARSCHKOW, KATAWUT CHUASIRIPATTANA, MATTHEW LYLE, School of Physics, The University of Sydney, BERNARD DELLEY, Paul-Scherrer-Institut, CATHY STAMPFL, School of Physics, The University of Sydney — The system Cu/ZnO is industrially important as a catalyst for methanol synthesis and water-gas-shift reactions. The pairing of copper and zinc oxide is crucial to catalytic efficacy; however, the atomic-scale interactions between the two phases are far from resolved. This presentation will focus on three heterojunctions of relevance to catalytic action, namely, Cu(111):ZnO(0001), Cu_2O(110):ZnO(0001), and Cu_2O(111):ZnO(0001). We use density functional theory to characterize these interfaces in terms of their environment-dependent structure and energetics. This allows us to assess the relative stability of competing structures, and discuss their possible roles in an active catalyst.

[1]This work was supported by the Australian Research Council under Discovery Grant No. DP0770631.

9:00AM A10.00006 Hydrogen Adsorption on polar ZnO(0001)-Zn - extending equilibrium surface phase diagrams to kinetically stabilised structures , MIRA TODOROVA, Dept. for Computational Materials Design, Max-Planck-Institut fuer Eisenforschung GmbH, Duesseldorf, Germany, MARKUS VALTINER[1], Dept. for Interface Chemistry and Surface Engineering, Max-Planck-Insitut fuer Eisenforschung GmbH, Duesseldorf, Germany, JOERG NEUGEBAUER, Dept. for Computational Materials Design, Max-Planck-Institut fuer Eisenforschung GmbH, Duesseldorf, Germany — Hydrogen adsorption on the Zn-terminated polar ZnO(0001) surface is studied by a combination of density-functional theory calculations and *atomistic thermodynamics*. Going beyond the thermodynamic limit and constructing meta-stable phase diagrams we extend the concept of equilibrium surface phase diagrams to include kinetically stabilised surface reconstructions. Using this approach we were able to identify new and hitherto not reported structures that become stable under non-equilibrium extreme H-rich conditions. Experimental situations that realise such conditions will be discussed.

M. Valtiner, M. Todorova, and J. Neugebauer, Phys. Rev. B **82**, 165418 (2010).

[1]Other Affiliation: Dept. for Chemical Engineering, University of California, Santa Barbara, CA 93106-5080, USA

9:12AM A10.00007 DFT Study on ZnO Nanoplate Towards Magnetic Property , SEUNG SOON JANG, JI-IL CHOI, JUNG-IL HONG, ZHONG LIN WANG, ROBERT SNYDER, Georgia Institute of Technology, School of Materials Science and Engineering — Using a GGA+U method and Density Functional Theory, we present a theoretical study for the existence of a magnetic moment in ZnO nanoplate without any extrinsic doping of magnetic impurities. Nanoplate are configured with a Zn-terminated (0001) surface and O-terminated $(000\bar{1})$ surfaces. The surface reconstruction was considered by optimizing the structures. Using GGA PBE, we calculated the spin density of states for both spin states and individual density of states for each orbital to clarify the degree of contributions. Compared to the electronic configuration of bulk wurtzite ZnO, net spins are observed in ZnO nanoplates depending on the plate thickness, which is thought to be due to large changes in the degree of hybridization throughout the plate. As the electronic configuration of a ZnO nanoplate is converged to that of bulk ZnO with increasing plate thickness, its net spin disappears. Specifically, It is found that the net spin of the ZnO nanoplate disappears when its thickness increases beyond $\sim$ 6 nm. In our presentation, we will discuss the change of the electronic configurations as a function of the plate thickness with a rationalization of this change.

9:24AM A10.00008 Ultrathin film growth of iron oxides on YSZ(001) and (111) , GARY KELLOGG, IVAN ERMANOSKI, Sandia National Laboratories — We use low energy electron microscopy (LEEM) and low energy electron diffraction (LEED) to study in real time the growth of iron oxides on the (001) and (111) surfaces of yttriastabilized zirconia (YSZ). Investigations of the FeO_x-YSZ system are motivated by its use as a working oxide for thermochemical fuel production via splitting of H_2O and CO_2. LEED patterns obtained from YSZ(001) during Fe deposition in $\sim 10^{-6}$ Torr O_2 at 600°C and above indicate first-layer growth of FeO(111) and second-layer growth of Fe_2O_3(0001). LEEM imaging shows highly anisotropic first-layer growth into four non-equivalent domains (two rotations and two stacking orientations). Distinct LEEM-IV (intensity-voltage) spectra are obtained for the two stoichiometries providing unique fingerprints of the observed oxide phases. On YSZ(111), growth $>$800°C in O_2 is similar to (001) in that FeO is observed in the first layer and Fe_3O_4 in the second. Sandia is a multiprogram laboratory operated by Sandia Corporation, a subsidiary of Lockheed Martin, for the U.S. DOE's NNSA under contract DEAC0494AL85000. Funding was provided through Sandia's LDRD Office.

9:36AM A10.00009 *In Situ* Synchrotron Studies of a Model Catalyst: WO_x/α-Fe_2O_3 , MARTIN MCBRIARTY, ZHENXING FENG, Northwestern University, JOSEPH LIBERA, JEFFREY ELAM, Argonne National Laboratory, DONALD ELLIS, MICHAEL BEDZYK, Northwestern University — Statistically averaging surface-sensitive X-ray techniques are employed to elucidate the surface morphology of a model oxide-supported heterogeneous catalyst, tungsten oxide (WO_x) on hematite (α-Fe_2O_3). Atomically flat α-Fe_2O_3 (0001) single crystals were coated with sub-monolayer WO_x by atomic layer deposition (ALD). *In situ* X-ray standing wave (XSW) imaging with X-ray fluorescence (XRF) was used to determine W position relative to bulk-like cation lattice sites under nominally reducing and oxidizing chemical conditions. X-ray absorption fine structure (XAFS) reveals details of W coordination, bond length, and chemical state on WO_x-coated hematite single crystals and nanopowders. Synchrotron characterization results are compared with morphologies predicted by density functional theory (DFT) calculations for clean WO_x/α-Fe_2O_3 surfaces. Thermodynamics and atomic configurations for H_2O and CO adsorption are also predicted. Excited-state self-consistent field (SCF) calculations are used to model X-ray photoelectron spectroscopy (XPS) results.

9:48AM A10.00010 First-Principles Investigations of Oxygen Vacancies on SnO2 Nanofilms[1] , DANIEL CELLUCCI, STEVEN LEWIS, University of Georgia — The n-type semiconductor tin dioxide (SnO2) has long been used as the working material for robust, inexpensive oxidizable-gas sensors. In recent years, advances in nanofabrication have made possible the well-controlled formation of SnO2 nanocrystals. Since gas sensing in SnO2 involves changes in surface resistivity as a function of gas concentration, nanocrystalline SnO2 holds great promise for high-sensitivity gas sensors, due to the high surface-to-volume ratio. A key feature of the sensing mechanism is the facile formation and destruction of oxygen vacancies at (or near) the surface. In this talk I will discuss our ongoing first-principles investigations of surface oxygen vacancies in SnO2 nanofilms. We have focused on vacancy formation among the so-called bridging oxygen atoms on the (110) surface of rutile SnO2, as a function of vacancy concentration and film thickness, studying the effect on local atomic and electronic structure. This work is the first phase of a longer-term investigation of surface vacancy phases on SnO2 (110) as a function of temperature and oxygen vapor pressure.

[1]National Science Foundation, Grant #CMMI-0856719.

10:00AM A10.00011 Microstructural relaxation phenomena on laser-modified fused silica surfaces , MANYALIBO MATTHEWS, THOMAS SOULES, JAMES STOLKEN, RYAN VIGNES, STEVEN YANG, SELIM ELHADJ, Lawrence Livermore National Laboratory — Laser-driven phase transformations and associated morphological deformations on vitreous SiO_2surfaces are presented. Direct imaging of Si-O-Si asymmetric stretch transverse-optic (TO) mode shifts using a combination of scanning Infrared and Raman spectromicroscopy revealed the creation of the high pressure phase stishovite through the nonlinear absorption of ultraviolet laser pulses. Structural relaxation at $\sim$1900 K of modified surfaces back to the amorphous state could be correlated with Si-O bond angle shifts and used to describe the thermally-driven transformation kinetics. Kohlrausch relaxation functions are applied through finite element modeling of the calculated sub-surface thermal histories to extract reasonable values for the activation enthalpy and annealing point relaxation time of laser-modified silica. Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration under Contract DE-AC52-07NA27344.

10:12AM A10.00012 Polarizing-Depolarizing fields competition on $PbTiO_3$ nanocapacitors[1] , MIGUEL ANGEL MENDEZ POLANCO, ILYA GRINBERG, ANDREW RAPPE, University of Pennsylvania, Department of Chemistry — We analyzed the stability of various interfacial atomic arrangements in $PbTiO_3$ (PTO) based nanocapacitors, using density functional theory (DFT). We observed that particular constructions induce a large polarization enhancement via a net field depolarizing-to-polarizing swap within the PTO layers, as revealed by analysis of electrostatic potential profiles. In contrast to those with a dominant depolarizing field, possessing a polarization below that of the bulk, the polar structures are stable in the thin-film regime. Interface atomic relaxation is also observed to be a key factor in determining the overall stability of the different capacitor configurations. This boosted charge screening capacity along with appropriate engineering of the interface chemistry, are potential how-to pointers to alleviate the critical thickness in ferroelectric-based nanocapacitors.

[1]The authors acknowledge financial and computational support from ONR, DoE and DoD.

10:24AM A10.00013 ABSTRACT WITHDRAWN –

10:36AM A10.00014 Growth of vanadium dioxide thin films using magnetron sputtering , FANGFANG SONG, B.E. WHITE, Binghamton University — The unique electronic properties of vanadium dioxide have been a focus of intense experimental and theoretical investigation. Although the origin of the metal-insulator transition in this material is still under investigation, the magnitude of the resistivity change at the metal-insulator transition and closeness of the transition temperature to room temperature suggest this material has high potential for future electronic devices. However, the existence of a large number of distinct stable vanadium oxide phases offers a particular challenge to the growth of thin films of this material. In this work, we present our experimental investigation of vanadium dioxide thin film deposition. RF and DC Magnetron sputtering are used for thin film deposition and the effect of oxygen partial pressure, substrate material, and deposition temperature are studied. The impact of deposition conditions on the structural and morphological properties of the thin films, as determined by x-ray diffraction and scanning electron microscopy, will be discussed. Results indicate that on the technologically relevant silicon dioxide surface, the transitional phase of vanadium dioxide can be stabilized with an appropriate post deposition anneal.

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A11 FIAP: Semiconductor Growths D222

8:00AM A11.00001 Kinectic Monte Carlo Simulation of Strained Heteroepitaxial Growth[1] , PETER SMEREKA, University of Michigan, TIM SCHULZE, University of Tennessee — An efficient algorithm for the simulation of strained heteroepitaxial growth with intermixing in 2+1 dimensions is presented. The talk will first describe a KMC solid-on-solid model that has been modified to incorporate elastic interaction. The simulation of such models is computationally difficult due to the need to repeatedly update the elastic displacement field. This hurdle can be overcome by using local updates of the displacement field combined with a multigrid approach for global updates (when needed). The validity of this technique can be theoretically justified. This algorithm is efficient enough to allow the simulation of heteropitaxy on macroscopic time scales. Simulations will have 100 million to 10 billion atomistic moves. Results will be presented showing how various parameters (e.g. temperature, misfit, and deposition rate) effect the morphology of growing films. Annealing simulations of a single 3d island reveal something akin to the pyramid to dome transition observed for Ge islands on Si. Simulations of stacked quantum dots will be presented, these simulations show the capping layer can erode the dots and the alignment of the dots is somewhat different than is often proposed in the literature.

[1]Funded by NSF.

8:12AM A11.00002 Fabrication and characterization of cryogenic complementary devices on Si/SiGe heterostructures , T.M. LU, Princeton University, C.-H. LEE, National Taiwan University, D.C. TSUI, Princeton University, C.W. LIU, National Taiwan University — We have fabricated cryogenic complementary devices using undoped Si/SiGe heterostructures which contain an electron quantum well and a hole quantum well. The highest temperature in the fabrication process is as low as 440°C, preserving the quality of the epitaxial films. By properly biasing the gate voltage, two-dimensional (2D) electrons and holes are induced capacitively in the quantum wells. The electron mobility, $\sim 2\times 10^4$ cm^2/Vs, is significantly lower than that in a heterostructure without any hole quantum well. Nevertheless, the induced 2D electrons show the integer and fractional quantum Hall effect characteristics. The mobility of the 2D holes is $\sim 7\times 10^3$ cm^2/Vs, consistent with previous reports, and is limited by alloy scattering. A proof-of-principle inverter is demonstrated.

8:24AM A11.00003 Mechanisms of Stranski Krastanov Growth , ARVIND BASKARAN, University of California, Irvine, PETER SMEREKA, University of Michigan, Ann Arbor — During the Heteroepitaxial growth of strained semiconductor films (like Ge on Si) the self assembly of quantum dots is observed. This is often reported in experiments to take place though the Stranski Krastanov (SK) growth mode, where the film grows in a layer by layer fashion up to a certain critical thickness after which islands (dots) form. In this talk we present a study of the SK growth mode using a solid on solid Kinetic Monte Carlo model. The importance of the use of such an discrete stochastic model and its merits over the continuum approach will be outlined. Entropy is found to play a very crucial role in the SK growth mode. The mechanism of the SK growth is understood in the context of a delicate balance of the energy and entropy. This is joint work with Peter Smereka.

8:36AM A11.00004 High-purity germanium crystal growth for DUSEL experiments , WENCHANG XIANG, YONGCHEN SUN, DONGMING MEI, YUTONG GUAN, CHAO ZHANG, The University of South Dakota, CUBED TEAM — High-purity Germanium single crystals can be fabricated into ultra-low background detectors for dark matter and neutrinoless double-beta decay experiments at DUSEL. If the crystals are grown in underground environment, the cosmogenic production can be minimized and hence the crystals can be ultra-pure for the next generation experiments at DUSEL. Growing high-purity germanium crystals represents one of the most difficult tasks in semiconductor field. We adopt Czochralski method in growing single crystal in order to understand various technical challenges. With the pioneers' work done in the past, we are moving rapidly toward growing high quality single crystals on the surface. With the available valuable papers and accumulation of the growing experience, our growing process is being improved on weekly basis. This paper will report the grown crystals produced by our equipment and address versions issues with the growing processes.

8:48AM A11.00005 Strain-promoted growth of Mn silicide nanowires on Si(001)[1] , KAZUSHI MIKI, HONGJUN LIU, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan., JAMES H.G. OWEN, CHRISTOPH RENNER, Université de Genève, Section de Physique/DPMC, Quai Ernest-Ansermet 24, 1211 Genève 4 — We have discovered a method to promote the growth of Mn silicide nanowires on the Si(001) at 450°C. Deposition of sub-monolayer quantities of Mn onto a Si(001) surface with a high density of Bi nanolines results in the formation of nanowires, 5-10 nm wide, and up to 600 nm long. These nanowires are never formed if the same growth procedure is followed in the absence of the Bi nanolines. The Haiku core of the Bi nanoline is known to induce short-range stress in the surrounding silicon surface, straining neighbouring dimers, and repelling step edges [1]. We discuss the possible mechanisms for this effect, including the effect of the Bi nanolines on the surface stress tensor and alteration of the available diffusion channels on the surface.

[1] J. H. G. Owen, K. Miki, and D. R. Bowler J. Mat. Sci. 41 4568-4603 (2006)

[1]This research was partially supported by the Ministry of Education, Science, Sports and Culture, Grant-in-Aid for Scientific Research, the Iketani Science and Technology Foundation.

9:00AM A11.00006 Hyperthermal epitaxy of enriched ^{28}Si , KEVIN DWYER, University of Maryland, College Park, JOSHUA POMEROY, National Institute of Standards and Technology — In the effort to produce devices suitable for quantum computation, it is necessary to increase as much as possible the T_2 coherence time of the electron or nuclear spin being used as a qubit. For silicon devices this means using isotopically enriched ^{28}Si. This is because ^{28}Si has no net nuclear spin while the spin of ^{29}Si present in natural Si (4.67%) interacts with the qubit spin and reduces the T_2 time greatly. Sufficiently long T_2 times are necessary for successful operation of quantum computers and we will demonstrate a method for producing epitaxial layers of ^{28}Si on a Si substrate. Ideally, the silicon layers produced must not only be isotopically enriched, but chemically pure and defect free for best performance. These qualities are produced by deposition from a hyperthermal energy beam line using a mass selecting magnet. Depositing silicon epilayers at hyperthermal energies allows for greater manipulation of layer quality. This process is tested and calibrated initially using carbon dioxide. As a preliminary test, isotopically enriched ^{13}C is implanted into semiconductor grade silicon and analyzed by secondary ion mass spectroscopy as an independent check on estimated levels of isotopic and chemical purity.

9:12AM A11.00007 Anti-phase domain suppression and increased electron mobilities in InSb epilayers and quantum wells on off-axis Ge(211) and GeOI(001) substrates[1] , MUKUL C. DEBNATH, TETSUYA D. MISHIMA, MICHAEL B. SANTOS, University of Oklahoma, KHALID HOSSAIN, ORIN W. HOLLAND, Amethyst Research Inc. — We report on the molecular beam epitaxy of InSb epilayers and Si δ-doped InSb/$Al_xIn_{1-x}Sb$ quantum wells (QWs) on off-axis Ge(211) and Ge-On-Insulator (GeOI)-On-Si substrates. The high carrier mobilities in n-type InSb and p-type Ge QWs provide a motivation to integrate these structures on a single substrate for an improved CMOS technology. Growth on GeOI substrates may also make possible the integration of InSb infrared detectors with Si transistors. We evaluate the suppression of anti-phase domains (APDs) through analysis of Reflection High-Energy Electron Diffraction (RHEED) patterns obtained during growth on off-axis substrates. The narrowest X-ray rocking curve width is 100 arc sec for a 4.0-μm-thick InSb epilayer. The highest room temperature electron mobilities of a 4.0-μm-thick InSb epilayer and an InSb QW are 64,000 and 23,500 cm^2/V-s for growth on off-axis Ge(211) and GeOI(001) substrates, respectively. We attribute the single-domain RHEED patterns, reduced X-ray rocking curve widths, and increased electron mobilities to the suppression of APDs in the structures grown on off-axis Ge(211) and GeOI(001) substrates.

[1]This work was supported by OCAST and NSF Grant DMR-0520550.

9:24AM A11.00008 Synthesis of large-area graphene on cobalt film by thermal cracker enhanced gas source molecular beam epitaxy , NING ZHAN, GUOPING WANG, JIANLIN LIU, Department of Electrical Engineering,University of California, Riverside, QUANTUM STRUCTURES LABORATORY TEAM — Recently, synthesis of large-area graphene has become increasingly important. Various metal substrates have been tested. Among these substrates, cobalt (Co) has been used to absorb carbon and form hexagonal structures on its surface. Nevertheless, only small graphene piece or nano carbon islands have been achieved. Here, we propose a method to grow graphene on Co using thermal cracker enhanced gas source molecular beam epitaxy. Atomic carbon beam provided by thermal cracker impinges to Co film and forms graphene epitaxially. Raman spectroscopy and transmission electron microscopy measurements confirmed mis-oriented stacking order between layers rather than strict AB Bernal stacking. The coverage of single layer and bi-layer is more than 90%. Growth temperature- and time-dependent analyses indicate a narrow growth window for the growth of few-layer graphene.

9:36AM A11.00009 Studies on magneto-transport properties of dilute magnetic semiconductors , R. GUPTA, A. GHOSH, Missouri State University, Y. KOLEKAR, Pune University, K. GHOSH, P. KAHOL, Missouri State University — Diluted magnetic semiconductors (DMS) are rare group of promising semiconductors in which a fraction of the constituent ions is replaced by magnetic ions. This study is aimed to understand the magneto-transport properties of magnetic ion doped In2O3 thin films. The films were grown under different temperature and partial oxygen pressures by pulsed laser deposition. The films were characterized using various techniques such as X-ray diffraction, UV-VIS spectroscopy and magneto-transport. Anomalous magneto-resistive (MR) behavior has been observed for these films, which largely depends on growth conditions. For example, Co doped In2O3 films show presence of negative as well as positive MR at low temperatures. However, the film grown at 400 0C at a partial oxygen pressure of 1×10-4 mbar shows negative MR with a maximum value of around -0.3%. Films grown under higher partial oxygen pressures show large positive MR. Maximum positive MR of 8.9% is seen for the film grown at partial oxygen pressure of 4.3×10- 4 mbar at 400 0C. The effect of growth conditions on MR properties of these films will be presented in detailed. This work is supported by National Science Foundation (Award Number DMR-0907037).

9:48AM A11.00010 Phase evolution and microstructure growth of $CuInSe_2$ by sonochemistry , EMRE YASSITEPE, University of Delaware, WILLIAM N. SHAFARMAN, Institute of Energy Conversion, University of Delaware, S.ISMAT SHAH, University of Delaware — Non toxic chemical routes that enable formation of high quality $CuInSe_2$ thin films with high materials utilization are desired for low production cost of solar cells. Sonochemistry provides a well known route to form reactive surfaces in metallic particles and , in the literature, CuSe has been reactively formed by using organic precursors. We will present results of the effects of ultrasound on the reactivity between Cu, In and Se elemental particles. The reaction between these elements facilitates binary selenide phase formation which promotes single phase growth of $CuInSe_2$ with further annealing. XRD analyses showed that binary phases of $CuSe_2$, CuSe and In_4Se_3 are formed by sonication. Annealing these binary phases led to the single phase formation of $CuInSe_2$ at 350 °C. We have found that if In has not reacted with Se during sonication, the structure is not completely transformed to $CuInSe_2$ at 350 °C.

10:00AM A11.00011 Structural and magnetic properties of Cr and Co doped indium oxide dilute magnetic semiconductors , K. GHOSH, E. NAHLIK, M. LANGHOFF, R. GUPTA, Missouri State University, Y. KOLEKAR, Pune University, P. KAHOL, Missouri State University — Dilute magnetic semiconductors have attracted considerable attention for development of next generation multifunctional spintronics devices. Indium oxide is a wide band gap semiconductor with unique optical and electrical properties. Here, we investigate the effect of Co and Cr doping on structural and magnetic properties of Indium oxide. Different amounts of Co and Cr were doped in In2O3 using solid state reaction method. Structural and magnetic properties have been measured using standard techniques. X-ray diffraction analysis confirmed single phase Indium oxide with no impurity phases due to addition of Co and Cr. Magnetization (M) as a function of applied magnetic field (H) and temperature (T) were collected on all the samples using a superconducting quantum interference device magnetometer. M vs T measurements for Co doped Indium oxide showed the presence of a hump around 50K which could be due to paramagnetic to ferromagnetic transition and the M vs H field study show the hysteresis behavior which confirms the ferromagnetism. This work is supported by National Science Foundation (Award Number DMR-0907037)

10:12AM A11.00012 High-Purity Germanium Crystal Characterization for DUSEL Experiments[1] , DONGMING MEI, CHAOYANG JIANG, OLEG PEREVOZCHIKOV, NICK WEINANDT, YONGCHEN SUN, The University of South Dakota, CUBED COLLABORATION — Understanding the nature of neutrinos and dark matter was identified by a National Academy of Sciences panel as one of the key problems facing physicists today. The CUBED (Center for Ultra-Low Background Experiments at DUSEL) collaboration is working on the development of techniques to manufacture crystals in an underground environment with unprecedented purity levels that may be used by experiments proposed for DUSEL. Growing high-purity germanium crystals depends strongly on the understanding of various impurities in the grown crystals and developing new techniques to eliminate them. This paper will present the characterization techniques to identify the impurity levels according to their energy levels and distributions. The results will provide feedback for the crystal growth process that would eliminate the impurities in the grown crystals for DUSEL experiments.

[1]DOE grant DE-SC0004768 and the South Dakota 2010 Center

10:24AM A11.00013 Stable Nanocrystals vs. Ostwald Ripening: A Theoretical Investigation , MICHAEL CLARK, SANAT KUMAR, Columbia University, KUMAR GROUP TEAM — Previous studies have shown that stable, monodisperse-sized nanocrystals (NCs) have been produced through the use of strongly binding surfactants, e.g. Au NCs with alkylthiols or Co NCs with oleic acid, to name a few. Through a first-principles theoretical investigation, we determine that these stable sized NCs are in an equilibrium state, and we establish what conditions lead to stable, monodisperse nanocrystals instead of polydisperse nanocrystals undergoing Ostwald ripening. Our results further describe how the equilibrium NC size can be tuned through experimentally adjustable parameters (concentration, temperature, reactant proportions), providing novel concepts for controlling the synthesis of monodisperse nanocrystals. Our theoretical results are compared directly with experimental NC syntheses, providing additional insight into the microscopic properties and dynamics of these stable NC mixtures.

10:36AM A11.00014 Extreme electronic sensitivity of carbon nanotubes to internal wetting , DI CAO, Arizona State University — It is now possible to pass a solution of an analyte through the interior of individual single-walled carbon nanotube (SWCNT) nanofluidic channels in a planar device connecting two fluid reservoirs. By building field-effect transistor connections onto the SWCNT nanofluidic channel, we have discovered that internal wetting of the SWCNT by pure water turns semiconducting tubes on, and renders them insensitive to back gating. Transistor action is restored when the devices are dried under vacuum. In contrast, external wetting has little effect. Theoretical simulations recapitulate this behavior, showing that the difference in response to internal and external wetting is a consequence of nanoconfinement, which enabled water molecule structure ordering and enhanced the water-CNT interaction. The dipole field of ordered water locks the CNT potential and the water-CNT interaction modifies the electronic structure of the CNT.

10:48AM A11.00015 CN-VFET Based Organic Nonvolatile Memory Elements Using a Floating Gate , PO-HSIANG WANG, BO LIU, MITCHELL MCCARTHY, ANDREW RINZLER, Dept. of Physics, UNIVERSITY OF FLORIDA, GAINESVILLE FL 32611 TEAM — We have demonstrated organic nonvolatile memory elements based on carbon nanotube enabled vertical field effect transistors (CN-VFETs) with a hybrid dielectric embedded floating metal gate used for charge storage. The electric field concentration around the high aspect ratio carbon nanotubes (acting as the source electrode in the vertical transistor) makes them excellent sources of charge injection of both polarities into the floating gate. This results in a large, fully programmable, hysteresis in cyclic transfer curves without sacrificing carrier mobility in the vertical organic channel layer. These features may provide for cost-effective, relatively high-density organic memory devices compared to more conventional TFT architecture organic devices.

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A12 GERA DMP: Focus Session: Electricity-to-Light Conversion: Solid State Lighting I D223/224

8:00AM A12.00001 Surface phase matched templates for GaN hetroepitaxial growth[1] , PRAVEEN KUMAR, NPL New Delhi India, JITHESH KUYYALIL, SHIVAPRASAD SM, JNCASR Bangalore India — Surface structural modifications are performed on Si(111)-7x7 surface, to find the appropriate template for high quality GaN growth. Adsorption of Ga forms stable superstructural phases of (1x1), (6.3x6.3) and (rt3xrt3) at 1.5ML, 0.8ML and 0.33ML respectively on a (7x7) reconstructed Si(111) surface. Using PA-MBE system, GaN of 0.75microns is grown at a relatively low temperature of 450oC on each of these phases. The films formed grow in the wurtzite phase with c-axis perpendicular to the Si(111) substrate surface. Now XRD, PL, XPS, AFM, FESEM and RHEED are employed to evaluate the structural, optical, compositional and morphological aspects of the GaN films. It is clearly observed that the 0.33ML (rt3xrt3) Ga phase results in the best quality GaN films, followed by the (6.3x6.3) phase and then the (1x1) phase. The (rt3xrt3) unit cell dimension matches with 2xa of GaN unit cell size, and thus GaN grows epitaxially on this surface with oriented single crystal grains. Thus, the results clearly demonstrate the possibility of employing low coverage metal induced surface phases as templates to form matched GaN films of high structural & optical quality.

[1]One of the authors acknowledge UGC for SRF -fellowship.

8:12AM A12.00002 Quantum Photovoltaics via Coherent Drive[1] , KONSTANTIN DORFMAN, ANATOLY SVIDZINSKY, MARLAN SCULLY, Texas A&M University — We study the fundamental limit to photovoltaic efficiency that is widely thought to be due to detailed balance between radiative recombination and radiative absorption. Quantum coherence in fact can break the detailed balance yielding vanishing emission of incident resonant radiation with nonzero absorption. This results in the enhancement of the quantum efficiency of the photovoltaic (PV) cell as compared to the "two-level" system. Similar to lasing without inversion and photo-Carnot quantum heat engine, in a quantum dot PV cell with coherently driven doublet in the excited state it is possible to suppress the radiative recombination and increase the quantum limit of photovoltaic operation compare to classical one. Our approach is consistent and does not violate the laws of thermodynamics.

[1]The NSF Grant No. EEC-0540832 (MIRTHE ERC), the Office of Naval Research, and the Robert A. Welch Foundation (A-1261).

8:24AM A12.00003 New Type of Core-Shell Nanocrystal Quantum Dots for Applications in Light Emitting Diodes (LEDs) , B.N. PAL, S. BROVELLI, Y. GOSH, V.I. KLIMOV, J.A. HOLLINGSWORTH, H. HTOON, LANL, CHEMISTRY DIVISION TEAM, CENTER FOR ADVANCED SOLAR PHOTOPHYSICS TEAM, CENTER FOR INTEGRATED NANOTECHNOLOGIES TEAM — We demonstrate a proof of principle for LEDs based on giant nanocrystal quantum dots (g-NQDs). These dots consist of a CdSe core overcoated with a thick CdS shell built one monolayer at a time. Our device structure is composed only of a PEDOT:PSS coated indium-tin oxide (ITO) anode and a LiF-Al cathode. These simple devices exhibit a maximum external quantum efficiency (EQE) and luminance of 0.12% and 1000 Cd/m2 respectively when 16 shell g-NQDs are used for the active layer. This performance is already comparable to that of more sophisticated all-inorganic NQD LEDs. Thick shell (>13 monolayer) g-NQD devices show EQEs about one order of magnitude higher than those of thin-shell (4 monolayer) NQD devices, as well as much greater stability for operation under ambient conditions. Although current g-NQD devices do not set any new performance records, this work demonstrates a significant potential of g-NQDs for LED applications.

8:36AM A12.00004 Lattice-mismatched phosphide-based LEDs for color mixing white light applications , KIRSTIN ALBERI, National Renewable Energy Laboratory — The most promising means of achieving high efficiency white light emitting diodes (LEDs) with high color rendering indices (CRI) is to combine individual red (615 nm), yellow (573 nm), green (535 nm) and blue (459 nm) solid-state LEDs in a four color RYGB architecture. Due to their high bandgaps and the availability of bulk substrates, phosphide-based alloys are currently leading candidates for achieving the longer wavelengths, of which AlGaInP lattice-matched to GaAs has been extensively explored. In a departure from this approach, we investigate phosphide alloys at compositions that are lattice-mismatched with respect to GaAs for color mixing white light applications. Lifting the lattice-matching requirement extends the options for active and cladding layer design and optimization, thereby providing additional avenues for reducing carrier loss pathways and improving device efficiency. This talk covers our work on issues central to the success of this technology: metamorphic growth of high quality epilayers, the competing trade-off between operating wavelength and intervalley carrier transfer loss, and the availability of optimal cladding layers for high power operation. Support from the DOE EERE-SSL and BES-DMS programs and the LDRD program at NREL is gratefully acknowledged.

9:12AM A12.00005 Ab initio study of MOCVD synthesis of InN and GaN , WERONIKA WALKOSZ[1], Argonne National Laboratory, PETER ZAPOL, MATTHEW J. HIGHLAND, PAUL H. FUOSS, GREGORY B. STEPHENSON — A detailed understanding of MOCVD growth of group III nitrides is important for improved control over their properties and performance in a wide range of applications. Because of the relative instability of InN, chemically active precursors such as NH_3 are typically used to provide the high nitrogen activity needed for growth. Our goal is to understand the mechanism and species involved in active nitrogen formation on the growth surface. Here we present results of density functional theory calculations for the decomposition of NH_3 on InN and GaN (0001) surfaces through reaction intermediates such as adsorbed NH_2 and NH. The calculated equilibrium surface structures along with the reaction barriers for the dissociation pathways of NH_3 on these surfaces are described. Kinetic modeling based on the calculated barriers to determine reaction mechanisms and effective nitrogen activities is discussed. The results will be used to elucidate chemical kinetics on GaN and InN (0001) surfaces under MOCVD growth conditions with the aim to optimize synthesis conditions and precursors for effective growth of metastable nitrides. Work supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-06CH11357.

[1]Materials Science Division

9:24AM A12.00006 Band Gap Tuning and Structural Transformation in GaN through Equi-biaxial In-plane Strains and Alloying with InN , LIANG DONG, Department of Physics, University of Connecticut, S. PAMIR ALPAY, Department of Physics and Institute of Materials Science, University of Connecticut — Gallium nitride (GaN)-based semiconductor devices play a key role in modern optoelectronics and photovoltaics. Structural and electronic properties of the GaN can be tuned through external/internal stresses or by alloying it with InN. In this study, we present an *ab initio* analysis using density functional theory to understand the effects of equi-biaxial strains and indium additions to the crystallographic structure, electronic properties, and polarization of GaN and band bending in GaN-InN heterostructures. It is shown that internal strains in GaN may result in significant changes in the band gap and may even give rise to structural transformations from wurtzite to a graphite-like semi-metallic phase. For the InGaN alloys, possible stable crystal structures (besides the prototypical wurtzite structure), lattice parameters, the band gap, and the spontaneous polarization are calculated as function of indium composition.

9:36AM A12.00007 Structural and Optical properties of Si-doped AlN , SASHIKANTH MAJETY, BED PANTHA, ASHOK SEDHAIN, JING LI, HONGXING JIANG, JINGYU LIN, Texas Tech University — A lot of research has focused on controlling the conductivity in AlN by Silicon doping. AlN has the widest bandgap (∼6.1 eV) among III-Nitride semiconductors and exhibits excellent properties such as high temperature stability, high thermal conductivity, and deep ultraviolet transparency. In the AlN material system, doping causes crystal imperfections which can affect the structural and optical properties of the AlN epilayers. In this work, we investigated the impact of Si incorporation on the structural and optical properties of AlN epilayers. The formation of edge dislocations in Si-doped AlN is explained by the built-up tensile stress in the epilayers as revealed by X-ray diffraction measurement. Photoluminescence (PL) studies revealed that the full width at half maximum of both band-edge emission and impurity related transitions are correlated with the density of screw dislocations, N_{screw}, which is found to increase with increasing doping concentration of Si (N_{Si}). In addition, it was formulated that the band-edge (impurity) PL emission linewidth increases linearly with increasing N_{screw} at a rate of ∼3.3±0.7 meV/10^8 cm^{-2} (26.5±4 meV/10^8 cm^{-2}), thereby establishing PL measurement as a simple and effective method to estimate screw dislocation density in AlN epilayers.

9:48AM A12.00008 Causes of yellow luminescence in GaN , ANDERSON JANOTTI, University of California Santa Barbara — Although GaN is already used in light-emitting diodes and laser diodes, the origins of a number of frequently observed sub-band-gap luminescence bands are still under debate. For instance, the broad yellow luminescence that is invariably seen in n-type GaN has been long attributed to Ga vacancies. However, its presence in semi-insulating or p-type material, in which the Ga-vacancy concentration is low, has remained unexplained. The yellow luminescence has also been associated with the presence of carbon impurities, yet no credible, C-related configuration has been suggested. Using first-principles calculations we investigate the electronic and structural properties associated with defects and impurities in GaN. We employ a hybrid functional method to overcome the well-known band-gap problem of density functional calculations, and obtain accurate, quantitative results for defect transition levels. We find that C substituting for N (C_N) is a deep acceptor in GaN, with an ionization energy of 0.90 eV, in contrast to the commonly accepted view that C_N acts as a shallow acceptor. Incorporating C_N will therefore not result in p-type conductivity [1]. By inspecting the calculated configuration coordinate diagrams, we find that the absorption and emission lines of C_N are in remarkable agreement with the experimental results for yellow luminescence. This solves the longstanding puzzle regarding the nature of the defect responsible for yellow emission in C-containing GaN, and suggests that previous experimental data, analyzed under the assumption that C_N acts as a shallow acceptor, should be revisited. Work performed in collaboration with J. L. Lyons and C. G. Van de Walle, and supported by the NSF and by the UCSB Solid State Lighting and Energy Center.

[1] J. L. Lyons, A. Janotti, and C. G. Van de Walle, Appl. Phys. Lett. 97, 152108 (2010).

10:24AM A12.00009 Hybrid functional calculations of DX centers in AlN, GaN and AlGaN[1] , LUKE GORDON, JOHN L. LYONS, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106-5050 — The group-III nitrides have important commercial applications in optoelectronic devices. To achieve high-efficiency UV lasers and LEDs, AlN substrates and high Al-content AlGaN alloys will likely be required. A better understanding of the role of defects and impurities in AlN is crucial. One of the outstanding problems in the study of AlN and high-Al-content AlGaN is the formation of the so-called DX centers, which consist of donor impurities that self-compensate by turning to acceptors as the Fermi level approaches the conduction band. In this work, we employ density functional calculations using a hybrid functional to investigate the possibility of DX-center formation for Si and O donors in AlN and GaN. The functional includes a portion of Fock exchange and gives band gaps and lattice parameters very close to the experimental values, allowing for quantitative predictions of defect levels. Based on the analysis of the stability of DX centers in AlN and GaN, we discuss the onset of DX behavior in AlGaN alloys.

[1]This work was supported by NSF and by the UCSB SSLEC.

10:36AM A12.00010 Role of nitrogen vacancies and related complexes in compensation and luminescence of Mg-doped GaN , QIMIN YAN, ANDERSON JANOTTI, University of California at Santa Barbara, MATTHIAS SCHEFFLER, UCSB and Fritz-Haber-Institut, D-14195 Berlin, CHRIS G. VAN DE WALLE, University of California at Santa Barbara — Using first-principles calculations with the hybrid functional method (HSE), we investigate the effects of nitrogen vacancies and related complexes on the electrical and optical properties of Mg-doped GaN. We obtain information about the expected defect concentration, stable charge states, and defect levels by calculating the formation energies of vacancies and Mg−vacancy complexes. The $3+$ state of the nitrogen vacancy and the $2+$ state of the complex are found to be most stable when the Fermi level is near the valence-band maximum (VBM). Our calculations also enable us to study the role of these defects in luminescence. Vacancy-dopant complexes (including $\mathrm{Mg_{Ga}}-V_{\mathrm{N}}$) have been proposed as the origin of a deep level involved in the red (1.8 eV) photoluminescence (PL) band often observed in Mg−doped GaN. We investigate the optical absorption and emission energies by calculating the configuration coordinate diagram for the vacancy and for the $\mathrm{Mg_{Ga}}-V_{\mathrm{N}}$ complex. The emission, in which an electron in the conduction band is transferred to $(\mathrm{Mg_{Ga}}-V_{\mathrm{N}})^{2+}$, resulting in $(\mathrm{Mg_{Ga}}-V_{\mathrm{N}})^{+}$, peaks at 1.81 eV. Our calculated emission lines thus indicate that $\mathrm{Mg_{Ga}}-V_{\mathrm{N}}$ is a likely source for the red luminescence observed in Mg-doped GaN.

10:48AM A12.00011 Effects of strain on effective masses in GaN and AlN[1] , CYRUS E. DREYER, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106-5050 — Strain caused by lattice mismatch or alloying is present in almost all heterostructure-based semiconductor devices. One of the fundamental effects of strain on semiconducting materials is to alter their band gap and thus the effective mass of their carriers. Because of the lack of native substrates for GaN and the mismatch between different layers, these effects are particularly important in GaN/AlGaN based devices. Using first-principles calculations, we have investigated the effects of hydrostatic and c-plane biaxial strain on the band structure of GaN and AlN, specifically on the band gap and effective mass in the direction parallel and perpendicular to the c direction. In general, the effective mass decreases with increased hydrostatic or biaxial tensile strain, as expected from k.p theory. However, the opposite trend is observed for the effective mass of AlN in the c direction under biaxial strain. This is explained by analyzing the strained band structure of AlN using a two-band Kane model.

[1]This work was supported by NSF and by the UCSB Solid State Lighting and Energy Center.

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A13 DFD DPOLY: Focus Session: Polymer Colloids: Structure, Function, and Dynamics I D225/226

8:00AM A13.00001 Osmotic pressure of microgel suspensions , JUAN JOSE LIETOR-SANTOS, BENJAMIN SIERRA-MARTIN, JUSTIN FREDERICK, YESENIA LAPORTE, GEORGE MARKOU, ALBERTO FERNANDEZ-NIEVES, Georgia Institute of Technology — Microgels are crosslinked-polymeric networks in the colloidal domain, whose size can be change in response to external stimuli. They are soft particles by construction and can exhibit a very different behavior compared to hard sphere suspensions. In some cases, this different behavior has been understood by alluding to particle de-swelling at low volume fractions. For this to happen, the suspension osmotic pressure at such volume fraction should be comparable to the particle bulk modulus. In this work, we independently measure the bulk modulus of microgel particles and the suspension osmotic pressure and find that both magnitudes become comparable at a volume fraction corresponding to a liquid-to-solid transition, which we asses using rheology. Interestingly, in the solid region, the shear and compressional moduli of the suspension exhibit the same behavior with volume fraction, in analogy to emulsions. However, by contrast to emulsions, they are almost two orders of magnitude apart. This reflects the contributions from the internal modes of the microgel particles, which are absent for the case of an emulsion drop.

8:12AM A13.00002 Particle Charging and Interaction in Nonpolar Colloidal Dispersions Mediated by Nonionic Surfactants , SVEN BEHRENS, Georgia Tech — The electrostatic stabilization of colloidal dispersions is usually considered the domain of polar media only, but some surfactants are known to raise the conductivity of liquids with low electric permittivity and to mediate charge-stabilization of nonpolar dispersions. Here we report an example of the counterintuitive electrostatic effects of nonionic surfactants on colloidal particles in nonpolar solvents. PMMA particles in hexane solutions of sorbitan oleate (Span) surfactants exhibit a field-dependent electrophoretic mobility. In the zero field limit, we find large surface potentials whose decay with increasing surfactant concentration resembles the salt-induced screening in aqueous solutions. The amount of surface charge and screening ions in the nonpolar bulk is further characterized via ensemble measurements of the particles' pair interaction energy. In contrast to the behavior reported for systems with *ionic* surfactants, we observe particle charging and a screened Coulomb type interaction both above and below the surfactant's critical micelle concentration.

8:24AM A13.00003 Experimental Studies of the Brownian Diffusion of Boomerang Colloidal Particle in a Confined Geometry , AYAN CHAKRABARTY, FENG WANG, BHUWAN JOSHI, QI-HUO WEI, Kent State University — Recent studies shows that the boomerang shaped molecules can form various kinds of liquid crystalline phases. One debated topic related to boomerang molecules is the existence of biaxial nematic liquid crystalline phase. Developing and optical microscopic studies of colloidal systems of boomerang particles would allow us to gain better understanding of orientation ordering and dynamics at "single molecule" level. Here we report the fabrication and experimental studies of the Brownian motion of individual boomerang colloidal particles confined between two glass plates. We used dark-field optical microscopy to directly visualize the Brownian motion of the single colloidal particles in a quasi two dimensional geometry. An EMCCD was used to capture the motion in real time. An indigenously developed imaging processing algorithm based on MatLab program was used to precisely track the position and orientation of the particles with sub-pixel accuracy. The experimental finding of the Brownian diffusion of a single boomerang colloidal particle will be discussed.

8:36AM A13.00004 Effect of Boundary Mobility on the Dynamics of Confined Colloidal Suspensions , GARY L. HUNTER, KAZEM V. EDMOND, ERIC R. WEEKS, Emory University — We use high-speed confocal microscopy to study the influence of boundary mobility on the dynamics of confined colloidal suspensions. Experiments in molecular super-cooled liquids show that confinement can enhance or hinder sample mobility, depending on whether the confining boundary is "soft" (mobile) or "hard" (immobile). We confine suspensions of PMMA microspheres within emulsion droplets of different sizes to examine the consequences of confinement. By changing the viscosity of the external, continuous phase, we also vary the boundary mobility of our samples. In this way, we decouple the effects of confinement and boundary mobility, and draw comparisons between colloidal suspensions and molecular liquids.

8:48AM A13.00005 Observing liquid-gas nucleation in a colloid-polymer solution , RYAN MCGORTY, VINOTHAN N. MANOHARAN, Harvard Unversity, Dept. of Physics — We study liquid-gas nucleation in a colloid-polymer solution. Though the colloidal particles are too small to resolve, we are able to observe nucleating droplets due to the refractive index mismatch between the two fluid phases. By using digital holographic microscopy and thermally-responsive colloids we are able to observe the micron-sized nucleating droplets and their fluctuations in three-dimensions. From the droplets' fluctuations we can back out the interfacial tension. Additionally, our three-dimensional imaging technique allows us to capture individual nucleation events and their rate of occurrence. We hope that our data will allow us to better understand nucleation kinetics.

9:00AM A13.00006 Measuring the translational and rotational diffusion of colloidal clusters with digital holographic microscopy , JEROME FUNG, KRISTOPHER ERIC MARTIN, RYAN MCGORTY, DAVID M. KAZ, REBECCA W. PERRY, Harvard University, JOHN A. KELLER, Eastern Nazarene College, GUANGNAN MENG, VINOTHAN N. MANOHARAN, Harvard University — We measure the rotational and translational diffusion coefficients of individual non-spherical colloidal clusters undergoing three-dimensional Brownian motion. We image clusters comprised of spheres approximately 1 μm in diameter using digital holographic microscopy. Fitting the measured holograms to exact electromagnetic scattering calculations allows us to determine cluster positions and orientations with millisecond temporal resolution and $\sim$10 nm spatial resolution. For dimers of polystyrene spheres in an aqueous solution, our measurements of the coefficients for rotational diffusion as well as translational diffusion parallel and perpendicular to the dimer axis are consistent with theory. We discuss the extension of this work to non-axisymmetric trimers and potential applications.

9:12AM A13.00007 Density of States of a Two-Dimensional NIPA-Polystyrene Colloidal Crystal[1] , MATTHEW GRATALE, PETER YUNKER, KE CHEN, ARJUN YODH, Department of Physics and Astronomy, University of Pennsylvania — In this work we are interested in how "dopants" affect the vibrational properties of crystals. We study the vibrational density of states of a two-dimensional colloidal crystal consisting of a mixture of hard polystyrene particles and soft NIPA microgel particles. Thus, depending on the particles involved, multiple inter-particle potentials are present in these crystals. The number ratio of hard to soft particles is varied, creating crystals consisting primarily of soft particles doped with hard particles and vice versa. We employ video microscopy to derive the phonon density of states of corresponding "shadow" crystals with the same geometric configuration and interactions as the experimental colloidal system, but absent damping [1,2,3]. Preliminary data reveal low frequency plane-like waves in all crystals, regardless of composition. Participation in higher frequency modes is often enhanced in one species of particles and diminished in the other.

[1] Chen *et al.*, PRL 105, 025501 (2010). [2] Kaya *et al.*, Science 329, 656 (2010). [3] Ghosh *et al.*, PRL 104, 248305 (2010).

[1]This work is supported by NSF grant DMR-0804881, MRSEC grant DMR-0520020, and NASA grant NNX08AO0G.

9:24AM A13.00008 Structure and dynamics of confined colloid-polymer mixtures , JACINTA CONRAD, Department of Chemical and Biomolecular Engineering, University of Houston, BINH TRINH, GILDARDO CEBALLOS, Department of Chemical and Biomolecular Engineering, University of Houston — Colloidal processing routes typically require attractive suspensions to be flowed through fine geometries such as microchannels, nozzles, or thin films. To elucidate the effects of confinement on attractive suspensions during processing, we use confocal microscopy to image the structure and dynamics of model colloid-polymer mixtures as a function of confinement dimensionality and thickness, colloid volume fraction, and the strength and range of the attraction. We characterize the phase behavior of the confined suspensions, and find that confinement induces non-uniform structural changes within colloidal gels.

9:36AM A13.00009 Controlling the size distribution of self-assembled colloidal clusters[1] , NICHOLAS SCHADE, Harvard Department of Physics, JESSE COLLINS, JONATHAN FAN, MIRANDA HOLMES-CERFON, Harvard SEAS, VINOTHAN MANOHARAN, Harvard Department of Physics — Using a combination of experiment and simulation, we investigate the structures that form when spherical colloidal particles cluster around spheres of different sizes in a binary mixture. We use either oppositely charged particles or particles coated with complementary DNA sequences to form the clusters. Using optical microscopy, we examine the effect of the stoichiometric ratio, the size ratio, and the type of interaction on the distribution of clusters. These parameters serve as useful control mechanisms for the synthesis of nanostructures with tunable properties. For example, a high density of tetrahedral clusters of metallo-dielectric spheres could be used to create a bulk, isotropic metamaterial.

[1]We acknowledge support from NSF grant no. ECCS-0709323 as well as the DOE Office of Science Graduate Fellowship Program.

9:48AM A13.00010 Dynamics of interfacial breach by colloidal spheres , DAVID M. KAZ, RYAN MCGORTY, Harvard University, MADHAV MANI, University of California at Santa Barbara, VINOTHAN N. MANOHARAN, Harvard University — We present observations of individual colloidal spheres as they approach and penetrate a flat aqueous interface. Polystyrene spheres with various surface chemistries (sulfate, carboxyl, etc) are brought to the boundary between an oil phase (decane) and an aqueous phase (water+glycerol+NaCl) using radiation pressure from a tightly focused laser. Holographic images are recorded at up to 24,000 frames per second and subsequently compared with Mie-scattering calculations to obtain positional data at a resolution of 5nm in x,y, and z. Typical trajectories consist of an approach to the interface that is dominated by hydrodynamics; a discontinuous jump at the point of penetration (POP); and a very long timescale relaxation that is logarithmic in time. We find that the concentration of salt in the aqueous phase must be above a certain threshold (depending on species) for breach to occur. Well above this threshold, trajectories just prior to the POP are characterized by short-timescale features that are non-monotonic in salt concentration. DLVO type calculations reproduce some aspects of these features, but the non-monotonicity remains mysterious.

10:00AM A13.00011 Sub-diffusion of DNA Coated Particles Near a Complementary DNA Covered Surface[1] , LANG FENG, QIN XU, Center for Soft Matter Research, New York University, RUOJIE SHA, NADRIAN SEEMAN, Chemistry Department, New York University, PAUL CHAIKIN, Center for Soft Matter Research, New York University — We have measured the diffusive behavior of micrometer sized colloids in a DNA covered particle-surface system. Near the particle-surface melting temperature of $\sim 45^\circ$ C we observe conventional diffusion but as temperature is lowered we see a crossover to sub-diffusion over a narrow temperature range. The sub-diffusive behavior is intimately related to the broad distribution of local trapping times. We present a theoretical model which explains the sub-diffusion exponent μ in $< R^2(t) > \sim t^\mu$, which ranges from $\mu = 1$ at 44.7° C to $\mu = 0.33$ at 44.1° C. From the distribution of number of DNA bonds we calculate the trapping time distribution and average trapping time. When the measurement time exceeds the average trapping time the system is in equilibrium and exhibits conventional diffusion. When the measurement time is less than the average trapping time the system is not in equilibrium and is sub-diffusive.

[1]NASA NNX08AK04G

10:12AM A13.00012 Multiple-Stage Melting and Freezing of Colloidal Crystallites with Short-range Attraction , LIQUAN PEI, Department of Physics, University of Massachusetts Amherst, J.R. SAVAGE, Department of Physics, Cornell University, A.D. DINSMORE, Department of Physics, University of Massachusetts Amherst — We study the dynamics of melting and freezing in a model colloidal system with short-range, temperature tunable attraction. In particular, we mix micron-sized, charge stabilized polystyrene spheres with salt and the surfactant micelles. The micelles induce depletion attraction whose range is less than 2% of the sphere diameter and whose magnitude changes strongly with temperature. We use optical microscopy to record the dynamics of freezing and melting following temperature changes. We use particle tracking algorithms to identify the particles with sub-pixel resolution. For samples with area fraction less than 40%, we have observed that melting and freezing occur in multiple stages, with a metastable liquid phase appearing in both processes. For the freezing sample at area fraction 55%, we have found that the gas droplets are nucleated from high area fraction backgound. The data also show how nucleation dynamics are affected by the metastable gas-liquid binodal. We are also investigating the role of the second, metastalbe solid phase in melting and freezing. Our results are relevant to systems where non-equilibrium states may play a role in phase separation.

10:24AM A13.00013 Colloidal aggregation in microgravity by critical Casimir forces , SANDRA VEEN, PETER SCHALL, University of Amsterdam, MARCO POTENZA, MATTEO ALAIMO, University of Milan, STEFANO MAZZONI, European Space Agency, GERARD WEGDAM, University of Amsterdam, VAN DER WAARLS ZEEMAN INSTITUTE, UNIVERSITY OF AMSTERDAM COLLABORATION, OPTICS AND MICROGRAVITY RESEARCH LABORATORY, UNIVERSITY OF MILAN COLLABORATION, PHYSICAL SCIENCE UNIT, EUROPEAN SPACE AGENCY COLLABORATION — We study aggregation and crystal growth of spherical Teflon colloids in binary liquid mixtures in microgravity by the critical Casimir effect. The critical Casimir effect induces interactions between colloids due to the confinement of bulk fluctuations (density or concentration) near the critical point of liquids. The strength and range of the interaction depends on the length scale of these fluctuations which increase as one approaches the critical point. The interaction potential can thus be tuned with temperature. We follow the growth of structures in real time with Near Field Scattering. Measurements are performed in microgravity in order to study pure diffusion limited aggregation, without disturbance by sedimentation or flow.

10:36AM A13.00014 Particle interactions in colloids are revealed in a nonlinear effect in light transmission , JINSUK SONG, DANIEL OU-YANG — Studies on interactions between particles in highly concentrated suspensions are rare because the solutions are opaque and the interpretations from methods such as diffusing wave spectroscopy are often complicated. We propose a simple method of probing particle interactions in the opaque solution by measuring light transmission affected by optically induced particle concentration enhancement. The increase in the particle concentration with the input light intensity depends on the interactions between particles. We demonstrate how this method can be used to determine single particle trapping energy and the virial coefficients in aqueous suspensions of 190 nm polystyrene spheres.

10:48AM A13.00015 Nano-dumbells pack densely to form birefringent photonic crystals , JASON FORSTER, JIN-GYU PARK, Yale, MANISH MITTAL, University of Delaware, VINODKUMAR SARANATHAN, HEESO NOH, CARL SCHRECK, RICHARD PRUM, COREY O'HERN, HUI CAO, Yale, ERIC FURST, University of Delaware, ERIC DUFRESNE, Yale — Monodisperse spherical colloidal particles robustly self-assemble into crystals at high concentration. We study the the self-assembly of polymer nano-dumbells and find that they crystallize only under strong confinement - in thin films less than three particles thick. On the other hand, external electric fields can readily align dumbbell- shaped particles to make a birefringent suspension. When the electric field is turned off, the dumbbells rapidly lose their orientational order and the birefringence quickly goes away. However, if the solvent is removed with the electric field on, the particles self-assemble into a novel dense crystalline packing hundreds of particles thick. We describe the essential physics of self-assembly of these structures through an interplay of the applied electric field and capillary forces.

Monday, March 21, 2011 8:00AM - 10:48AM –

Session A14 FEd: Focus Session: New Ways of Communicating Physics D227

8:00AM A14.00001 The Need For "Pleasure in Finding Things Out:" The Use of History and Our Greatest Scientists for Human Survival and Scientific Integrity , JOSHUA BORCHARDT, North Dakota State University — Why Homo sapiens search for interesting things and the methods of which we do so. The use of philosophical, theoretical, and demonstrated processes for exploration of the natural, and not so natural world are presented based on the ideas and wishes of some of History's greatest scientists, with concentration on Richard P. Feynman's lens on scientific discovery and pursuit, for which the abstract gets its title. This talk is presented towards the layman as well as the physicist, and gives insight to the nature of discovery and what it means to have pleasure in finding things out for the betterment of all mankind.

8:12AM A14.00002 Energy Experiments for STEM Students , JOHN FANCHI, TCU — Texas Christian University (TCU) is developing an undergraduate program that prepares students to become engineers with an emphasis in energy systems. One of the courses in the program is a technical overview of traditional energy (coal, oil and gas), nuclear energy, and renewable energy that requires as a pre-requisite two semesters of calculus-based physics. Energy experiments are being developed that will facilitate student involvement and provide hands-on learning opportunities. Students participating in the course will improve their understanding of energy systems; be introduced to outstanding scientific and engineering problems; learn about the role of energy in a global and societal context; and evaluate contemporary issues associated with energy. This talk will present the status of experiments being developed for the technical energy survey course.

8:24AM A14.00003 Physics Learning Strategies with Multi-touch Technology , MARK POTTER, SUNY Oswego, C. ILIE, SUNY Oswego Physics Dept., D. SCHOFIELD, SUNY Oswego CS Dept. — Advancements in technology have opened doorways to build new teaching and learning methods. Through conjunctive use of these technologies and methods, a classroom can be enriched to stimulate and improve student learning. The purpose of our research is to ascertain whether or not multi-touch technology enhances students' abilities to better comprehend and retain the knowledge taught in physics. At their basis, students learn via visual, aural, reading/writing, and kinesthetic styles. Labs provide for all but the aural style, while lectures lack kinesthetic learning. Pedagogical research indicates that kinesthetic learning is a fundamental, powerful, and ubiquitous learning style [1]. By using multi-touch technology in lecture, not only can we accommodate kinesthetic learners, but we can also enrich the experiences of visual learners. Ushering to this wider array of students will hopefully lead to an increase in meaningful learning.

[1] Wieman, C.E, Perkins, K.K., Adams, W.K., -Oersted Medal Lecture 2007: "Interactive Simulations for teaching physics: What works, what doesn't and why," American Journal of Physics. 76 393-99.

8:36AM A14.00004 Why the New York Times Science Tuesday section is only eight pages and what to do about it , BRIAN SCHWARTZ, The Graduate Center of CUNY — Communicating science to the public is the responsibility of all scientists and necessary for an informed electorate and as an inspiration to young minds. Yet successful national strategies for communicating science and the venues for such communication seem limited. Science museums and TV programs like NOVA reach millions of people but still only a very small fraction of the US population. In terms of daily science reporting very few newspapers have a devoted science reporter and it is only the New York Times which has a significant weekly reporting section on science (and health). What can one do about reaching wider and new audiences? We recently ran an NSF sponsored international conference entitled Communicating Science to the Public through the Performing Arts (www.sciartconference2010.com). At the conference there were sessions on science and theater, science and TV and film, science and dance, science and music and science festivals, cafes and events (web.gc.cuny.edu/sciart). Using these new approaches one can reach a new and wider audience and one can also take advantage of the seemingly insatiable interest of the press in the arts. Examples of successful new strategies for communicating science will be presented, evaluated and shown to be replicable at a relatively modest cost of time and money.

9:12AM A14.00005 Teaching Physics Through Comic Books , REBECCA THOMPSON[1], TASSIA OWEN, American Physical Society — Comics have been around as a form of entertainment for decades. They are often as seen as one of the distracting vices of kids (and adults!), but comics and their more adult version, the graphic novel, are increasingly valued as a legitimate genre of literature. The APS Outreach Department has created three comic books, one featuring Nikola Tesla and his battles with the evil Thomas Edison, and two about laser super hero Spectra and her continuing battles with the nefarious Miss Alignment. These comics have struck a delicate balance between education and entertainment being well received by both the comic book and education communities. By creating a compelling comic story that has correct physics, it is possible to use this under-appreciated medium to excite middle-school students who might otherwise be turned off by traditional teaching methods. One lesson-learned is that It is very important to make sure first and foremost that the students enjoy the story and that they feel a connection to the characters. Students are thus hooked and once they are drawn in, the learning happens automatically..

[1]APS Head of Public Outreach

9:24AM A14.00006 Khan Academy: the world's free virtual school[1] , JOSHUA A. DIJKSMAN, Duke University, SALMAN KHAN, Khan Academy — Khan Academy offers an unprecedented set of educational material for science and math education, in the form of short, free, publicly available video clips. With a growing set of already over 2000 videos, it is easily the most exhaustive collection of structured educational material on the Internet. The content is made in digestible 10-20 minute chunks; the granular nature of the material allows learners to fill in almost any of their knowledge "gaps." Importantly, the conversational style used in the videos offers a fresh, new perspective on math and science instruction. With our 2 M$ funding grant from Google and support from the Gates foundation, we envision covering all topics that would appear in typical high-school or collegiate-level Math and Science courses, and translating these videos to the major languages across the globe. Moreover, we also offer a free and fully integrated assessment system, which allows students to practice problems at their own pace and focus on the appropriate instruction to fill in their individual gaps. Many testimonials have already proven our methods to be a highly successful educational tool. Our goal is to allow educators to improve their teaching, but above all to bring simple, rewarding and enjoyable education to the minds of many young students.

[1]Supported by Google, the Gates Foundation, donors and volunteers.

9:36AM A14.00007 How to Talk Science to Homer Simpson , MICHAEL LUCIBELLA, The American Physical Society — Communicating scientific information to the general public is an important but often underappreciated skill. Researchers who can clearly and concisely describe the science they do are critical to helping create a scientifically literate public, something that is sorely lacking in this country. Public understanding of science is crucial because people who understand and appreciate science are more likely to support research funding, the public has to vote on issues of science and technology more than ever, and it helps sow the next generation of scientists. Plus there are many people interested in learning about science who but don't have the training to digest technical language. Writing or talking to a public with minimal background in science and or the media is very different from communicating members of the scientific community. I'll go over a few strategies to keep your message as clear as possible, and will offer some communication guidelines that will ensure that the media and public understand what you say.

9:48AM A14.00008 School for Scientific Thought: Saturday sessions that bring high school and STEM graduate students together , ELISABETH GWINN, Physics Department, UCSB, WENDY IBSEN, CNSI, UCSB — The School for Scientific Thought (http://csep.cnsi.ucsb.edu/k12/sst) is a Saturday morning program that exposes high school students to current research in STEM fields, through 5-week miniclasses that are conceived, developed and taught by graduate students. Now in its second year of sponsorship by UCSB's California Nanosystems Institute, this NSF-supported program provides graduate students with a creative opportunity to communicate their own favorite science to a young audience. The experience solidifies the graduate student's own knowledge while developing expository skills during a limited time commitment that allows them to also progress in their research objectives. High school students make contact with positive scientist role models while learning about exciting topics that are beyond the high school curriculum. SST courses have ranged from "Surfing the Waves of Light and Matter" to "Nanotechnology: Using the Very Small to Solve the World's Problems". The selection of graduate student instructors and recruitment of high school students will be discussed. SST is an outgrowth of the NSF GK-12 program "Let's Explore Applied Physical Science" (LEAPS).

10:00AM A14.00009 The Changing Landscape of Science News , JAMES RIORDON, American Physical Society — Social media are revolutionizing the ways that people communicate and the ways they get their news. Traditional news outlets are in decline, and no subject area is declining faster than science news. Every day there are fewer professional science journalists working in traditional media. On the other hand, ever greater numbers of scientists, science enthusiasts, and online journalists are turning to blogs, podcasts, eBooks, twitter feeds, and social media sites like Facebook and Tumbler to spread news about science. I will present an overview of the state of science journalism and speculate on the likely directions it seems to be heading. I will also offer some general guidelines to help scientists understand what makes a good science news story, as well as suggesting ways that they can get their work in the news.

10:12AM A14.00010 Interactive NMR: A Simulation Based Teaching Tool for Fundamentals to Applications with Tangible Analogies[1] , SARAH GRIESSE-NASCIMENTO, Boston University, JOSHUA BRIDGER, Dover Sherborn HS, KEITH BROWN, ROBERT WESTERVELT, Harvard University — Interactive computer simulations increase students' understanding of difficult concepts and their ability to explain complex ideas. We created a module of eight interactive programs and accompanying lesson plans for teaching the fundamental concepts of Nuclear Magnetic Resonance (NMR) and Magnetic Resonance Imaging (MRI) that we call interactive NMR (iNMR). We begin with an analogy between nuclear spins and metronomes to start to build intuition about the dynamics of spins in a magnetic field. We continue to explain T1, T2, and pulse sequences with the metronome analogy. The final three programs are used to introduce and explain the Magnetic Resonance Switch, a recent diagnostic technique based on NMR. A modern relevant application is useful to generate interest in the topic and confidence in the students' ability to apply their knowledge. The iNMR module was incorporated into a high school AP physics class. In a preliminary evaluation of implementation, students expressed enthusiasm and demonstrated enhanced understanding of the material relative to the previous year.

[1]Funded by NSF PHY-0646094 grant

10:24AM A14.00011 ALPhA: The Advanced Laboratory Physics Association , ERIC BLACK, California Institute of Technology, LOWELL MCCANN, University of Wisconsin at River Falls, JONATHAN REICHERT, TeachSpin, Inc., GABE SPALDING, Illinois Wesleyan, JOHN ESSICK, Reed College, DAVID VAN BAAK, Calvin College, STEVE WONNELL, Johns Hopkins University — The Advanced Laboratory Physics Association (ALPhA) is a group of people with a shared interest in teaching physics labs at the advanced undergraduate or graduate level. ALPhA works closely with the American Physical Society (APS), the Optical Society of America (OSA), and the American Association of Physics Teachers (AAPT) to develop new methods for teaching modern experimental physics. In the summer of 2010 we initiated the ALPhA Immersion Program, a three-day short course where instructors visit a lab, do one or more of the local experiments (home-built or commercial) with the local instructor, and learn the experiments well enough to incorporate them into their own programs. These immersions were very well received, with attendees filling up all available slots. In this talk I will describe ALPhA and the Immersions Program and solicit input from the broader community.

10:36AM A14.00012 Back to the old questions: physics as culture , LEONARDO COLLETTI, Dipartimento di Fisica and INFN, Università di Trento, 38123 Povo (TN), Italy — My thesis is that, when communicating physics to a large public, more effort should be put into presenting it as an invaluable cultural resource. In fact, by insisting only, as it often happens, on its strategic role as technology booster, one would rather understate physics' very core values. People do certainly appreciate new devices which make their life easier, but they also love thinking about general questions, such as "What is the Universe?" and "How do we know something about it?", which make life truly worth living. I am convinced that not introducing properly the large public to the intellectual beauty of physics' ideas, would represent a waste of knowledge which may result in a society that is even poorer than that resulting from scarce investment in innovation. I will propose a variety of approaches that can be used to highlight the conceptual richness of physics at the aesthetic and inspiring level. Not unlike art and literature, physics can be offered in a way that shows its transformative power of our vision of the universe and its capability of matching human desire for understanding.

Monday, March 21, 2011 8:00AM - 10:48AM –
Session A15 DMP GMAG FIAP: Focus Session: Spins in Semiconductors - Spin Dynamics D171

8:00AM A15.00001 "Listening" to the spin noise of electrons and holes in semiconductor quantum dots[1] , SCOTT CROOKER, National High Magnetic Field Laboratory, Los Alamos National Lab — The coherence and dynamical properties of spins in semiconductors are usually studied with powerful techniques based on optical pump-probe or spin resonance methods. Such methods are necessarily perturbative, in that one measures the (dissipative) response of the spins resulting from an external drive or excitation field (*eg*, free-induction decays). However, in accord with the fluctuation-dissipation theorem, the intrinsic fluctuations of the spin system - if experimentally measurable - can also reveal the same dynamical properties (such as g-factors and decoherence times) without ever perturbing the spin ensemble from thermal equilibrium. This talk describes how we measure electron and hole spin dynamics in semiconductors by passively "listening" to these small spin noise signals [1]. We employ a spin noise spectrometer based on a sensitive optical Faraday rotation magnetometer that is coupled to a digitizer and field-programmable gate array (FPGA), to acquire noise spectra from 0-1 GHz in real time with picoradian/root-Hz sensitivity. In doped (In,Ga)As/GaAs quantum dots, both electron and hole spin fluctuations generate distinct noise peaks whose shift and broadening with magnetic field directly reveal their g-factors and dephasing rates. A large, energy-dependent anisotropy of in-plane hole g-factors is clearly exposed, reflecting systematic variations in the average confinement potential. In contrast with conventional pump-probe studies, noise signals increase as the probed volume shrinks, suggesting possible routes towards non-perturbative, sourceless magnetic resonance of few-spin systems.

[1] PRL **104**, 036601 (2010); PRB **79**, 035208 (2009).

[1]In collaboration with Yan Li, D. Smith, J. Brandt, C. Sandfort, A. Greilich, D. Reuter, A. Wieck, D. Yakovlev and M. Bayer; supported by LANL-LDRD programs.

8:36AM A15.00002 Understanding the modulation frequency dependence of continuous wave optically/electrically detected magnetic resonance , SANG-YUN LEE, SEOYOUNG PAIK, DANE R. MCCAMEY, CHRISTOPH BOEHME, Department of Physics and Astronomy, University of Utah — Continuous wave optically and electrically detected magnetic resonance spectroscopy (cwODMR/cwEDMR) are powerful methods which allow the investigation of the microscopic nature of paramagnetic states involved in spin-dependent transitions, like recombination and transport. Although experimentally similar to conventional electron spin resonance (ESR), there exist limitations when applying conventional theoretical models originally developed for ESR to explain how the observables (luminescence and electric current) of cwODMR and cwEDMR behave under the influences of various experimental parameters. Here we present closed-form solutions for the modulation frequency dependence of cwODMR and cw EDMR based on an intermediate pair recombination model [1] and discuss ambiguities which arise when attempting to distinguishing the dominant spin-dependent processes underlying experimental data. These include: 1) a large number of quantitatively different models cannot be differentiated, 2) signs of signal are determined not only by recombination, but also by other processes like dissociation, intersystem-crossing, pair generation, and even an experimental parameter, modulation frequency.
[1] D. Kaplan, I. Solomon, and N. Mott, Journal de Physique Lettres 39, 51 (1978).

8:48AM A15.00003 Observation of Long Spin Coherence Times in CdSe/CdS Colloidal Nanostructures , K.J. VAN SCHOOTEN, Department of Physics and Astronomy, University of Utah, Salt Lake City, Utah, 84112, USA, J. HUANG, D.V. TALAPIN, Department of Chemistry, The University of Chicago, Chicago, Illinois 60637, USA, W.J. BAKER, C. BOEHME, J.M. LUPTON, Department of Physics and Astronomy, University of Utah, Salt Lake City, Utah, 84112, USA — Spin states in colloidal quantum dots have been intensively studied over the past decade, usually through various all optical time-resolved pump-probe techniques of excitonic fine-structure. Coherence times measured in this manner, which are usually limited to T_2^*, have ranged in order from 1ps to 1ns, thus limiting the potential to use these types of quantum dots in quantum memory schemes. Here, we describe coherence times (T_2) on the order of 100ns for optical excitations in ensembles of CdSe/CdS heterostructure colloidal nanocrystals at 10K. In contrast to the more conventional pump-probe techniques, we employ a time-correlated optically-detected magnetic resonance scheme to measure the true T_2 of optically generated excitations via a Hahn echo sequence. A strong temperature dependence of the spin-dependent luminescence rate is observed, demonstrating that longitudinal spin-relaxation in these strongly spin-orbit coupled semiconductors is thermally activated.

9:00AM A15.00004 Universal scheme for optically-detected T_1 measurements , JOHN COLTON, KEN CLARK, TYLER PARK, DALLAS SMITH, SCOTT THALMAN, Brigham Young University — A two laser pump-probe scheme for measuring spin flip (T_1) lifetimes in GaAs-related materials has been developed. The pump and probe beams are switched on and off electronically, with pulse widths and delays controlled by a two-channel pulse generator. The effect of the pump beam on the probe beam is seen by monitoring the Kerr rotation of the reflected probe beam. The technique has broad applicability, and should work for any material in which Kerr rotation spin measurement can be employed. The authors have applied this technique to a lightly-doped GaAs layer (n=3E14 cm^{-3}), to compare it with two other samples (at slightly higher[1] and slightly lower[2] doping levels) whose T_1 dependence on field had substantial qualitative and quantitative differences from each other. Results for this sample will be presented.

[1]Colton et al., Phys. Rev. B **75**, 205201 (2007).
[2]Fu, et al., Phys. Rev. B **74**, 121304(R) (2006).

9:12AM A15.00005 Ultrafast Measurement of Critical Slowing Down of Hole-Spin Relaxation in Ferromagnetic GaMnAs , AARON PATZ, TIANQI LI, Ames Laboratory and Department of Physics and Astronomy, Iowa State University, ILIAS PERAKIS, Department of Physics, University of Crete, Greece, XINYU LIU, JACEK FURDYNA, Department of Physics, University of Norte Dame, JIGANG WANG, Ames Laboratory and Department of Physics and Astronomy, Iowa State University — We have studied ultrafast photoinduced hole spin relaxation in GaMnAs via degenerate ultrafast magneto-optical Kerr spectroscopy. Near-infrared pump pulses strongly excite the sample, and probe pulses at the same photon energy reveal subpicosecond demagnetization accompanied by energy and spin relaxation of holes manifesting themselves as a fast (∼200fs) and a slow (ps) recovery of transient MOKE signals. By carefully analyzing the temporal profiles at different temperatures, we are able to isolate femtosecond hole spin relaxation processes, which are subject to a critical slowing down near the critical temperature of 77K. These results demonstrate a new spectroscopy tool to study the highly elusive hole spin relaxation processes in heavily-doped, correlated spin systems, and have important implications for future applications of these materials in spintronics and magnetic-photonic-electronic multifunctional devices.

9:24AM A15.00006 A Model Study of Photomagnetization in Diluted Magnetic Semiconductors , S.N. BEHERA, IIT/Bhubaneswar, S.M. BOSE, Drexel University, J.T. SCHICK, Villanova University — In the context of application to spintronics, photon induced magnetization or photomagnetization (PM) of diluted magnetic semiconductors (DMS) like $Hg_{1-x}Mn_xTe$ [1] has been the subject of many recent investigations. We present results of a model calculation of the dependence of the PM on the photon power in a DMS for different temperatures and different magnetic impurity concentrations. The model which includes kinetic energies of the charge carriers created by the incident light, the attractive Coulomb interaction between the electrons and the holes treated in the mean field approximation, the coupling of the photon with the exciton density, and the magnetic interaction between the spins of the charge carriers and the magnetic moments of the magnetic impurity atoms in the semiconductor is solved exactly using the equation of motion of the Green's functions method. Expressions for the densities of spin up and spin down charge carriers, and their magnetization and that of the magnetic impurities obtained in the form of a set of coupled equations are solved self consistently to determine the PM. Interestingly there is a temperature dependent threshold in photon power for the appearance of the PM. A detailed study of the dependence of the PM on different parameters will be presented.

[1] H. Krenn et al., PRL **55**, 1510 (1985).

9:36AM A15.00007 Dynamic Magnetic Polarization in Semi-magnetic II-VI Quantum Dots via Electrical/Optical Carrier Injection , BAHMAN ROUSTAI, University of Cologne, RAMIN ABOLFATH, U. Texas at Dallas, THOMAS BRABEC, U. Ottawa, PAWEL HAWRYLAK, NRC, Ottawa — Theory of Dynamic Magnetic Polarization (DMP), the enhancement of collective spin polarization of magnetic impurities (MI) in semi-magnetic II-VI quantum dots is presented. DMP, known for nuclear spins, is the result of the transfer of electron's spin to MI's spin polarization as a function of time. DMP has been recently observed in various opto-electronic experiments [1]. We study the interplay of optically/electrically pumped electrons from the leads to the quantum dot and their effects on DMP in the dot. The interaction of MI's with electron spin and orbital degrees of freedom is modeled. In the weak coupling (t>>J), the DMP is the result of electron tunneling followed by the exchange interaction J with MI. In the strong coupling (J>>t) the electrons in the lead and the magnetic impurity in the dot form a Kondo-type bound state resulting in even stronger DMP.

[1] Ochsenbein et al. Nature Nanotechnology 4, 681 (2009).

9:48AM A15.00008 Carrier spin polarization and magneto-polaron formation in colloidal quantum dots[1] , SAVAS DELIKANLI, ANDREAS RUSS, LARS SCHWEIDENBACK, SUNGJIN KIM, JOSEPH MURPHY, ALEXANDER CARTWRIGHT, ATHOS PETROU, HAO ZENG, SUNY at Buffalo — We present a magneto-optical study of magnetic polarons in Mn-doped II-VI colloidal quantum dots. The polarons are formed due to the exchange coupling between the spins of the holes and those of the Mn ions, both of which are localized in the dots. The long lifetime of the excitons allows the observation of the complete formation process of the magneto polaron. The spin alignment occurs at the time scale of hundreds of ps. The extra energy is dissipated through spin lattice interactions, during the next hundreds of nanoseconds. The dependence of these effects on quantum confinement are studied in different systems.

[1]Research Supported by: NSF DMR 0547036, NSF (ECS0824220) and ONR (N000140910113).

10:00AM A15.00009 Non-equilibrium Magnetic Ordering in Quantum Dots , JAMES PIENTKA, RAFAL OSZWALDOWSKI, IGOR ZUTIC, JONG HAN, University at Buffalo, ANDRE PETUKHOV, South Dakota School of Mines and Technology — We study semiconductor Quantum Dots (QDs) with magnetic impurities. The magnetism in these systems can be controlled in ways not possible in bulk semiconductors [1]. Robust magnetic effects have been observed recently in both colloidal and self-assembled QDs [2,3]. Here, we develop a rate-equations approach to describe the carrier-mediated magnetic ordering in QDs. In this situation, the magnetic properties are different from the steady-state scenario, due to different carrier spin density, which affects the magnetic-impurity alignment. We focus on a type-II QD band profile, where the electrons reside in the barrier, while the holes are localized in the QD interior, which contains the magnetic impurities. Supported by DOE-BES, US ONR, AFOSR, NSF-DMR and NSF-ECCS CAREER.

[1] R. M. Abolfath, A. G. Petukhov, and I. Zutic, Phys. Rev. Lett. **101**, 207202 (2008); I. Zutic and A. G. Petukhov, Nature Mater.**4**, 623 (2009).
[2] R. Beaulac et al., Science **325**, 973 (2009).
[3] I. R. Sellers, R. Oszwaldowski, et al., Phys. Rev. B **82**, 195320 (2010).

10:12AM A15.00010 Magneto-optical studies of magnetic polarons in type-II (Zn,Mn)Te/ZnSe quantum dots[1] , BIPLOB BARMAN, ANDREAS RUSS, LARS SCHWEIDENBACK, JOSEPH MURPHY, RAFAL OSZWALDOWSKI, IAN SELLERS, ATHOS PETROU, IGOR ZUTIC, BRUCE MCCOMBE, ALEXANDER CARTWRIGHT, SUNY Buffalo, ANDRE PETUKHOV, South Dakota School of Mines & Technology, WU-CHING CHOU, WEN CHUNG FAN, National Chiao Tung University — We have recorded time-resolved emission spectra from a series of MBE grown (Zn,Mn)Te/ZnSe quantum dots (QDs) at 7 K in the 0 - 4 tesla magnetic field range. The photoluminescence (PL) spectra were analyzed into their $\sigma+$ and $\sigma-$ circularly-polarized components. The holes in this type-II system are confined in the (Zn,Mn)Te QDs, while the electrons reside in the surrounding ZnSe matrix. The PL intensity, peak energy, and circular polarization were recorded as a function of time and magnetic field. These studies show evidence of exchange coupling between the holes and Mn spins in the (Zn,Mn)Te QDs, which leads to the formation of magnetic polarons. The time scale of polaron formation is shorter than the recombination time in this type-II system. We discuss our results within the framework of a model that describes the magnetic polaron formation in this system.

[1]This work is supported by NSF, ONR, DOE-BES, AFOSR, and the Rustgi professorship.

10:24AM A15.00011 Prediction of extremely long mobile electron spin lifetimes at room temperature in low-Z wurtzite semiconductor quantum wells , NICHOLAS HARMON, WILLIAM PUTIKKA, The Ohio State University, ROBERT JOYNT, University of Wisconsin — Many proposed spintronics devices require mobile electrons at room temperature with very long spin lifetimes. One route to achieving this is to use quantum wells with tunable spin-orbit (SO) parameters. Research has focused on materials with the zincblende structure such as GaAs, which however, do not have long spin lifetimes at room temperature. We show that low-Z materials with the wurtzite structure are much better suited for spintronics applications. Their hexagonal symmetry implies that SO couplings can be completely canceled over a very wide range of electron momenta at zero temperature. Low-Z materials possess smaller SO couplings resulting in long spin lifetimes at room temperature. This leads to predictions of spin lifetimes exceeding 2 ms at helium temperatures in wurtzite AlN and, most relevant to spintronic devices, spin lifetimes up to 0.5 μs are predicted for tuned AlN wells at room temperature.

10:36AM A15.00012 Conductance signatures of spin correlations and quantum phase transitions in parallel quantum dots[1] , ARTURO WONG, Ohio U., WILLIAM LANE, Jacksonville U., LUIS DIAS, U. of Sao Paulo, KEVIN INGERSENT, U. of Florida, NANCY SANDLER, SERGIO ULLOA, Ohio U. — Semiconductor quantum dots provide a highly controllable environment to study strongly correlated phenomena and quantum phase transitions (QPT). A parallel double-quantum-dot system, in which dot 1 is in the Kondo regime and dot 2 behaves as a non-interacting resonant level, shows a QPT separating Kondo-screened and local-moment phases [1]. In this work, we use the numerical renormalization-group approach to explore the effect of a nonzero Coulomb interaction U_2 in dot 2. When dot-2 level is fixed at the Fermi energy, a critical value of U_2 separates local-moment and Kondo-screened phases. By contrast, if U_2 is increased keeping particle-hole symmetry in dot 2, the system evolves from a local-moment regime to an underscreened spin-1 regime. Signatures of these behaviors can be experimentally identified through the conductance of the system. We also calculated the spin-spin correlations between the dots and between each dot and the leads to identify how the spin-spin interactions are distributed throughout the structure.
[1] L. G. G. V. Dias da Silva, N. P. Sandler, K. Ingersent, and S. E. Ulloa, Phys. Rev. Lett. 97, 096603 (2006).

[1]Supported by NSF Grant DMR-0710581.

Monday, March 21, 2011 8:00AM - 11:00AM –
Session A16 DMP GMAG: Focus Session: Magnetic Nanostructures I D173

8:00AM A16.00001 Cantilever torque magnetometry studies of the in-plane to out-of-plane transition in a single nickel magnetic nanorod , ERIC W. MOORE, SANGGAP LEE, STEVEN A. HICKMAN, JONILYN G. LONGENECKER, JOHN A. MAROHN, Cornell University — Torque magnetometry, using attonewton-sensitivity cantilevers, is extremely sensitive to both the average magnetic moment and magnetization fluctuations within a small magnetic tip. Operating at $T = 4\,\mathrm{K}$ with such a system, we study in-plane to out-of-plane magnetization switching in a single, electron beam lithographically defined nickel nanorod, of radius $r \approx 50\,\mathrm{nm}$. Numerous, simultaneous, peaks are visible in cantilever frequency, dissipation and jitter as well as Barkhausen like steps. A analytic model is developed that achieves order of magnitude agreement with the frequency and dissipation peaks.

8:12AM A16.00002 Interedge magnetic coupling in metal-terminated graphene nanoribbons[1] , YAN WANG, CHAO CAO, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida — Graphene nanoribbons (GNRs) with armchair or zigzag edges, a novel organic material system produced by cutting graphene along two crystallographic directions, have recently attracted considerable attention in spintronics. GNR with zigzag edges is known to be magnetic with two spin-polarized edge states, which are ferromagnetically ordered but antiferromagnetically coupled to each other. Most of the previous studies focus ribbons with zigzag edges and hydrogen terminations. Here we present a first-principles study[2] of zigzag and armchair GNRs terminated with 3*d* transition-metals and noble metals. Specifically, we investigate the long-range interedge magnetic coupling as a function of the ribbon's width. We also show that the proposed hybrid metal-terminated GN[3]Rs can be excellent candidate for spintronic applications.

[1]This work was supported by US/DOE/BES/DE-FG02-02ER45995.
[2]Y. Wang, C. Cao, and H.-P. Cheng, Phys. Rev. B 82, 205429 (2010).
[3]Y. Wang and H.-P. Cheng, submitted.

8:24AM A16.00003 Magnetic Properties of Single Crystal Nickel Nanowires[1] , JIMMY KAN, KEITH CHAN, ERIK SHIPTON, ERIC FULLERTON, University of California - San Diego — Toward the goal of understanding magnetism in confined dimensions, we have synthesized Nickel nanowires (NWs) by chemical vapor deposition and characterized their magnetic properties. By tuning chemical vapor deposition synthesis parameters, we can controllably synthesize a variety of morphologically dissimilar Ni products onto untreated amorphous SiO2||Si substrates [1]. These structures include polycrystalline core-shell NWs, single-crystal cubes, in-plane wires, and vertically-oriented single crystal arrays. To probe the magnetic properties of individual NWs, we combined magneto-transport, XPEEM, and magnetic modeling. For polycrystalline NWs, the magnetic properties are dominated by shape anisotropy. However, for single-crystal NWs, there is a competition between the shape anisotropy along the (001) direction and magneto-crystalline anisotropy along the (111) direction. This gives rise to complex magnetic stripe domain patterns along the wires, interesting magneto-transport properties, and novel reversal modes not typically observed in magnetic wires.

[1] K.T. Chan, J.J. Kan, E.E. Fullerton, et al., "Oriented Growth of Single-Crystal Ni Nanowires onto Amorphous SiO2," Nano Letters, Oct. 2010

[1]This research is supported by NSF Award #DMR-0906957.

8:36AM A16.00004 Tunable magnetism in nanomaterials and systems , WANLIN GUO, Nanjing University of Aeronautics and Astronautics, ZHUHUA ZHANG — Tunable magnetism in nanomaterials and systems are especially attractive and hold great promise for applications in nanoelectronics and spintronics. Here we show some of our recent findings along this direction. First, we present a novel magnetoelectric effect in graphene nanoribbons settled on silicon substrates whereby the ribbon edge magnetization can be tuned linearly by applied bias voltage (**Phys.Rev.Lett**, **103**, 187204, 2009), and this effect is robust to material and geometry variations (**Phys.Rev.B** 81, 155428, 2010). We also realize an electrical control of magnetism in ZnO ribbons (**ACS Nano 4**, 2124, 2010**)**, and even a tunable magnetic ordering in sandwich nanowires by changing charge states (**J.Am.Chem.Soc**.**132**, 10215, 2010). Contrast to the zero-gap graphene, both hexagon-BN sheets and nanotubes are generally insulating. We provide two efficient recipes to narrow the wide gap of BN: applying external electric fields for nanoribbons and increasing tube curvature for nanotubes. Of more interesting is that ferromagnetic ordering is obtained in BN nanotubes by fluorination and it can be remarkably modulated by applying radial pressure (**J.Am.Chem.Soc**.**131**, 6874, 2009). Our revealed control of magnetism in a wide range of nanomaterials may open up new vistas towards spintronics.

8:48AM A16.00005 Magnetic Properties of Iron-added Titanium Oxide Nanotubes[1] , EUGEN PANAITESCU, PEGAH HOSSEINPOUR, LAURA H. LEWIS, LATIKA MENON, Northeastern University — Titanium oxide represents a promising candidate as the support material for dilute magnetic semiconductors (DMSs), especially in a nanostructured form. Titania nanotubes ordered arrays produced by anodization have been used in this study as the base material for the addition of a ferromagnetic component, iron in particular. Several routes such as titanium-iron films co-deposition before anodization, anodization in iron cations containing solutions, and post-anodization iron deposition have been used for the incorporation of iron into the titanium oxide nanotubes matrix. Samples morphology and structure was analyzed by electron microscopy, and by EDS and XRD spectroscopy. Subsequent magnetic measurements were performed on both amorphous and crystalline samples, and compared with references such as blank nanotubes and commercial anatase nanoparticles powder.

[1]Work supported by the NSF Grant DMR-0906608

9:00AM A16.00006 Synthesis and Characterization of CoFe nanowires , PO-CHING TSAI, YAJING ZHANG, GIRIJA S. CHAUBEY, NARAYAN POUDYAL , CHUANBING RONG, J. PING LIU, Department of Physics, The University of Texas at Arlington, Arlington, TX 76019 — CoFe and CoNi nanocrystals with different size, shape and compositions were successfully synthesized via a non-catalyst chemical solution method. It was found that the structure and morphology of the nanocrystals with high aspect ratio can be controlled by varying parameters such as solvent amount, surfactant ratio, reducing agent and heating rate. The elongation of the nanowires can be adjusted by changing surfactant ratio and catalyst amount. It has also been observed that the growth mechanisms for CoFe and CoNi nanowires are different. Magnetic properties of the nanocrystals are size and shape dependent. By optimizing the synthesis conditions, nanowires with enhanced magnetization and coercivity can be obtained.

9:12AM A16.00007 Focused electron beam induced deposition of magnetic nanostructures[1] , JOSE M. DE TERESA, CSIC-University of Zaragoza (Spain) — Nanopatterning strategies of magnetic materials normally rely on standard techniques such as electron-beam lithography using electron-sensitive resists. Focused electron beam induced deposition (FEBID) is currently being investigated as an alternative single-step route to produce functional magnetic nanostructures. Thus, Co-based [1] and Fe-based [2] precursors have been recently investigated for the growth of magnetic nanostructures by FEBID. In the present contribution, I will give an overview of the existing literature on magnetic nanostructures by FEBID and I will focus on the growth of Co nanostructures by FEBID using $Co_2(CO)_8$ as precursor gas. The Co content in the nanostructures can reach 95% [3]. Magnetotransport experiments indicate that full metallic behaviour is displayed with relatively low residual resistivity and standard anisotropic magnetoresistance (0.8%) [3]. The coercive field of nanowires with changing aspect ratio has been determined in nanowires with width down to 150 nm by means of Magneto-optical Kerr Effect [4] and the magnetization reversal has been imaged by means of Magnetic Force Microscopy, Scanning Transmission X-ray Microscopy as well as Lorentz Microscopy experiments. Nano-Hall probes have been grown with remarkable minimum detectable magnetic flux. Noticeably, it has been found that the domain-wall propagation field is lower than the domain-wall nucleation field in L-shaped nanowires, with potential applications in magnetic logic, sensing and storage [5]. The spin polarization of these Co nanodeposits has been determined through Andreev-Reflection experiments in ferromagnetic-superconducting nanocontacts and amounts to 35% [6]. Recent results obtained in Fe-based nanostructures by FEBID using $Fe_2(CO)_9$ precursor will be also presented [7].

[1] I. Utke et al., Appl. Phys. Lett. 80 (2002) 4792-4794
[2] M. Takeguchi et al., Nanotechnology 16 (2005) 1321-1325
[3] A. Fernández-Pacheco et al, J. Phys. D: Appl. Phys. 42 (2009) 055005
[4] A. Fernández-Pacheco et al, Nanotechnology 20 (2009) 475704
[5] A. Fernández-Pacheco et al, Appl. Phys. Lett. 94 (2009) 192509
[6] S. Sangiao et al, Solid State Communications, in press
[7] R. Lavrijsen et al, Nanotechnology, submitted

[1]I acknowledge the collaboration in this field with A. Fernandez-Pacheco, R. Cordoba, L. Serrano, S. Sangiao, L.A. Rodriguez, C. Magen, E. Snoeck, L. Morellon, M.R. Ibarra.

9:48AM A16.00008 Memory effect in magnetic nanowire arrays[1] , XIAOMING KOU, XIN FAN, Department of Physics and Astronomy, University of Delaware, RANDY DUMAS, Department of Physics, University of California, Davis, QI LU, Department of Physics and Astronomy, University of Delaware, YAPING ZHANG, Department of Physics, University of Science and Technology Beijing, HAO ZHU, XIAOKAI ZHANG, Spectrum Magnetics, LLC, KAI LIU, Department of Physics, University of California, Davis, JOHN XIAO, Department of Physics and Astronomy, University of Delaware — A memory effect has been demonstrated in magnetic nanowire arrays. The magnetic nanowire array has the ability to record the maximum magnetic field that the array has been exposed to after the field has been turned off. The origin of the memory effect is the strong magnetic dipole interaction among the nanowires. Switching field distributions among nanowires was studied with a first order reversal curve technique to elucidate the discrepancy between the experimental result and the theoretical explanation. Based on the memory effect, a novel and extremely low cost EMP detection scheme is proposed. It has the potential to measure magnetic field pulses as high as a few hundred Oe without breaking down.

[1]This work has been supported by NSF DMR0827249 and NSF IIP-1013468. Work at UCD was supported by NSF DMR-1008791 and NSF ECCS-0925626.

10:00AM A16.00009 ABSTRACT WITHDRAWN –

10:12AM A16.00010 Magnetic hyperthermia in frozen and liquid ferrofluids , R. REGMI, Wayne State University, A. NAIK, University of Wisconsin, J.S. THAKUR, Wayne State University, P.P. VAISHNAVA, Kettering University, G. LAWES, Wayne State University — We report magnetic hyperthermia in dextran coated Fe_3O_4 nanoparticles suspended in an aqueous solution over a temperature range from -40 ^oC to +40 ^oC to investigate heating mechanisms in the solid and liquid states. We used an alternating magnetic field of 70 Oe at frequency of 395 kHz to produce heating in the 12 nm Fe_3O_4nanoparticles. We found that at the lowest and highest temperatures, ambient heat flow to or from the environment produced small but non negligible effects. After correcting for this ambient heat flow, we found an average magnetic heating of 4.7 W/g, 11.2 W/g, and 6.5 W/g in the solid, mixed solid-liquid, and liquid phases, respectively. These values in the solid and liquid phases are consistent for models for magnetic heating considering Neel heating only and Neel and Brownian heating together, respectively.

10:24AM A16.00011 Characterization of iron oxide-dextran magnetic nanoparticle suspensions , J. SHIH, R. BAI, W. CHIOU, R.M. BRIBER, University of Maryland, College Park, J.A. BORCHERS, C.L. DENNIS, NIST, Gaithersburg, MD, C. GRUETTNER, Micromod Partikeltechnologie, GmbH — Magnetic nanoparticles, with structures from core-shell to nanocrystallites in a matrix, are candidates for use in biomedical applications. "Superparamagnetic iron oxide" (SPIO) nanoparticles are nanocrystallites of iron oxide in a dextran matrix, with sizes between 20nm and 250nm. Dynamic light scattering (DLS), transmission electron microscopy (TEM), atomic force microscopy (AFM), and hysteresis measurements were used for structural and magnetic characterization. Additionally, cryoquench-TEM was performed, allowing direct imaging without false aggregation from drying. The DLS-determined size of the particles is 250nm, but cryoquench-TEM yields a smaller size of 150nm. In addition, the particles are relatively well-dispersed, but dimers and trimers are observed. This corresponds with the evidence of weak interactions in magnetic hysteresis measurements. Further magnetic characterization will provide information on how the magnetic properties of these SPIO particles correlate with their size and structure.

10:36AM A16.00012 Thermosensitive Nanostructured Media for imaging and Hyperthermia Cancer Treatment[1] , KAREN MARTIROSYAN, University of Texas at Brownsville — Hyperthermia has been used for many years to treat a wide variety of tumors in patients. The most commonly applied method of hyperthermia is capacitive heating by using microwave. Magnetic fluids based on iron oxide (Fe3O4), stabilized by biocompatible surfactants are typically used as heating agent. However, significant limitations of using commercial available magnetic particles are non-selectivity and overheating of surrounding normal tissues. To improve the efficacy of hyperthermia treatment we intend to develop Curie temperature (Tc)-tuned nanostructured media having T2 relaxation response on MRI for selective and self-controlled hyperthermia cancer treatment. As an active part of this media we fabricated superparamagnetic, biocompatible and dextran coated ferrite nanoparticles Mg1+xTixFe2(1-x)O4 at 0.3<x<0.5 with low Curie temperature. To tune Tc we produced a large number of ferrites powders with x=0.05 by aqueous combustion synthesis. This process typically involves a reaction in a solution containing metal nitrates and different fuels, which are classified based on the type of reactive groups (e.g., amino, hydroxyl, carboxyl) connected to a hydrocarbon chain, such as glycine, hydrazine, or urea. Our experiments revealed that ferrite with formula Mg1.35Ti0.35Fe1.3O4 appears with Curie temperature within 46-50 $^\circ$C.

[1]NSF, grant # 0933140

10:48AM A16.00013 Magnetism of Au Nanoparticles on *Sulfolubus Acidocaldarius* S-Layer , JUAN BARTOLOME, F. BARTOLOME, L.M. GARCIA, A.I. FIGUEROA, ICMA, Universidad de Zaragoza - CSIC, Spain, T. HERRMANNSDOERFER, R. SKROTZKI, R. SCHOENEMANN, J. WOSNITZA, Dresden High Magnetic Field Laboratory, HZDR, Dresden, Germany, S. SELENSKA-POBELL, A. GEISSLER, T. REITZ, Institute of Radiochemistry, HZDR, Dresden, Germany, F. WILHELM, A. ROGALEV, ESRF, Grenoble, France — Au nanoparticles (NP) with diameters of a few nm have been synthesized on a protein S-layer of *Sulfolobus Acidocaldarius* bacteria. SQUID magnetization (1.8 K $<$ T $<$ 300 K and 0 $<$ B $<$ 7 T) shows superparamagnetic behavior at low-T. Its origin lays at the Au NP's, as has been proven by Au $L_{2,3-}$edge XMCD spectroscopy, performed in the range 2.2$<$T$<$20 K and up to B_{app}=17 T. XMCD analysis yields a total magnetic moment per Au atom μ_{Au}= 0.050(1) μ_B, a particle average moment m_{part}= 2.3 μ_B, Au orbital to spin moment ratio of m_L/m_S= 0.29, and Curie-like superparamagnetism. Au-S bonds are detected by S K-edge XAS measurements. Besides, EXAFS at the Au L_3-edge shows that the Au NP internal structure is fcc, and Au-S bonds are located at the particle surface. An increase of the hole charge carrier density in the Au 5d band due to electron transfer with the S-layer explains the Au magnetism. The observed magnetic moment per Au atom is 25 times larger than those previously found by XMCD in Au-thiol capped NPs.

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A17 DMP GMAG: Focus Session: Bulk Properties of Complex Oxides - Manganites I

D174

8:00AM A17.00001 Enhanced magneto-elastic coupling in hexagonal multiferroic $HoMnO_3$, MARIO POIRIER, JULIEN CAMIRAND LEMYRE, PIERRE-OLIVIER LAHAIE, Universite de Sherbrooke, LOREYNNE PINSARD-GAUDART, ALEXANDRE REVCOLEVSCHI, Universite Paris-Sud — From ultrasonic velocity measurements, we report a study of the magneto-elastic coupling occurring on elastic moduli C_{11} and C_{33} at the different magnetically induced phase transitions in $HoMnO_3$. Although both the Ho-Mn and Ho-Ho interactions soften the the elastic moduli, the largest softening in observed on C_{11} over a wide temperature range extending well beyond the Néel temperature. An in-plane orientation of the magnetic field reduces strongly the softening due to a stabilization of the Mn moments order; concurrently, the Ho magnetic order is destroyed. When the field is rather oriented along the c axis, the elastic softening is enhanced as if the Ho-Mn interactions were reinforced and the Mn order consequently destabilized. The phase diagram deduced from the elastic anomalies observed at the several phase transitions are in agreement with microwave measurements performed on the same sample. An in-plane anisotropy of the diagram is also proposed.

8:12AM A17.00002 Multiferroics in $Eu_{1-x}Tb_xMnO_3$ system[1] , YUNG-YUAN HSU, H.C. HSU, H.C. CHEN, W.Y. TSENG, C.D. YANG, National Taiwan Normal University, H.C. KU, National Tsing Hua University — A low-T phase diagram of the $Eu_{1-x}Tb_xMnO_3$ ($0 \leq x \leq 1$) is reported. Systematic substation of Tb into the system changes the perovskite lattice structure which further varies the electronic and magnetic behaviors of the system from a paraelectric-canted-AFM to a ferroelectric-spiral-AFM ground state. The Mn^{3+} spins ordered, presumably, in a collinear incommensurate sinusoidal antiferromagnetic structure below T_N = 52-45 K (x = 0 to 1). Then system enters a canted-AFM (weak- ferromagnetic) state below T_{cant} for the $x \leq 0.5$ compounds, which decreases from 42 K to 25 K with increasing x. For the $x \geq 0.5$ compounds, ferroelectricity was found below $T_C \sim 28$ K with a presumably spiral spin arrangement as that in $TbMnO_3$. At the boundary, $x = 0.5$, the multiferroics coexists with the weak-ferromagnetism. The Rietveld refinement shows an Mn-O2-Mn angle of 145.9° for the $Eu_{0.5}Tb_{0.5}MnO_3$ suggesting a critical Mn-O2- Mn angle of ∼146° that multiferroics appears at the smaller angle side.

[1]This work was supported by NSC of Taiwan under No. NSC -97-2112-M-003-001-MY3.

8:24AM A17.00003 Ferromagnetically charge ordered nanoclusters in $La_{0.52}Ca_{0.48}MnO_3$[1] , JING TAO, Brookhaven National Laboratory, D. NIEBIESKIKWIAT, Universidad San Francisco de Quito, Q. JIE, M. A. SCHOFIELD, L. WU, Q. LI, Y. ZHU, Brookhaven National Laboratory — A charge-ordered (CO) nanoscale phase was reported to appear in coincidence with the well known colossal magnetoresistance (CMR) in a wide doping range in manganites. The competition between the CO nanoscale phase and the surrounding ferromagnetic (FM) phase has been considered as the key to understand the CMR phenomenon. However, the role of this nanoscale phase in the CMR effect is not fully established because the magnetic and physical properties of the CO nanoscale phase remain elusive. In particular, the CO nanoscale phase was hypothesized to be antiferromagnetic, the same as its long range counterpart. Here we report the experimental evidences showing the unexpected magnetism and resistivity in the CO nanoclusters in $La_{0.52}Ca_{0.48}MnO_3$. Correlated with a number of bulk property measurements, the transmission electron microscopic observations strongly suggest that the CO nanoclusters are FM and probably conducting. Such results could substantially alter the role of the CO nanoclusters in the CMR.

[1]Research at BNL was sponsored by the U.S. DOE/BES under Contract No. DE-AC02-98CH10886.

8:36AM A17.00004 Structural and Magneto-electric properties of substituted $R\mathrm{MnO}_3$ crystals (R=*Sm, Gd*) , G. BALAKRISHNAN, D. O'FLYNN, DA-QIAN LIAO, R.A. MCKINNON, D.S. KEEBLE, M.R. LEES, Department of Physics, University of Warwick, UK, A. DAOUD-ALADINE, ISIS Facility, STFC, Didcot, UK — In order to understand the emergence of multiferroic behaviour in the $R\mathrm{MnO}_3$ type compounds, it is educational to study the relationship between ferroelectricity and magnetoelastically induced lattice modulations. The Mn-O-Mn bond angle is a crucial parameter in these systems and it varies with the ionic radii (r_R) of the R atoms. Multiferroic behaviour may be induced in large Rsystems by substituting the R site with a smaller ion (e.g. *Y, Lu*). We have studied the effect of substituting Y in *Sm*MnO_3 and *Lu* in *Gd*MnO_3 respectively. In the optimally substituted compounds, we observe a strong coupling between the magnetic and dielectric properties. We have investigated the local structural distortions in the MnO_6 octahedra in both these systems using single crystal X-ray studies. Additionally, neutron powder diffraction has been used to investigate the nature of the low temperature magnetic ordering in the Sm system. Investigations of the dielectric properties of the Y and *Lu* substituted crystals reveal anomalies in the dielectric properties coincident with an additional magnetic transition, indicative of multiferroic behaviour. We present detailed investigations of the magnetic, dielectric and structural properties on single crystals of selected compositions.

8:48AM A17.00005 Synthesis and Oxygen Content Dependent Properties of Hexagonal Manganites[1] , B. DABROWSKI, S. REMSEN, S. KOLESNIK, O. CHMAISSEM, J. MAIS, Department of Physics, Northern Illinois University, DeKalb, IL 60115, USA — Oxygen deficient samples of hexagonal ($P6_3cm$) $DyMnO_{3+\delta}$(δ=-0.04) were synthesized in Ar by intentional decomposition of the perovskite phase obtained in air. Hexagonal samples annealed under oxidizing conditions exhibit unusually large excess oxygen content (δ <0.4) and two new structural phases below 350 °C. We will demonstrate how structural, resistive, magnetic, and thermal expansion properties are sensitively dependent δ. Similar observations were made for other hexagonal manganites $RMnO_{3+\delta}$ indicating that their multiferroic properties can be controlled by the synthesis and annealing conditions.

[1]Work supported by NSF-DMR-0706610.

9:00AM A17.00006 Spin and Lattice excitations in Ferromagnetic Insulating Manganites[1] , DALGIS MESA, JIANDI ZHANG, Dept. of Physics, Louisiana State University, Baton Rouge, LA 70802, USA, JAIME FERNANDEZ-BACA, FENG YE, MARK HAGEN, Neutron Scattering Science Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, T. TOMIOKA, YOSHINORI TOKURA, National Institute of Advanced Industrial Science and Technology (AIST), Japan — Though double-exchange interaction has been recognized as a major driving force for the couple magnetic and electronic phase transition, the nature of insulating ground state with ferromagnetic ordering in low-doping manganites is still not fully understood. Here we report on an inelastic neutron scattering study of spin and lattice excitations in the ferromagnetic insulating (FMI) phase of $La_{1-x}Ca_xMnO_3$ with x(Ca) = 0.2. Dispersion relations for both phonons and spin waves along high-symmetry directions were obtained for temperatures of 5 and 225 K, respectively. At low temperatures, our results indicate an anomalous softening and broadening of the magnons near the zone boundary, especially when the magnon energy E ∼ 20 meV, where a longitudinal optical phonon is present. Additional phonon and magnon branches observed will also be discussed.

[1]Acknowledgement: NSF DMR1005562

9:12AM A17.00007 X-ray Absorption Spectroscopy studies of photo-induced and magnetic-field-induced phase transitions in $Pr_{0.7}Ca_{0.3}MnO_3$, YI ZHU, MATTEO RINI, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California, 94720, USA, JOHN FREELAND, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois, 60439, USA, ROBERT SCHOENLEIN, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California, 94720, USA — Changes in the electronic structure underpinning the ultrafast photo- and magnetic-field-induced insulator to metal phase transition in $Pr_{0.7}Ca_{0.3}MnO_3$ are compared directly via x-ray absorption near edge spectroscopy (XANES). Static and time-resolved XANES at the O K-edge and Mn L-edge directly monitor the evolution of the density of Mn-3d/O-2p electronic states as the system is driven across phase boundaries. Our results reveal the non-thermal nature of the photoinduced phase transition and show that the CMR magnetic-field-induced and the photoinduced phase-transitions rely on identical rearrangements of the electronic structure.

9:24AM A17.00008 Striped Multiferroic Phases in Narrow Bandwidth Hole-Doped Manganites[1] , SHUHUA LIANG, Univ. of Tennessee, ORNL, SHUAI DONG, Southeast University, China, CENGIZ SEN, UTK, ORNL, MARIA DAGHOFER, IFW Dresden, ELBIO DAGOTTO, UTK, ORNL — A novel phase with diagonal charge stripes and a complex spin arrangement that allows for ferroelectricity to develop has been recently reported in a model for hole-quarter-doped manganites (S. Dong et al., Phys. Rev. Lett. **103**, 107204 (2009)). The study of this "spin-orthogonal stripe" (SOS) phase is here generalized to other hole doping fractions $x = 1/N$ ($N = 3, 5, 6, ...$), to search for analogous multiferroic states. In this effort, the two-orbital double-exchange model for manganites is studied, employing variational, Monte Carlo, and zero temperature optimization techniques. The phase diagrams obtained by varying the electron-lattice and superexchange couplings also contains exotic C_xE_{1-x} phases. A systematic procedure to construct new C_xE_{1-x}/SOS_x phases is discussed. Both the Dzyaloshinskii-Moriya interaction and exchange-striction effect may work in these C_xE_{1-x}/SOS_x phases, giving rise to ferroelectricity. In addition, these SOS_x/C_xE_{1-x} phases can be extended into many other similar states, with (almost) degenerate energies but different multiferroic properties.

[1]This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

9:36AM A17.00009 Magnetic imaging of domains and walls in multiferroic $ErMnO_3$, YANAN GENG, EDWARD LOCHOCKI, NARA LEE, YOUNGJAI CHOI, SANG-WOOK CHEONG, WEIDA WU, RUTGERS CENTER FOR EMERGENT MATERIALS & DEPT OF PHYSICS & ASTRONOMY, RUTGERS UNIV, PISCATAWAY TEAM — Multiferroic hexagonal rare-earth manganities $RMnO_3$ (R = Ho... Lu, Y, Sc) have generated great interest because of the coexistence of ferroelectric and magnetic orders. Herein we conducted low temperature magnetic force microscopy (LT-MFM) studies on flux-grown $ErMnO_3$ single crystals. The ferroelectric transition T_C is ∼1300 K while antiferromagnetic transition T_N is ∼ 80 K. We observed intriguing behaviors of magnetic domains & walls in $ErMnO_3$ from the temperature and magnetic field dependence of local magnetic contrast. In addition, we will present results of comparison between LT-MFM images and room temperature piezoresponse force microscopy (PFM) images of the same sample to understand the mechanism of cross-coupling between ferroelectricity & magnetism in $RMnO_3$.

9:48AM A17.00010 Multiferroic Perovskite Manganites with Symmetric Exchange Striction , SHINTARO ISHIWATA, Dept. of Appl. Phys. and Quantum-Phase Electronics Center (QPEC), University of Tokyo — Orthorhombic perovskite manganites have been extensively studied as a representative system hosting versatile multiferroic phases such as the cycloidal spin phase and the E-type antiferromagnetic phase with an exchange striction mechanism. Recently, the latter phase has been the subject of growing interest for a potentially giant polarization as large as 60000 $\mu C/m^2$, which might involve a significant contribution from the orbital polarization.[1] However, while several groups have reported ferroelectricity in this phase, further experimental progress on the clarification of the multiferroic properties and the microscopic mechanism has been hampered by the difficulty in sample preparation. In this talk, we report a series of multiferroic perovskite $RMnO_3$ with R = Dy-Yb, $Eu_{1-x}Y_x$ and $Y_{1-y}Lu_y$, synthesized under high pressure and show the complete phase diagram.[2,3] The magnitude of the polarization in the E-type phase was estimated to be about 5000 $\mu C/m^2$ (10 times larger than that of the *bc*-cycloidal phase) and an enhanced magnetoelectric response was discovered near the first-order phase boundary. Furthermore, we have succeeded in synthesizing single crystals of perovskite $YMnO_3$ under a high pressure and succeeded in structure refinements for the E-type phase with a polar space group of $P2_1nm$.[4] This work demonstrates for the first time the quantitative estimation of ferroelectric lattice displacements induced by a magnetic order. This work was done in collaboration with D. Okuyama, Y. Kaneko, Y. Takahashi, H. Sakai, K. Sugimoto, K. Yamauchi, S. Picozzi, Y. Tokunaga, R. Shimano, Y. Taguchi, T. Arima and Y. Tokura, and in part supported by JSPS FIRST program.

[1]S. Picozzi *et al.*, Phys. Rev. Lett. **99**, 227201 (2007).
[2]S. Ishiwata *et al.*, Phys. Rev. B **81**, 100411(R) (2010).
[3]Y. Takahashi *et al.*, Phys. Rev. B **81**, 100413(R) (2010).
[4]D. Okuyama *et al.*, manuscript in preparation.

10:24AM A17.00011 Dynamical Magnetoelectric Phenomena in the Multiferroic Mn Perovskites , MASAHITO MOCHIZUKI, Dept. of Applied Physics, Univ. of Tokyo — Electric manipulation of magnetic structures is an urgent issue in the field of spintronics. Concurrently magnetic and ferroelectric materials, i.e., multiferroics offers a promising route to attain this goal, and its dynamical aspects are now attracting a great deal of interest. In this talk, we will discuss the recent progress of theoretical study on the dynamical magnetoelectric phenomena in the multiferroic Mn perovskites $RMnO_3$ (R=Tb, Dy, $Eu_{1-x}Y_x$, ...). In these materials, a spiral order of the Mn spins induces spontaneous electric polarization through breaking the inversion symmetry, and thus the strong coupling between electric and magnetic dipoles is realized. Using an accurate spin Hamiltonian describing $RMnO_3$, we first study the electromagnon excitation in these materials at THz frequencies, i.e., collective motion of spins with oscillating electric dipoles activated by the electric-field component of light. The optical spectra with two specific peaks are explained by a symmetric magnetostriction model for the spiral spin order with higher harmonic components. After clarification of its mechanism and nature, we then study the nonlinear dynamical processes of magnetic system caused by the intense electromagnon excitations through the optical pumping. The excitation by the electric field can be more intense and faster than that by the magnetic field. This necessarily leads to novel and intriguing phenomena which can never be expected in the conventional magnetic-field-induced magnon excitation. As one of the most interesting phenomena, we will theoretically propose a picosecond optical switching of spin chirality in $RMnO_3$. We will demonstrate that by tuning strength, shape and length of the optical pulse, we can control the spin chirality at will. This proposal will pave a new way to control the magnetism in the picosecond/THz time domain.

[1] M. Mochizuki, N. Furukawa and N. Nagaosa, PRL **104**, 177206 (2010)
[2] M. Mochizuki and N. Nagaosa, PRL **105**, 147202 (2010)
[3] M. Mochizuki and N. Furukawa, PRB **80**, 134416 (2009).

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A18 GMAG DMP: Focus Session: Low D/Frustrated Magnetism - Pyrochlore, et al.

D172

8:00AM A18.00001 From Two Dimensional Correlations to a Disordered Ground State in the XY Pyrochlore, $Yb_2Ti_2O_7$[1] , KATE ROSS, Department of Physics and Astronomy, McMaster University — The tetrahedral geometry of the cubic pyrochlore lattice lends itself to strong geometric frustration, which has the effect of suppressing transitions to long range magnetic order (LRO) for certain types of magnetic exchange and single-ion anisotropy. $Yb_2Ti_2O_7$, whose magnetic Yb^{3+} ions decorate the pyrochlore lattice, is known to have ferromagnetic exchange combined with XY single-ion anisotropy. Hence it is not expected to be frustrated, and should develop an LRO state below some Tc on the order of the exchange energy ($\theta_{CW} \simeq$ 600mK). Indeed, $Yb_2Ti_2O_7$ displays a specific heat anomaly around 240mK, but this does not lead to an LRO state. Our recent triple-axis neutron scattering results have revealed that the specific heat anomaly is directly related to a change in dimensionality of the magnetic correlations, causing a transition from an unusual two-dimensionally correlated state above Tc to a short range correlated 3D state below Tc. Combined with recent specific heat results, we argue that the exact transition temperature depends on the precise level of weak structural disorder in the samples, implying that structurally perfect samples may lead to a fully developed LRO state below Tc. Furthermore, our earlier time-of-flight neutron scattering measurements revealed that even for the structurally imperfect systems, an ordered state can easily be induced by the application of a small magnetic field at low temperatures, as evidenced by the appearance of sharp spin wave excitations [1].

[1] K. A. Ross, J. P. C. Ruff, C. P. Adams, J. S. Gardner, H. A. Dabkowska, Y. Qiu, J. R. D. Copley, and B. D. Gaulin. Phys. Rev. Lett. 103, 227202 (2009)

[1]Work at McMaster University supported by NSERC of Canada.

8:36AM A18.00002 Order and disorder in the local and long-range structure of the spin-glass pyrochlore, $Tb_2Mo_2O_7$, YU JIANG, Lawrence Berkeley National Laboratory, ASHFIA HUQ, Oak Ridge National Laboratory, CORWIN H. BOOTH, Lawrence Berkeley National Laboratory, GEORG EHLERS, Oak Ridge National Laboratory, JOHN E. GREEDAN, McMaster University, JASON S. GARDNER, Indiana University and National Institute of Standards and Technology — The structure of $Tb_2Mo_2O_7$ is investigated using two techniques: the long-range lattice structure was measured using neutron powder diffraction, and local structure information was obtained from extended x-ray absorption fine structure measurements. While the long-range structure appears generally well ordered, enhanced mean-squared site displacements on the O(1) site and the lack of temperature dependence of the strongly anisotropic displacement parameters for both the Mo and O(1) sites indicates some disorder exists. Likewise, the local structure measurements indicate some Mo-Mo and Tb-O(1) nearest-neighbor disorder exists, similar to that found in the related spin-glass pyrochlore, $Y_2Mo_2O_7$. Although the freezing temperature in $Tb_2Mo_2O_7$, 25 K, is slightly higher than in $Y_2Mo_2O_7$, 22 K, the degree of local pair distance disorder is actually less in $Tb_2Mo_2O_7$. This apparent contradiction is considered in light of the interactions involved in the freezing process.

8:48AM A18.00003 An Exchange Hamiltonian for $Yb_2Ti_2O_7$, JORDAN THOMPSON, PAUL MCCLARTY, University of Waterloo, HENRIK RøNNOW, Laboratory for Quantum Magnetism, EPFL, LOUIS-PIERRE REGNAULT, CEA-Grenoble, ANDREAS SORGE, Network Dynamics Group, MPI for Dynamics and Self-Organization, MICHEL GINGRAS, University of Waterloo — $Yb_2Ti_2O_7$ is a pyrochlore material with many strange properties at low temperature. Specific heat measurements on this material find evidence for a first order phase transition at a temperature of $\mathrm{T_c} \approx 240$ mK, but several experiments fail to find any evidence of long range order below $\mathrm{T_c}$. In order to understand the behaviour of the magnetic moments of the Yb^{3+} ions below $\mathrm{T_c}$ it is necessary to quantift how they interact. I will present work based on using diffuse neutron scattering measurements to find a magnetic interaction Hamiltonian for $Yb_2Ti_2O_7$. We propose a Hamiltonian based on all of the symmetry allowed interactions on the pyrochlore lattice, along with long-range dipolar interactions. Using the energies of the symmetry allowed nearest-neighbor exchange interactions as free parameters, we perform simulated annealing to minimize the difference between experimental neutron scattering and neutron scattering computed from our exchange Hamiltonian using the random phase approximation. I will present the results of this fitting, and discuss the predictions of the resulting model for the behaviour of $Yb_2Ti_2O_7$, including calculations of the local susceptibility.

9:00AM A18.00004 Low temperature freezing and dynamics in Tb2Sn2O7[1] , MARIA MATTHEWS, MARIA DAHLBERG, Pennsylvania State University, PAWINA JIRAMONGKOLCHAI, ROBERT CAVA, Princeton University, PETER SCHIFFER, Pennsylvania State University — We have probed the low temperature magnetic behavior of the ordered spin ice material Tb2Sn2O7 through ac magnetic susceptibility measurements of both the pure material and samples with small percentages of Ti substituted on the Sn sublattice.. Our aim is to qualitatively probe the nature low temperature spin state of the stanate by slowly adjusting the chemical composition towards a known spin liquid— terbium titanate. In pure Tb2Sn2O7, we observe a clear signature for the previously reported ordering transition at Tc = 850 mK, and we also observe evidence for dynamic freezing at temperatures well below Tc, confirming the persistence of significant magnetic fluctuations deep in the spin-ordered regime. We found that the long range ordering transition was completely suppressed by substitution with as little as 5 percent Ti, whereas larger Ti substitution resulted in a spin-glass-like spin freezing transition near 250 mK. The suppression of ordering with minimal substitution demonstrates a remarkable fragility to the spin ordering in this system.

[1]This research was supported in part by the NSF Grant No. DMR-070158.

9:12AM A18.00005 Magnetic Diffuse Scattering in spinels GeCo2O4 (GCO) and GeNi2O4 (GNO) , P. MANUEL, M.K. CRAWFORD, D.T. ADROJA, L.C. CHAPON, S. HARA, Y. YOSHIDA, S.I. IKEDA, J.W. LYNN, Y. CHEN, R.A. FISHER — Materials exhibiting geometrical magnetic frustration have been very topical in condensed matter physics due to their large ground state degeneracy usually leading to a great variety of behavior. GCO and GNO are spinels where the Co/Ni ions form a sublattice identical to the pyrochlore. This topology naturally leads to magnetic frustration which can be relieved to permit the appearance of longrange magnetic order. GCO has a Néel temperature of 21 K, below which a tetragonal distortion is observed. However, our heat capacity measurements show only about half of the entropy expected when integrated up to 75 K. This strongly suggests the existence of frustration which is evidenced by our neutron data where strong diffuse scattering (DF) is observed. GNO also exhibits strong DF at the same q-position but with different shape. We will present the neutron data alongside a Monte-Carlo analysis of the DF and the implications on the nature and strength of the different interactions in these two systems.

9:24AM A18.00006 Dimerized Excitations in $La_4Ru_2O_{10}$[1] , JOHN-PAUL CASTELLAN, R. OSBORN, S. ROSENKRANZ, Argonne National Laboratory, Argonne, IL 60439, M.B. STONE, S.E. NAGLER, M.A. LUMSDEN, Oak Ridge National Laboratory, Oak Ridge, TN 37831, P. KHALIFAH, SUNY Stony Brook, Stony Brook, NY 11794. — The interplay between orbital, spin and charge degrees of freedom is at the forefront of condensed matter physics. The discovery of orbital ordering in $La_4Ru_2O_{10}$ [1] offers a unique opportunity to study orbital phenomena in a 4d transition metal oxide. $La_4Ru_2O_{10}$ undergoes a structural phase transition at ∼158K, below which there is a spin gap of ∼40 meV caused by Ru-O-Ru dimerization. We have performed single crystal time-of-flight neutron scattering measurements on the ARCS spectrometer at the SNS in "sweep" mode, a new technique in which neutron events are measured during continuous sample rotation, in order to quickly and efficiently map out four-dimensional volumes of S(q,w). With this method, we measured the structure factors and full dispersion of the singlet-triplet excitations as a function of **Q** and w. A model of the orbital ordering producing the magnetic excitations and the event-based technique used for their measurement will be discussed.

[1] P. Khalifah, et al., Science **297**,2237 (2002)

[1]Supported by U.S. Department of Energy, Office of Science, under contract No. DE-AC02-06CH11357.

9:36AM A18.00007 Strong spin-orbit coupling in ordered double perovskites , GANG CHEN, University of Colorado Boulder, LEON BALENTS, UCSB — We construct and analyze a microscopic model for insulating rock salt ordered double perovskites, with the chemical formula $A_2BB'O_6$, where the B' atom has a $4d^2$ or $5d^2$ electronic configuration and forms a face centered cubic (fcc) lattice. The combination of the triply-degenerate t_{2g} orbital and strong spin-orbit coupling favors an effective local spin moment $j = 2$. Moreover, due to strongly orbital-dependent exchange, the effective spins have substantial biquadratic and bicubic interactions (fourth and sixth order in the spins, respectively). This leads, at the mean field level, to several interesting phases with high magnetic multipolar orders. We discovered a fundamental difference between integer spin system (considered in present work) and half-integer spin system (studied in previous work), that is, there exists a spin nematic ground state at zero temperature for integer-spin system. We also address the finite temperature properties of different phases. Existing and possible future experiments are discussed in light of these results.

9:48AM A18.00008 Interplay between Lattice Distortion and Spin-Orbit Coupling in Double Perovskites , TYLER DODDS, University of Toronto, TING-PONG CHOY, Universiteit Leiden, YONG BAEK KIM, University of Toronto — We develop anisotropic pseudo-spin nearest-neighbour antiferromagnetic Heisenberg models for monoclinically distorted double perovskites. We focus on these $A_2BB'O_6$ materials that have magnetic moments on the $4d$ or $5d$ transition metal B′ ions, which form a face-centred cubic lattice. In these models, we consider tetragonal distortion of B′-O octahedra, affecting relative occupancy of t_{2g} orbitals, along with geometric effects of the distortion and spin-orbit coupling. The resulting pseudo-spin-$1/2$ models are solved in the saddle-point limit of the Sp(N) generalization of the Heisenberg model. The spin S in the SU(2) case generalizes as a parameter κ controlling quantum fluctuation in the Sp(N) case. We consider two different models that may be appropriate for these systems. In particular, using Heisenberg exchange parameters for La_2LiMoO_6 from a spin-dimer calculation [T. Aharen *et al.*, Phys. Rev. B **8**1, 224409 (2010)], we conclude that this $S = 1/2$ system may order, but must be very close to a disordered spin liquid state.

10:00AM A18.00009 Elastic and inelastic neutron scattering study on $(CuCl)LaTa_2O_7$, SEUNGHUN LEE, KAZUKI IIDA, University of Virginia, ATSUSHI KITADA, YOSHIHIRO TSUJIMOTO, HIROSHI KAGEYAMA, Kyoto University, BELLA LAKE, HZB, SEIKO KAWAMURA, J-PARC, KAZUHISA KAKURAI, JAEA, YIMING QIU, MARK GREEN, NCNR, UNIVERSITY OF VIRGINIA TEAM, KYOTO UNIVERSITY COLLABORATION, HELMHOLTZ-ZENTRUM BERLIN COLLABORATION, JAPAN ATOMIC ENERGY AGENCY COLLABORATION, NIST CENTER FOR NEUTRON RESEARCH COLLABORATION — A quasi-two-dimensional frustrated spin system, $(CuCl)La(Nb_{1-x}Ta_x)_2O_7$, shows a quantum phase transition upon doping of Ta ions from a singlet state to an ordered state at $x \sim 0.4$. $(CuCl)LaNb_2O_7$ has been reported as the first ferromagnetically coupled Shastry-Sutherland singlets with the triplet excitations centered at 2 meV. We report elastic and inelastic neutron scattering measurements on a powder sample of $(CuCl)LaTa_2O_7$ with and without an magnetic field. Our results show that upon cooling this system undergoes a magnetic ordering below 7 K with a characteristic wave vector of $Q = (1/2\ 0\ 1/2)$. The magnetic excitations in the ordered phase are dominated by a nearly dispersionless mode centered at 2 meV similar to the triplet excitations observed in $(CuCl)LaNb_2O_7$. Under field, however, the 2 meV mode in $(CuCl)LaTa_2O_7$ splits into two modes, clearly indicating that it is a spin wave expected for an ordered state.

10:12AM A18.00010 Structure and phase transitions of a magnetic kink crystal , SEBASTIAN MUEHLBAUER, ANDREY ZHELUDEV, ETH Zurich, Neutron Scattering and Magnetism Group, Switzerland, EKATERINA POMJAKUSHINA, PSI, Villingen, Switzerland — The insulator $Ba_2CuGe_2O_7$ crystallizes in the non-centrosymmetric space group $P-4_21m$ allowing for the Dzyaloshinskii-Moriya interaction. Below T_N=3.2K $Ba_2CuGe_2O_7$ exhibits an almost antiferromagnetic cycloidal magnetic order. For H parallel to the c-axis, the cycloid distorts to solitions or kink domain walls. Using small angle neutron scattering and neutron diffraction the structure and phase transitions of a magnetic kink crystal have been examined in $Ba_2CuGe_2O_7$. A magnetic phase transition seen with SANS and complementary measurements of the magnetization is interpreted in terms of a transition from a Neel domain wall with the propagation vector $parallel$ to its plane of spin rotation to a Bloch domain wall with a propagation vector $perpendicular$ to its plane of spin rotation. Indicated by the occurrence of satellite reflections with even and odd harmonics around the AF Neel point (1,0,0) and around the FM zone center (0,0,0) it was further shown that the AF cycloidal magnetic structure of $Ba_2CuGe_2O_7$ is considerably distorted by the staggered Dzyaloshinskii vector D_z.

10:24AM A18.00011 Neutron Scattering Study of Frustration and Magnetic Order in Spinels[1] , GREGORY MACDOUGALL, Oak Ridge National Laboratory — The 'A-site spinels' are materials with magnetic cations constrained to lie on the diamond sublattice of the spinel structure. These systems have been of increasing interest, as novel theoretical and experimental results have emphasized the central role of frustration arising from competing interactions. In particular, the sub-family of diamond lattice antiferromagnets with spin-only degrees-of-freedom is predicted to exhibit novel 'spiral-spin-liquid' and order-by-disorder physics (Bergman et al., Nature Physics (2007)). Real systems MnSc2S4 (Krimmel et al., PRB (2006)) and CoAl2O4 (Krimmel et al., Physica B (2006)) have been studied with powder neutron diffraction, and the results are argued to be consistent with this theory. However, as has been expressed on several occasions, studies on single-crystals are needed for a definitive answer. Here I will discuss neutron scattering results on single-crystalline CoAl2O4, which have given a much more complete picture of magnetic correlations in this material. Both elastic and inelastic measurements have been made using triple-axis and cold chopper spectrometry. With decreasing temperature, we observe intense diffuse scattering centred about locations in reciprocal space associated with collinear antiferromagnetism. At T* 6.5K, we further observe an unexpected change in the diffuse scattering lineshape, coupled with the emergence of well-defined spin-wave excitations. This temperature has been associated with an anomalous spin glass transition in the past, but we argue instead that the available data implies a first-order phase transition to an ordered state, possibly via the order-by-disorder mechanism. The ground state is degenerate, and kinetically frozen walls separating different domains give rise to the broadened scattering at magnetic wavevectors. This scenario may be present in many other frustrated systems. If time permits, I will also talk about new results on crystals of related systems MnAl2O4 and FeAl2O4.

[1]Research sponsored by the US Department of Energy, Basic Energy Sciences, Division of User Facilities

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A20 FIAP/DMP GERA/DCOMP: Focus Session: Physics of Energy Storage Materials I – Cathodes and Electrolytes D168

8:00AM A20.00001 Extracting the LiV3O8 Phase diagram by cluster expansion[1] , TONGHU JIANG, MICHAEL FALK, Department of Materials Science and Engineering, Johns Hopkins University — LiV3O8 as a lithium battery cathode material has many advantages over current commercialized counterparts, which has prompted interest in improving its electrochemical behavior. However, no clear picture of its structural chemistry and phase behavior has emerged from experimental investigations. In the current work, LiV3O8 was studied using computational methods. A cluster expansion was constructed based on energetic data from density functional theory calculation. The CE was employed to reveal structural information regarding this material. DFT calculation using the local density approximation were found to be deficient in correctly predicting ground states leading to mismatch between experimental and computational results, while generalized gradient approximation gives closer agreement with experimental data. A tentative phase diagram was obtained with the help of Metropolis Monte Carlo calculations.

[1]Research supported by National Science Foundation, Cyber Discovery and Innovation under award 102776511027729.

8:12AM A20.00002 Magnetic and spectroscopic characterization of C-$LiFePO_4$ nanoparticles for cathode material for Li ion batteries , AMBESH DIXIT, K. BAZZI, M.B. SAHANA, C. SUDAKAR, Wayne State University, M. NAZRI, 2Applied Sciences Inc., Cedarville, Ohio, P.P. VAISHNAVA, Kettering University, Flint, Michigan , V. NAIK, University of Michigan-Dearborn, V.K. GARG, A.C. OLIVEIRA, Universidade de Brasilia, Instituto de Fisica, G.A. NAZRI, R. NAIK, Wayne State University — We synthesized pure and carbon coated $LiFePO_4$ nanoparticles (size ∼25 nm) by sol-gel technique. All the samples were characterized by X-ray diffraction, XPS, SQUID, and Mossbauer spectroscopy measurements. The elemental chemical states for Li 1s, Fe 2p, P 2p, O 1s and C 1s were examined by using XPS for $LiFePO_4$ and compared with those of C-$LiFePO_4$ material. Temperature dependent magnetic measurements suggest an antiferromagnetic transition ∼50 K in both $LiFePO_4$ and C-$LiFePO_4$ samples. The role of various phases, such as $LiFePO_4$ Fe_xP, α-Fe and Fe_3O_4 identified by Fe^{57} Mossbauer spectroscopy, will be discussed in relationship with the electrochemical properties of the cathode materials.

8:24AM A20.00003 First-principles modeling of Li-air battery materials , MAXWELL RADIN, Mechanical Engineering Department, University of Michigan, DONALD SIEGEL, Department of Physics, University of Michigan — Of the many possible battery chemistries, the so-called "Li-air" system is noteworthy in that its theoretical capacity (∼5 kWh/kg, including mass of oxygen) exceeds that of any electrochemical system. Perhaps more importantly, the simplified composition of its air cathode – involving only the inlet of oxygen from the atmosphere – has the potential to provide cost benefits in comparison to the Li-ion systems of today. Although the first rechargeable Li-air battery was demonstrated by Abraham and Jiang 14 years ago, its performance in many dimensions remains poor, and relatively little computational work has been done to elucidate performance-limiting phenomena. This talk will introduce the basic properties and main performance issues associated with Li-air batteries. Opportunities for first-principles modeling to assist in overcoming these obstacles will be highlighted.

8:36AM A20.00004 Materials Challenges and Opportunities of Lithium-ion Batteries for Electrical Energy Storage , ARUMUGAM MANTHIRAM, University of Texas at Austin — Electrical energy storage has emerged as a topic of national and global importance with respect to establishing a cleaner environment and reducing the dependence on foreign oil. Batteries are the prime candidates for electrical energy storage. They are the most viable near-term option for vehicle applications and the efficient utilization of intermittent energy sources like solar and wind. Lithium-ion batteries are attractive for these applications as they offer much higher energy density than other rechargeable battery systems. However, the adoption of lithium-ion battery technology for vehicle and stationary storage applications is hampered by high cost, safety concerns, and limitations in energy, power, and cycle life, which are in turn linked to severe materials challenges. This presentation, after providing an overview of the current status, will focus on the physics and chemistry of new materials that can address these challenges. Specifically, it will focus on the design and development of (i) high-capacity, high-voltage layered oxide cathodes, (ii) high-voltage, high-power spinel oxide cathodes, (iii) high-capacity silicate cathodes, and (iv) nano-engineered, high-capacity alloy anodes. With high-voltage cathodes, a critical issue is the instability of the electrolyte in contact with the highly oxidized cathode surface and the formation of solid-electrolyte interfacial (SEI) layers that degrade the performance. Accordingly, surface modification of cathodes with nanostructured materials and self-surface segregation during the synthesis process to suppress SEI layer formation and enhance the energy, power, and cycle life will be emphasized. With the high-capacity alloy anodes, a critical issue is the huge volume change occurring during the charge-discharge process and the consequent poor cycle life. Dispersion of the active alloy nanoparticles in an inactive metal oxide-carbon matrix to mitigate this problem and realize long cycle life will be presented.

9:12AM A20.00005 Vacancy-driven anisotropic defect distribution in $LiFePO_4$[1] , JAEKWANG LEE, WU ZHOU, JUAN CARLOS IDROBO, Department of Physics and Astronomy, Vanderbilt University, Nashville, STEPHEN PENNYCOOK, Materials Science & Technology Division, Oak Ridge National Laboratory Oak Ridge, SOKRATES PANTELIDES, Department of Physics and Astronomy, Vanderbilt University, Nashville — It has been reported that iron cations occupying Li sites (Fe_{Li}) in $LiFePO_4$ are locally aggregated rather than homogeneously distributed in the lattice.[1] Here we report a combination of density-functional calculations, statistical mechanics, electron-energy-loss spectra (EELS) and show the following. There is a strong binding energy between $Fe_{Li}$and a lithium vacancy (V_{Li}), leading to clustering of Fe_{Li} along the b-axis, as observed, corresponding to the shortest separation of the Fe_{Li}-V_{Li} pair. EELS data find that a small fraction of Fe atoms are Fe^{3+}, which can be accounted for in terms V_{Li}-Fe_{Li}-V_{Li} clusters formed along the b-axis.

[1]S.-Y. Chung et al. Angew. Chem. 48, 543 (2009). This work was supported in part by the DOE Mater. Sci. and Eng. Div. and DOE grant FG02-09ER46554.

9:24AM A20.00006 Polaron formation and transport in olivine cathode materials , MICHELLE JOHANNES, Naval Research Laboratory, KHANG HOANG, Naval Research Laboratory; George Mason University — One of the critical factors limiting Li ion battery performance is electronic conduction through the cathode material. In the olivine structure type materials, such as $LiFePO_4$, the parent materials are insulators with a gap of approximately 4 (or more) eV. The withdrawal of an electron results not in a band-type hole state, but rather a localized polaronic state. Transport then occurs via hopping of the polaron through the crystal. The measured electronic conduction in olivine materials depends on the transition metal cation type. In this study, we use density functional theory to compare formation of polarons in olivine materials with different transition metal cations: Mn, Fe, Co, and Ni. We show that the underlying electronic structure of the fully lithiated material (or fully delithiated material) essentially determines whether or not polaron formation is possible in localized d-states or whether the holes that result from adding or removing an electron reside in oxygen-derived states. We also investigate the facility of polaronic hopping by calculating the barrier between adjacent polaron sites in each of the four materials.

9:36AM A20.00007 First-principles studies of native defects in olivine phosphates , KHANG HOANG, George Mason University and Naval Research Laboratory, MICHELLE JOHANNES, Naval Research Laboratory — Olivine phosphates Li$M$$PO_4$ (M=Mn, Fe, Co, Ni) are promising candidates for rechargeable Li-ion battery electrodes because of their energy storage capacity and electrochemical and thermal stability. It is known that native defects have strong effects on the performance of olivine phosphates. Yet, the formation and migration of these defects are not fully understood, and we expect that once such understanding has been established, one can envisage a solution for improving the materials' performance. In this talk, we present our first-principles density-functional theory studies of native point defects and defect complexes in Li$M$$PO_4$, and discuss the implications of these defects on the performance of the materials. Our results also provide guidelines for obtaining different native defects in experiments.

9:48AM A20.00008 Electronic structure of lithium borocarbide as a cathode material for a rechargeable Li-ion battery: First-principles calculation , QIANG XU, CHUNMEI BAN, ANNE DILLON, SUHUAI WEI, YUFENG ZHAO, National Renewable Energy Laboratory — Traditional cathode materials, such as transition-metal oxides, are heavy, expensive, and often not benign. Therefore, alternative materials without transition metal elements are highly desirable in order to design high-capacity Li-ion batteries of light weight and low price. Here we report on potential application of the LiBC compound as cathode materials, in which graphene-like BC sheets are intercalated by Li ions. The crystal structure and properties of LiBC were firstly reported by Wörle et al. in 1995. Importantly, it was found that the 75% Li ions can be retrieved out of the compound without changing the layered structure. We have performed first-principles calculations based on density functional theory, as implemented in the Vienna Ab-initio Simulation Package. According to our calculation, the layered Li_xBC structure can be well preserved at $x > 0.5$. The reversible electrochemical reaction, LiBC $\leftrightarrow$ $Li_{0.5}BC$ + 0.5Li, gives an energy capacity of 609mAh/g and an open-circuit voltage of 2.42V. The volume change is only about 5% during the charging and discharging process. All these results point to a potentially promising application of LiBC as a novel cathode material for high-capacity Li-ion batteries in replacement of the transition metal oxides.

10:00AM A20.00009 Competing stability of inverse and normal spinel structures for lithium battery cathodes , JISHNU BHATTACHARYA, CHRISTOPHER WOLVERTON, Northwestern University — Transition metal oxides comprise of an important class of cathode materials in rechargeable lithium ion batteries. Many of these materials occur in the spinel crystal structure, in which metal atoms are present in octahedral and tetrahedral interstices of a close-packed oxygen sublattice. Depending on whether the Li or the transition metal ions are found in the tetrahedral sites, one can form either the "normal" or "inverse" spinel structures. In the present study, we calculate from first principles the relative stability of the inverse vs. normal spinel for a series of transition metal oxides both at lithiated and delithiated limits. We find trends in the stability of the normal vs. inverse spinel are a strong function of lithium content, and explain these results in terms of the preference for metal/Li tetrahedral/octahedral coordination. Despite the similarities between these two structures, they can have a profound effect on the Li diffusivity. We also use our framework to address the stability of multicomponent inverse spinel electrodes, such as $LiNiVO_4$.

10:12AM A20.00010 Atomistic Simulation Study of Lithium Manganese Oxides for Li-Ion Batteries , PHUTI NGOEPE, KENNETH KGATWANE, RAPELA MAPHANGA, Materials Modelling Centre, Private Bag x1106, University of Limpopo, Sovenga 0727, South Africa, THI SAYLE, DEAN SAYLE, DEAS, Cranfield University, Defence Academy of the United Kingdom, Shrivenham, Swindon, SN6 8LA, UK. — Simulated amorphisation recrystallisation (A+R) technique has been successfully used to generate models of various nano-forms of the complex manganese dioxides [1]. We apply the method to study lithium insertion into the nano - spheres, sheets, rods and porous structures of the binary MnO_2. The variation of mechanical properties and microstructural features with lithium concentration are investigated. The bulk ternary Li_2MnO_3 provides structural integrity for lithium-ion battery cathodes and is electrochemically inactive. The nanocrystalline Li_2MnO_3 has a structure similar to that of the bulk, but shows different lithium intercalation properties [2]. We simulated such a nanophase by the A+R method, and the resulting microstructures provide insights into the origins of the electrochemical activity which renders it suitable for battery electrodes.

[1]. T.X.T. Sayle, R.R. Maphanga, P.E. Ngoepe, and D.C. Sayle, J. Am. Chem. Soc., 131, 6161, (2009).
[2]. G. Jain, J. Yang, M. Balasubramanian and J,J. Xu, Chem. Mater. **17**, 3850, (2005)

10:24AM A20.00011 Computer modeling of crystalline electrolytes – lithium thiophosphates and phosphates[1] , NICHOLAS LEPLEY, N.A.W. HOLZWARTH, Wake Forest University — During the last 5 years, lithium thiophosphate solid electrolyte materials have been developed[2] for use in all-solid-state rechargeable batteries. In particular, crystalline $Li_7P_3S_{11}$ has been characterized as a superionic conducting material having room temperature conductivities as high as 10^{-3} S/cm, which is 1000 times greater than that of the commercial solid electrolyte material LiPON. Building on our previous work,[3] we report computer modeling studies of this material as well as those of related phosphates and phosphonitrides. We present results on meta-stable crystal structures, formation energies, and mechanisms of Li ion migration. The calculational methods are based on density functional theory. The calculations were carried out using the Quantum Espresso (PWSCF) package.[4]

[1]Supported by NSF Grant DMR-0705239

[2]H. Yamane, M. Shibata, Y. Shimane, et al., *Solid State Ionics* **178**, 1162-1167 (2007).
[3]N. A. W. Holzwarth, N. D. Lepley, Y. A. Du, *J. Power Sources* (2010) [in press: doi:10.1016/j.jpowsour.2010.08.042]
[4]P. Giannozzi, S. Baroni, et al., *J. Phys.: Condens. Matter.* **21**, 394402 (2009); available from the website: http://www.pwscf.org/.

10:36AM A20.00012 Effect of electrolytes on the evolution of the solid electrolyte interphase (SEI) in Li-ion batteries: a Molecular Dynamics study , SANG-PIL KIM, VIVEK SHENOY, Brown University, BROWN UNIVERSITY TEAM — Controlling and understanding the atomic level reactions at the interface between electrode and electrolyte is a prerequisite for the improvement of the performance of Li-ion batteries. The solid electrolyte interphase (SEI), which forms on the negative electrode of Li-ion batteries, is known to significantly affect the battery performance leading to irreversible charge loss, exfoliation of graphite anode and affecting the safety. In spite of the large body of work on SEI, a quantitative understanding of the mechanisms of SEI formation is currently not available. In this work, we employ molecular dynamics simulations with reactive force fields to investigate the compositional and structural properties of the SEI. Our simulations capture the mechanisms of SEI formation as Li atoms react with different kinds of electrolytes (ethylene carbonate (EC), dimethyl carbonate (DMC), and their mixtures) and are able to quantitatively predict the properties in terms of the SEI thickness, byproducts, charge loss, and rigidity.

10:48AM A20.00013 Properties of Liquid Electrolytes for Li-ion Battery Applications from First Principles Molecular Dynamics Simulation , PAUL KENT, PANCHAPAKESAN GANESH, DEEN JIANG, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — A judicious choice of the liquid electrolytes used in battery systems is required to achieve a good balance between high energy storage, fast charging and long lifetime. Ethylene-carbonate (EC) and propylene-carbonate (PC) are popular electrolytes used for this purpose. To date, molecular-dynamics simulations typically rely on classical force-fields, which do not capture the true quantum-mechanical nature of the electrons, most important for the charging/discharging dynamics. We perform accurate first principles molecular-dynamics simulations of EC and PC with $LiPF_6$ at experimental concentrations to build solvation models which explain available Neutron and NMR results as well as to compute Li-ion solvation energies and diffusion constants. Our results throw light on why EC is a more popular choice for battery applications over PC. Insights into the formation of solid-electrolyte interphases in the presence of carbon electrodes in conventional Li-ion batteries will also be discussed, and perspectives into the likely future scope of these simulation methods presented. Supported by the Fluid Interface Reactions, Structures and Transport (FIRST) Center, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Basic Energy Sciences under Award Number ERKCC61.

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A21 GIMS: Focus Session: Advances in Scanned Probe Microscopy I – Novel Tip and Material Control D161

8:00AM A21.00001 Vacuum Phonon Tunneling in Variable Temperature STM[1] , IGOR ALTFEDER, ANDREY VOEVODIN, AJIT ROY, Air Force Research Laboratory — We demonstrate that the temperature of the terminating atom of STM tip can be directly measured by inelastic electron tunneling spectroscopy. A previously unknown mechanism of interfacial thermal transport, field-induced phonon tunneling, has been revealed by ultrahigh vacuum scanning tunneling microscopy. Using thermally broadened Fermi-Dirac distribution in the STM tip as in-situ atomic scale thermometer we found that thermal vibrations of the last tip atom are effectively transmitted to sample surface despite few angstroms wide vacuum gap. We show that phonon tunneling is driven by interfacial electric fields and thermally vibrating image charges, "thermal mirages". By comparing experimental data and theory, we show that the thermal energy transmitted through atomically narrow vacuum gap due to thermal vibration of image charges exceeds, by ten orders of magnitude, the Planck's thermal radiation energy. Reference: I. Altfeder, A. A. Voevodin, A. K. Roy, PRL 105, 166101 (2010)

[1]Research is funded by AFOSR

8:12AM A21.00002 A Dual Tip STM for Imaging the Superconducting Phase Difference[1] , ANITA ROYCHOWDHURY, M.A. GUBRUD, Physics Department, University of Maryland, College Park and Laboratory for Physical Sciences, DAN SULLIVAN, NASA/Goddard, MICHAEL DREYER, Physics Department, University of Maryland and Laboratory for Physical Sciences, J.R. ANDERSON, C.J. LOBB, F.C. WELLSTOOD, Physics Department, University of Maryland, College Park — We have built a dual tipped STM, with each tip capable of independently scanning a sample. We will use the STM at ultra-low (mK) temperatures to study superconducting samples. The two tips along with the superconducting sample constitute a SQUID. This configuration is designed to minimize fluctuations in the Josephson phase of one of the tips, which scans the sample, while the other tip acts as a reference junction. Calculations and separate experiments on test SQUIDs indicate this arrangement will enable us to measure spatial variations of the gauge-invariant phase difference at the atomic scale.

[1]This project was funded in part by NSF and the Laboratory for Physical Sciences.

8:24AM A21.00003 Nanoelectrical probing with multiprobe SPM Systems compatible with scanning electron microscopes , AARON LEWIS, Hebrew University of Jerusalem, ANDREY IGNATOV, HESHAM TAHA, Nanonics Imaging Ltd., OLEG ZHINOVIEV, ANATOLY KOMISSAR, ALEXANDER KROL, DAVID LEWIS, Nanonics Imaging Ltd. — A scanning electron microscope compatible platform that permits multiprobe atomic force microscopy based nanoelectrical characterization will be described. To achieve such multiple parameter nanocharacterization with scanning electron microscope compatibility involves a number of innovations both in instrument and probe design. This presentation will focus on how these advances were achieved and the results obtained with such instrumentation on electrical nano-characterization and electrical nano-manipulation. The advances include: 1. Specialized scanners; 2. An ultrasensitive feedback mechanism based on tuning forks with no optical feedback interference that can induce carriers in semiconductor devices; and 3. Unique probes compatible with multiprobe geometries in which the probe tips can be brought into physical contact with one another. Experiments will be described with such systems that will include multiprobe electrical measurements with metal and glass coated coaxial nanowires of platinum. This combination of scanning electron microscopes integrated with multiprobe instrumentation allows for important applications not available today in the field of semiconductor processing technology.

8:36AM A21.00004 Imaging and manipulation of nanoscale materials with coaxial and triaxial AFM probes , KEITH A. BROWN, R.M. WESTERVELT, Harvard SEAS and Physics — We present coaxial and triaxial Atomic Force Microscope (AFM) probes and demonstrate their applications to imaging and manipulating nanoscale materials. A coaxial probe with concentric electrodes at its tip creates a highly confined electric field that decays as a dipole field, making the coaxial probe useful for near field imaging of electrical properties. We show nearly an order of magnitude improvement in the step resolution of Kelvin probe force microscopy with coaxial probes. We further demonstrate that coaxial probes can image dielectric materials with the dielectrophoretic force. In addition to imaging, the capacitive structure that makes up the cantilever of a coaxial probe is used to locally mechanically drive the probe, making them self-driving probes. Finally, coaxial probes can create strong forces with dielectrophoresis (DEP) which we combine with the nanometer precision of the AFM to create a nanometer scale pick-and-place tool. We demonstrate 3D assembly of micrometer scale objects with coaxial probes using positive DEP and discuss the assembly of nanometer scale objects with triaxial probes using negative DEP.

8:48AM A21.00005 Deterministic Single Atom STM Tip Technology for Atomically Precise Manufacturing , JOSHUA BALLARD, JUSTIN ALEXANDER, ADRIAN RADOCEA, Zyvex Labs, MAIA BISCHOF, DAVID JAEGER, University of North Texas, JOHN RANDALL, Zyvex Labs, BRIAN GORMAN, Colorado School of Mines, JIM VON EHR, Zyvex Labs, RICK REIDY, University of North Texas — Deterministic tip fabrication for Scanning Tunneling Microscopy (STM) has long been an elusive goal, where the primary method of tip preparation usually includes significant "tip conditioning" once the tip has been incorporated into the STM. We have developed a process for generating reproducible single atom tips (SATs) with a small radius of curvature (r.o.c.) of less than 10nm. First, W(111) or W(110) tips are sputter sharpened using a self-limiting process to yield with r.o.c. of $<$3nm; the consistent r.o.c. greatly improves the reliability of the process. Next, we use a Field Ion Microscope (FIM) to perform field evaporation and analysis of the tips. Once a clear crystal structure is determined, an SAT is formed. Transmission Electron Microscopy is used to verify that after field evaporation the r.o.c. remains small. Correlations between FIM and tip performance in STM are determined, and long term STM stability is discussed.

9:00AM A21.00006 Atmospheric Stability of Tungsten STM Tips for Atomically Precise Manufacturing (APM) , MAIA BISCHOF, DAVID JAEGER, University of North Texas, JOSHUA BALLARD, JUSTIN ALEXANDER, JOHN RANDALL, Zyvex Labs, RICHARD REIDY, University of North Texas, BRIAN GORMAN, Colorado School of Mines, JIM VON EHR, Zyvex Labs, ATOMICALLY PRECISE MANUFACTURING CONSORTIUM COLLABORATION — In APM, STM tungsten tips are used to selectively remove or add surface atoms to build atomically precise 3D structures. Therefore, the development of stable atomically sharp tips is crucial for long term tip performance and process efficiency. These tips have been shown to be extremely sensitive to electrostatic discharge (ESD) events and some environmental conditions. However, recent work has demonstrated that tungsten tips with three to eight atoms at their apex can be stable structurally and chemically after days of ambient exposure with ESD-safe practices. Whereas macroscale W surfaces will oxidize under atmospheric oxygen, HRTEM and 3-D atom probe measurements confirm that no oxide is formed on these tips with an extremely stable surface structure; however, some oxygen does diffuse into the material. In addition to the description of the chemical and structural characterization employed in this work, several possible explanations for the stability of these tips will be offered.

9:12AM A21.00007 STM manipulation and measurement of charged species in semiconductors[1] , JAY GUPTA, Ohio State University — The scaling of transistors to nanometer dimensions requires more precise control of individual dopants in semiconductor nanostructures, as statistical fluctuations in dopant distributions can significantly impact device performance. Proposals for next-generation quantum- and spin-based electronics also rely on the tuning of the charge, spin and interactions of dopant atoms with local electric fields. Using a scanning tunneling microscope (STM), we demonstrate how to control the binding energy and ionization state of individual acceptors in p- GaAs [1]. Charged species such as native dopants, vacancies and adatoms directly influence the acceptor binding energy via the Coulomb interaction. In addition, a combination of defect- and tip-induced band bending can be used to remotely tune the acceptors' ionization state. We find that by applying voltage pulses with the STM tip, charged vacancies and adatoms can be positioned on the surface. These experiments suggest a new and direct method for quantifying the charge of adsorbates (e.g. adatoms or molecules) as well as defects (e.g. vacancies, antisites, interstitials) at semiconductor surfaces.

[1] D.H. Lee and J.A. Gupta (submitted)

[1]Work supported by the Arnold and Mabel Beckman Foundation

9:48AM A21.00008 Dirac Fermions in Nanoassembled Artificial Graphene[1] , KENJIRO K. GOMES, WONHEE KO, WARREN MAR, HARI C. MANOHARAN, Stanford University — In condensed matter, electronic properties derive from the energy band structure created by a periodic potential formed by the atoms that constitute a particular material. The power to design unique electronic states is ultimately tied to the power to design the atomic lattice. Utilizing the technique of atomic manipulation with a scanning tunneling microscope, we create an artificial lattice potential that reshapes the band structure of a normal 2D electron gas—found in the surface states of a normal metal—into a unique and distinct 2D gas of massless Dirac fermions. We present scanning tunneling spectroscopic measurements of nanoassembled honeycomb electron lattices, and we characterize their band structure through Fourier transform analysis of impurity scattering maps. The control of every atomic position in the lattice provides unprecedented control over physical parameters elusive in natural graphene systems. These abilities include atomically sharp doping configurations and the power to embed topological singularities, resulting in unique electronic states rarely encountered in natural systems.

[1]Supported by the DOE, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under contract DE-AC02-76SF00515.

10:00AM A21.00009 Topological properties of artificial graphene assembled by atom manipulation[1] , WONHEE KO, WARREN MAR, KENJIRO K. GOMES, HARI C. MANOHARAN, Stanford University — Graphene exhibits special electronic properties stemming from its two-dimensional (2D) structure and embedded relativistic Dirac cones. However, many proposed topologically ordered ground states remain elusive in conventional measurements due to the difficulty in arranging the necessary quantum textures into natural graphene. By exploiting atomic manipulation with a custom-built ultrastable scanning tunneling microscope, we have constructed graphene-like structures by arranging molecules to create a honeycomb lattice of electrons drawn from normal 2D surface states. Spectroscopy reveals a spectacular transformation of nonrelativistic massive 2D electrons into massless Dirac fermions carrying a chiral pseudospin symmetry. We demonstrate the tailoring of this new class of graphene to reveal signature topological properties: an energy gap and emergent mass created by breaking the pseudospin symmetry or changing the hopping term non-uniformly with a Kekulé bond distortion; gauge fields generated by applying atomically engineered strains; and the condensation of electrons into quantum Hall-like states and topologically confined phases.

[1]Supported by the DOE, Office of Basic Energy Sciences, Division of Material Science and Engineering under contract DE-AC02-76SF00515

10:12AM A21.00010 Self-navigation of STM tip toward a micron sized sample[1] , GUOHONG LI, ADINA LUICAN, EVA ANDREI, Department of Physics & Astronomy, Rutgers University, DEPARTMENT OF PHYSICS & ASTRONOMY, RUTGERS UNIVERSITY TEAM — Scanning probe microscopy (SPM) of small samples on insulating substrates, for example graphene devices, is of significant current interest as it can provide invaluable information on the electronic, structural chemical and optical properties of these materials. Accessing such samples with SPM often requires locating a micron sized area within a much larger region of several mm. This is a very difficult task because SPM is intrinsically nearsighted and in many cases combining it with larger scan probes such as optical microscopy is not practical. Here we report a simple capacitance-based method to navigate a STM tip operating at low temperatures in strong magnetic field which allows to find such small samples quickly and efficiently. The method consists of back-gate compensation, refocusing during the search, and distinguishing edges of conducting electrodes and the sample.

[1]Work Supported by DOE under DE-FG02-99ER45742, partially by NSF under NSF-DMR-0906711 and Lucent.

10:24AM A21.00011 Magnetic Particle Imagining with a Cantilever Detector , JACOB ALLDREDGE, JOHN MORELAND, NIST — We present a novel detection scheme for magnetic nano and micro particles using a magnetic force microscope (MFM) that allows for the local measurement of AC magnetic susceptibility. The method makes use of the nonlinearities in the magnetic response of a particle that come from its intrinsic magnetic susceptibility as well as its interaction with the surrounding environment. We excite the particle at subharmonic frequencies of the resonator detector to minimize cross talk similar to Magnetic Particle Imagining (MPI) (Gleich B, Weizenecker, J. Nature 435, 1214 2005) although here a cantilever acts as a detector instead of a tuned coil. This allows for the detection and characterization of magnetic particles with high signal to noise and low distortion making it ideal for characterizing magnetic nanoparticles over larger distances compared to typical scanned probe tip-sample separation. It also allows for the reconstruction of the local susceptibility curve.

10:36AM A21.00012 The importance of cantilever mechanics in the quantitative interpretation of Kelvin Probe Force Microscopy , KEVIN J. SATZINGER, Truman State University, KEITH A. BROWN, R.M. WESTERVELT, Harvard SEAS and Physics — A realistic interpretation of the measured contact potential difference (CPD) in Kelvin Probe Force Microscopy (KPFM) is crucial in order to extract quantitative information. Thus far, simulations of KPFM have treated the cantilever as a rigid object. We present a technique to simulate KPFM measurements by simulating a realistic three dimensional probe above a planar sample. We study three methods of weighing the probe-sample interactions to include cantilever mechanics. (1) The commonly-used force method treats the probe-sample interaction from all parts of the probe equally. This method only allows for translation of the probe. (2) The torque method allows for rotation of the probe, taking into account the fixed cantilever end. (3) The bending method acknowledges the flexibility of the cantilever by modeling it as an Euler-Bernoulli beam. We compare simulated step responses from each method to experimental data. We find the force and torque methods overestimate the effect of the cantilever and that the bending method produces the best agreement with experiment.

10:48AM A21.00013 Nm-Scale Surface Potential Transient Measurements of the E_C-0.57eV Trap in an AlGaN/GaN High Electron Mobility Transistor , D. CARDWELL, A.R. AREHART, S.A. RINGEL, J.P. PELZ, Ohio State University — AlGaN/GaN high electron mobility transistors (HEMTs) are intrinsically ideal for high frequency and high power applications, but have degraded performance due to charge trapping. A suspected virtual gate-related trap at E_C-0.57eV (with $\sim$30 ms emission time constant at 300 K) has been shown to have a significant impact on HEMT performance and reliability [1]. Using scanning Kelvin probe microscopy, we report on nm-scale measurements of surface potential transients consistent with the E_C-0.57 eV level at different locations across the surface of an AlGaN/GaN HEMT immediately after bias switching. We find that the amplitude of this surface potential transient is largest at locations close to the drain side of the gate, consistent with the "virtual gate model" where charge leaks and is stored near the gate edge in the drain –gate access region. Comparison of nm-scale measurements and electrostatic simulations will be discussed, to quantify the spatial distribution of this $\sim$30ms trap as a function of gate- and drain-biasing. Work supported by ONR-DRIFT (P. Maki).

[1] A.R. Arehart, S.A. Ringel, et al., IEEE International Electron Devices Meeting(IEDM), 2010, 20.1.

Monday, March 21, 2011 8:00AM - 10:48AM –
Session A22 DCMP: Charge Density Wave Materials D163

8:00AM A22.00001 New High Energy Scales in Quasi-One-Dimensional $K_{0.3}MoO_3$ Revealed by High Resolution Angle-Resolved Photoemission Spectroscopy , DAIXIANG MU, WENTAO ZHANG, LIN ZHAO, HAIYUN LIU, XIAOWEN JIA, SHANYU LIU, GUODONG LIU, XIAOLI DONG, JUN ZHANG, X.J. ZHOU, National Laboratory for Superconductivity, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, XIAOYANG WANG, QINJUN PENG, ZHIMIN WANG, SHENJIN ZHANG, FENG YANG, CHUANGTIAN CHEN, ZUYAN XU, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences — High resolution angle-resolved photoemission (ARPES) measurements have been carried out on $K_{0.3}MoO_3$, a proto-typical quasi-one-dimensional material that exhibits Peierls transition at 180 K. Two high energy scales around 100meV and 300meV are revealed in the dispersion measured using super-high resolution vacuum ultra-violet (VUV) laser-based ARPES measurements. These new high energy features emerge in the charge-density-wave state. The origin of these new energy scales will be discussed.

8:12AM A22.00002 Variable Temperature Scanning Tunneling Microscope study on CDW material 2H-$TaSe_2$, JIXIA DAI, YUE CAO, EDUARDO CALLEJA, DANIEL DESSAU, Department of Physics, University of Colorado at Boulder, Boulder, CO 80302, HELMUTH BERGER, Department de Physique, EPF Lausanne, CH-1015 Lausanne, Switzerland, KYLE MCELROY, Department of Physics, University of Colorado at Boulder, Boulder, CO 80302 — As a layered quasi-2D material, 2H-$TaSe_2$ has a very rich phase diagram including a second order phase transition at 122K, a first order phase transition at 90K, and a superconductivity transition at 133mK. With our UHV Scanning Tunneling Microscope, we have performed temperature-controlled STM work to study the incommensurate and commensurate CDW phases of 2H-$TaSe_2$, from 77K to 110K. We will present temperature and tunneling bias voltage dependant topograph data, together with IV and dI/dV spectra in order to help understanding the nature of these two different CDW phases and the gapping mechanism of this material.

8:24AM A22.00003 The Role of Electron-Phonon Coupling in the CDW phase transitions in $TaSe_2$, YUE CAO, ZHE SUN, QIANG WANG, JIXIA DAI, KYLE MCELROY, MICHAEL HERMELE, University of Colorado, HELMUTH BERGER, Institute of Condensed Matter Physics, EPFL, Switzerland, DANIEL DESSAU, University of Colorado — In this talk, we will report our research progress of the classical charge density wave material 2H-$TaSe_2$. The formation of the CDW can be driven by the electronic instability or by the interplay between electrons and phonons, which is an essential ingredient of CDW. In this talk, we will provide a novel analyzing technique that can help distinguish the two scenarios. We will discuss the three possible nesting schemes in this talk and compare its electronic instability. We employ a novel band dissected technique to analyze the characteristic correlation functions for the CDW phase. By comparing the electronic instability to the actual band folding in the incommensurate CDW phase, we can tell the role of electronic structure / electron phonon coupling in this material. This discussion will help improve our understanding of the CDW and of the nesting picture in general.

8:36AM A22.00004 Extended phonon collapse in the charge density wave compound $NbSe_2$, S. ROSENKRANZ, F. WEBER, J.P. CASTELLAN, R. OSBORN, A. SAID, Argonne National Laboratory, R. HOTT, R. HEID, Karlsruhe Institute of Technology, D. REZNIK, Univ. Colorado at Boulder — The soft-phonons in the charge density wave (CDW) compound $NbSe_2$ were investigated using high-resolution inelastic X-ray scattering. As the CDW transition at T_C=33K is approached from high temperature, we observe a breakdown of the dispersion with the phonons becoming overdapmed over an extended region around the CDW wavevector. This is in contrast to the cusp in the phonon dispersion expected from the commonly invoked electronic nesting scenario of the CDW transition. Instead, our results, combined with $ab\ initio$ calculations, show that the wavevector of the CDW order is dictated by the momentum dependence of the intrinsic electron-phonon coupling. The strong influence of electron-phonon matrix-elements could also be of importance to other systems, where CDW-like correlations have been attributed to unusual physical properties.
Work supported by US DOE BES-DMS DE-AC02-06CH11357.

8:48AM A22.00005 Pressure induced enhancement of CDW fluctuations in 1T-TiSe2[1] , Y.I. JOE, X.M. CHEN, University of Illinois, J. GECK, IFW-Dresden, Germany, M. VON ZIMMERMANN, DESY HASYLAB, Germany, S. YUAN, S.L. COOPER, PETER ABBAMONTE, University of Illinois — 1T-TiSe2 is atypical quasi 2-dimensional CDW material showing a 2x2x2 superlattice modulation at low temperature. It's is known that high pressure suppresses the CDW order and interestingly induces superconductivity. While it is not agreed what drives the CDW transition, it has been proposed that the CDW fluctuations are closely related to the emergence of superconductivity . Here we present a detailed high pressure X-ray diffraction study of the CDW order in -TiSe2. We can directly probe not only the order parameter but also the fluctuations of the CDW order. At low pressure we observe no sizable deviation from mean field predictions. For pressures above around 2.5GPa, however, we observe changes in the CDW line shape, indicating enhanced CDW fluctuations. Those results are consistent with previous high pressure transport measurements and suggest a relationship between the superconductivity and the charge density wave in this system.

[1]Funding DOE BES grant number DE-FG02-07ER46453

9:00AM A22.00006 Fluctuations of CDW order at a quantum phase transition , YEJUN FENG, J. VAN WEZEL, S. HARAVIFARD, G. SRAJER, J. MITCHELL, Argonne National Lab, JIYANG WANG, T.F. ROSENBAUM, University of Chicago, R. JARAMILLO, Harvard University, Z.-A. XU, Zhejiang University, Y. LIU, Penn State University — 2H-NbSe2 is the archetypical two-dimensional charge-density-wave system. Using x-ray diffraction in a diamond anvil cell, we track the evolution of the CDW order towards the buried quantum critical point inside the superconducting phase. We observe a pressure-dependent nesting vector as well as fluctuation broadening, and compare these results to the behavior of the three-dimensional spin-density-wave system, Chromium, at its quantum critical point.

9:12AM A22.00007 The effect of quantum fluctuations on charge ordered $NbSe_2$, JASPER VAN WEZEL, YEJUN FENG, JIYANG WANG, R. JARAMILLO, T.F. ROSENBAUM — Among materials displaying charge density wave order, $NbSe_2$ stands out because its ordering vector does not correspond to any obvious nesting properties of its Fermi surface or band structure. The well known Peierls mechanism is thus less effective in singling out an ordering vector for $NbSe_2$, and the transition is driven instead by an increase of the susceptibility over a wide range of wave numbers. As the CDW transition is suppressed towards zero temperature, such a broad susceptibility gives rise to quantum fluctuations with an equally broad span in wavelengths. Here, we examine the role of these quantum fluctuations as the critical point is approached. We compare our theoretical findings to recent measurements of the ordering wave vector of $NbSe_2$ under pressure and show that its properties can be understood as arising from the combined effect of the presence of quantum fluctuations and the coupling of the CDW order parameter to the lattice.

9:24AM A22.00008 Field-Effect Modulation of Charge Density Wave Conduction[1] , ETHAN GEIL, ROBERT THORNE, Cornell University — We have constructed field-effect devices, analogous to MOSFETs, with crystals of the charge-density wave (CDW) conductor NbSe3 as the channel. Applying a gate voltage across an oxide insulator modulates the carrier density in the NbSe3 and also applies a transverse electric field. Surprisingly, relatively small ($\sim$ 0.1%) changes in carrier density (as measured by the single particle conductivity) produce large ($\sim$ 40%) decreases in the threshold field for collective conduction. We discuss this result in terms of collective screening of the applied field and modulation of the CDW order parameter.

[1]This research was supported by NSF grant DMR 0805240.

9:36AM A22.00009 Torque dependence of the voltage-induced torsional strain in tantalum trisulfide associated with charge-density-wave depinning[1] , J. NICHOLS, H. ZHANG, J.W. BRILL, University of Kentucky — Crystals of orthorhombic tantalum trisulfide slowly twist (by $\sim 1/4$ degree) when voltages near the charge-density-wave depinning threshold are applied. We have studied how this hysteretic voltage-induced torsional strain (VITS) is affected by additional torques applied to the sample by attaching a magnetized steel wire to the center of the sample. The torsional strain in the crystal was measured by placing the sample in an RF cavity in a small, variable magnetic field. We have found that twisting the sample by a few degrees can have large effects on the induced strain: i) twisting can change the magnitude and dynamics of the VITS; ii) in some cases, twisting can change the direction of the VITS. The latter effect suggests that the VITS is caused by dislocation lines in the crystal causing transverse gradients in the CDW phase. As these gradients compress and dilate with alternating applied voltage, they can cause torsional strains in the crystal. A puzzle, however, is what causes the voltage-induced torsional strain to be so slow (time constants $\sim$ 1 sec near the depinning threshold).

[1]This research was supported by NSF grants DMR-0800367 and EPS-0814194.

9:48AM A22.00010 High Field Proton NMR Studies of Single Crystal $Per_2Pt[mnt]_2$[1] , ELIZABETH L. GREEN, J.S. BROOKS, NHMFL/FSU, P.L. KUHNS, A.P. REYES, NHMFL, S. BROWN, UCLA, M. ALMEIDA, Instituto-Tecnológico e Nuclear, Portugal — $Per_2Pt[mnt]_2$ is a quasi-one-dimensional organic conductor that has been studied for over thirty years. It consists of perylene and $Pt[mnt]_2$chains that undergo a spin-peierls (SP)-charge density wave (CDW) transition below 8 K. The phase diagram has previously been mapped out up to 42 T using transport measurements. The work we present here is the first single crystal NMR experiment, primarily focusing on the physics of the localized moment present on the platinum site. By measuring relaxation rates and spectra at high fields, up to 26 T, and low temperatures, down to 1.5 K, we were able to map out the SP phase boundary. Preliminary results indicate that the SP transition occurs at a lower temperature than the CDW boundary determined from transport, suggesting that the lattice instability on the perylene drives the dimerization of the platinum moment. Our ultimate goal is to use NMR spectra to observe the platinum moment in the field induced charge density wave (FICDW) state in the range 25-42 T.

[1]DMR-NSF-1005293

10:00AM A22.00011 Spin frustration and charge ordering in TMTTF salts , KAZUYOSHI YOSHIMI, NRI "RICS," AIST, Department of Physics, University of Tokyo, HITOSHI SEO, Advanced Science Institute, RIKEN, CREST JST, SHOJI ISHIBASHI, NRI "RICS," AIST, STUART BROWN, Department of Physics and Astronomy, UCLA — Quasi-one-dimensional organic conductors $(TMTTF)_2X$ salts exhibit various types of phase transitions such as magnetic ordering, charge ordering (CO), and superconducting transitions. Among them, $(TMTTF)_2SbF_6$ shows a peculiar behavior under pressure: a cooperative reduction of CO and anti-ferromagnetic (AF) phase transition temperatures by the application of pressure has been reported by NMR measurements [1]. This result naively does not coincide with the case for typical CO transitions, where CO suppresses the tendency toward magnetic ordering due to decrease of the effective spin exchange coupling. To explain this behavior, we investigate a 1/4-filled quasi-one-dimensional extended Hubbard model with Coulomb interactions and inter-chain hopping which causes spin frustration between the dimers on the one-dimensional chains. By numerical exact diagonalization method, we find that CO relaxes spin frustration and enhances two-dimensionality which stabilizes AF ordering. To compare our results with experiments, we determine the hopping parameters by first principles band calculation for several TMTTF salts and discuss the relation between spin frustration and CO.
[1] W. Yu et al., Phys. Rev. B. 70 121101 (2004).

10:12AM A22.00012 The Paired Electron Crystal: order from frustration in the quarter-filled band[1] , S. DAYAL, R.T. CLAY, Mississippi State University, H. LI, S. MAZUMDAR, University of Arizona — The effect of lattice frustration on two dimensional (2D) quantum spin models and the 2D half-filled Hubbard model has been intensively studied in order to understand the connections between antiferromagnetism (AFM), valence-bond ordered states, candidate spin-liquid states, and unconventional superconductivity. For several classes of unconventional superconductors, including the organic charge-transfer solids and superconducting spinels such as $LiTi_2O_4$, the correct starting point is however the quarter-filled rather than $\frac{1}{2}$-filled band. We present a study of the effect of frustration on the 2D $\frac{1}{4}$-filled interacting band. We demonstrate that in addition to the well known AFM state occurring with lattice dimerization, and Wigner crystal (WC) state, a paired insulating state occurs in the frustrated region of the phase diagram. This paired electron crystal (PEC) state has coexisting charge order and bond order and a spin-gap due to the formation of nearest-neighbor singlets in the pairs. We investigate fully the phase diagram, including effects of varying the strength of on-site and nearest-neighbor Coulomb interactions as well as electron phonon coupling strength. We present the full phase diagram showing the extent of AFM, PEC and WC phases.

[1]Supported by the DOE grant DE-FG02-06ER46315.

10:24AM A22.00013 The Paired Electron Crystal in quarter-filled organic superconductors[1] , R.T. CLAY, S. DAYAL, Mississippi State University, H. LI, S. MAZUMDAR, University of Arizona — In the 2D organic superconductors the underlying carrier density in the conducting layers is 1/2 electron per molecule. Because molecules often occur in dimer pairs, an effective model is frequently used with one electron per dimer. With strong electron-electron correlations, this effective model describes the occurrence of antiferromagnetism. Because of lattice frustration, κ-$(ET)_2Cu_2(CN)_3$ and other organics have been suggested to have spin liquid ground states. Recent experiments however have found strong lattice effects at low temperature in this material and raised uncertainty whether excitations are gapped or gapless. We argue that to resolve these issues one must go beyond the effective dimer model and instead start from the underlying 1/4-filled band. We have recently shown that in 2D 1/4-filled strongly correlated systems a commensurate insulating state forms that we have termed a Paired Electron Crystal (PEC). While in the antiferromagnetic state charge densities are uniform within a dimer, in the spin-gapped PEC state dimer charges become unequal and pairs of charge-rich sites are separated by pairs of charge-poor sites. We review the PEC concept and explain how it can provide a unified theoretical view of the 2D organics.

[1]Supported by DOE grant DE-FG02-06ER46315.

10:36AM A22.00014 Oscillating magnetothermopower in a Q2D organic conductor[1] , DANICA KRSTOVSKA, Ss. Cyril and Methodius University, Skopje, Macedonia and National High Magnetic Field Lab/FSU, Tallahassee, FL, USA — The beating oscillations of the interlayer thermopower with a large amplitude on both the magnetic field magnitude and an angle between the normal to the Q2D layer plane and the magnetic field are shown to occur when the cyclotron energy is comparable with the interlayer transfer integral. It is found that, in a Q2D organic conductor with a simple slightly warped FS, the amplitude of the quantum oscillations of the interlayer thermopower substantially exceeds the amplitude of its classical part due to the presence of features of the DoS of the charge carriers when their energy spectrum is quantized. The semi-classical Boltzmann theory predicts that the position of the beats in the magnetic oscillations of the interlayer thermopower are shifted with respect of those in the interlayer magnetoresistance. The shift is even bigger with increasing magnetic field. It might be expected that the difference between the beats in the interlayer thermopower and Shubnikov de Haass angular oscillations is not magnetic field dependent. However, experiments will be necessary for more detailed analysis of the magnetothermopower in Q2D organic metals to be made.

[1]I would like to thank the Fulbright Program for the financial support to this work.

Monday, March 21, 2011 8:00AM - 11:00AM –
Session A23 DCMP: Superconductivity: ARPES on BSCCO and SRO D165

8:00AM A23.00001 Deviation from $d_{x^2-y^2}$ gap form in Bi2201 revealed by photon-energy-dependent ARPES study , MAKOTO HASHIMOTO, SLAC, RUIHUA HE, LBNL, ROB MOORE, DONGHUI LU, SLAC, YOSHIYUKI YOSHIDA, HIROSHI EISAKI, AIST, ZAHID HUSSAIN, LBNL, ZHI-XUN SHEN, Stanford University — Previous ARPES studies on optimally doped cuprate superconductor Bi2201 with moderate incident photon energies ($>$ 20 eV) reported that the gap function deviates from simple $d_{x^2-y^2}$ functional form in the antinode, implying that the pseudogap is different from superconductivity. On the other hand, some other ARPES studies using low photon energies ($<$ 10 eV) found that simple $d_{x^2-y^2}$ functional form extends to the antinode, suggesting that the pseudogap has the same origin as superconductivity. We study this contradiction by photon-energy-dependent ARPES. We show that, at low photon energies, background signal is dominant in the antinode and conceals the true gap magnitude. This confirms that the gap function in optimally doped Bi2201 is not simple $d_{x^2-y^2}$ functional form, and supports that the pseudogap is different order from simple superconductivity.

8:12AM A23.00002 Laser-ARPES studies on Bi-2212 , I.M. VISHIK, W.-S. LEE, F. SCHMITT, Stanford University, T. SASAGAWA, Tokyo Institute of Technology, S. ISHIDA, University of Tokyo, K. FUJITA, Cornell University, S. UCHIDA, University of Tokyo, T.P. DEVEREAUX, Z.-X. SHEN, Stanford University — Temperature-dependent ARPES measurements of the gap function in $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi-2212) have given support for a 'two-gap' picture, where superconductivity and the pseudogap represent competing states, but the dichotomy between these gaps in momentum space and temperature is subtle. For instance, the pseudogap is observed by spectroscopy even below T_c, and ARPES observes superconducting quasiparticles in Bi-2212 even in the antinodal region, where the pseudogap is dominant. Thus, the gap measured at a particular momentum may contain contributions from both states. We have performed laser ARPES measurements on underdoped Bi-2212, using the superior energy resolution of this technique in conjunction with a detailed doping-and-temperature-dependence study, to elucidate the relative contributions of the pseudogap and superconducting gap at different temperatures and momenta. We report our findings on how the superconducting gap evolves into the pseudogap for various dopings.

8:24AM A23.00003 Structural origin of apparent Fermi surface pockets in angle-resolved photoemission of $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$, PHIL D.C. KING, W. MEEVASANA, University of St Andrews, J.A. ROSEN, University of British Columbia, A. TAMAI, E. ROZBICKI, University of St Andrews, R. COMIN, G. LEVY, D. FOURNIER, University of British Columbia, Y. YOSHIDA, H. EISAKI, NIAIST, Tsukuba, K.M. SHEN, Cornell University, N.J.C. INGLE, A. DAMASCELLI, University of British Columbia, F. BAUMBERGER, University of St Andrews — We observe *apparent* hole pockets in the Fermi surfaces of single-layer Bi-based cuprate superconductors from angle-resolved photoemission (ARPES). However, from an analysis of their polarization-dependence and detailed low-energy electron diffraction measurements, we show that these are not intrinsic, but due to multiple overlapping superstructure replicas of the main and shadow bands. We demonstrate that the hole pockets reported recently from APRES [Meng *et al.*, Nature **462**, 335 (2009)] have a similar structural origin, and are inconsistent with an intrinsic hole pocket associated with the electronic structure of a doped CuO_2 plane. The true nature of the Fermi surface topology in the enigmatic pseudogap phase therefore remains an open question.

8:36AM A23.00004 Photoemission Evidence for New Microscopic Scaling Relation in the Cuprate Superconductors[1] , JONATHAN RAMEAU, ZHIHUI PAN, HONGBO YANG, GENDA GU, PETER JOHNSON, Brookhaven National Laboratory — We use angle resolved photoemission spectroscopy (ARPES) to investigate the relationship between the superconducting gap at low temperature and the quasiparticle scattering rates in the normal state, on the Fermi arc, for optimal and underdoped Bi2212 cuprate high temperature superconductors. Combining these results with similar data on Bi2201 from the literature we find evidence of a new and simple microscopic scaling relation connecting the normal and superconducting states of the cuprates. The result suggests that while nodal-region Cooper pairs decohere above T_c they retain the signature of a strong pairing amplitude. The anomalous momentum dependence of excitation lifetimes on the Fermi arc, above T_c, are dominated by the same interactions that induce superconductivity at and below T_c.

[1]Supported by the Office of Science, Department of Energy

8:48AM A23.00005 Evidence for Strong Forward Scattering and Coupling to Acoustic Phonon Modes in the High-Tc Cuprates[1] , STEVEN JOHNSTON, IFW Dresden., I.M. VISHIK, W.S. LEE, Stanford University, F. SCHMITT, Stanford Universtiy, S. UCHIDA, University of Tokyo, K. KUJITA, Cornell University, S. ISHIDA, N. NAGAOSA, University of Tokyo, Z.X. SHEN, T.P. DEVEREAUX, Stanford University — The improved resolution of laser ARPES has revealed the presence of a new low-energy kink in the nodal dispersion of $Bi_2Sr_2Ca_2Cu_2O_{8+\delta}$, occuring at an energy below the maximum of the superconducting gap. This observation makes it difficult to interpret this renormalization in terms of coupling to any sharp bosonic modes. We examine coupling to the in-plane acoustic phonon branch via the modulation of the screened Coulomb interaction as an alternative explanation. We demonstrate that such a coupling is strongly peaked in the forward scattering direction and the resulting kink occurs at an energy shifted by the local gap $\Delta(\mathbf{k})$. Considerations for the reduction in screening with underdoping also provides a mechanism for understanding the doping dependence of the kink. These results indicate the importance of coupling to the acoustic branch with a strong forward scattering peak with important implications for the cuprates.

[1]Supported by the US Department of Energy under contract No. DE-AC02-76SF00515 and No. DE- FG03-01ER45929-A001.

9:00AM A23.00006 The single-particle self-energy and fluctuation spectrum of slightly underdoped Bi2212 from ARPES experiment , JIN MO BOK, JAE HYUN YUN, HAN-YONG CHOI, SungKyunKwan Univ., WENTAO ZHANG, X.J. ZHOU, Chinese Academy of Sciences, CHANDRA M. VARMA, University of California, SUNGKYUNKWAN UNIV. TEAM, CHINESE ACADEMY OF SCIENCES TEAM, UNIVERSITY OF CALIFORNIA TEAM — We extract the single particle self-energy $\Sigma(\theta,\omega)$ and Eliashberg function $\alpha^2F(\theta,\omega)$ of normal and superconducting state Bi2212 from ARPES experiments. The self-energies along the cuts at tilt angle θ were extracted by fitting ARPES momentum distribution curves. Then, using the extracted self-energy as input, the Eliashberg function is deduced by inverting the d- wave Eliashberg equation employing the adaptive maximum entropy method (MEM). The momentum dependence of self-energy was decomposed in terms of $\Sigma(\theta,\omega) = \Sigma_0(\omega) + \Sigma_4(\omega)cos4\theta$ at 16, 70, 80, 97, and 107 K. We will present the temperature evolution and momentum dependence of the deduced Eliashberg function and self-energy.

9:12AM A23.00007 Emergence of superconductivity in HighTc copper oxide superconductors via two crossovers , UTPAL CHATTERJEE, MIKE NORMAN, Argonne National Laboratory, MOHIT RANDERIA, Ohio State University, STEPHAN ROSENKRANZ, JUAN CARLOS CAMPUZANO, Argonne National Laboratory — From our detailed ARPES measurements on BISCO 2212 High Tc Superconductors we found that unlike in conventional superconductors, where there is a single temperature scale Tc separating the normal from the superconducting state, HTSCs exhibit with two additional temperature scales. One is T*, below which electronic excitations are gapped. And the other one is Tcoh, below which electronic states are long-lived. We observed that T* and Tcoh change strongly with doping. They cross each other near optimal doping. There is a region in the normal state where the single particle excitations are gapped as well as coherent. Quite remarkably, this is the region from which superconductivity with highest Tc emerges. Our experimental finding that the two crossover lines intersect is not consistent with a "single quantum critical" point near optimal doping, rather it is more naturally consistent with theories of superconductivity for doped Mott insulators.

9:24AM A23.00008 Low energy kink in the band dispersions of Sr_2RuO_4 studied by ARPES , CHUL KIM, Institute of Physics and Applied Physics, Yonsei University, CHOONGHYUN KIM, epartment of Physics and Astronomy, Seoul National University, Y.Y. KOH, Institute of Physics and Applied Physics, Yonsei University, JAEJUN YU, epartment of Physics and Astronomy, Seoul National University, M. ARITA, K. SHIMADA, Hiroshima Synchrotron Radiation Center, Hiroshima University, Y. YOSHIDA, National institute of Advanced Industrial Science and Technology, C. KIM, Institute of Physics and Applied Physics, Yonsei University — In Sr_2RuO_4 , incommensurate antiferromagnetic fluctuations (IAF) were reported to have 4 - 10 meV energy with $\mathbf{q} = (0.6\pi, 0.6\pi)$ while the lowest optical phonon is at 12meV. If an electron is coupled to AIF in Sr_2RuO_4, the electronic band dispersions will kink below 10meV. Then, one can attribute the low energy kinks below 10meV to the electron-IAF coupling. In spite of the fact that multiple kink energies were recently reported in Sr_2RuO_4, kinks below 10meV has not been observed. To look for the so far unobserved electron-IAF coupling in Sr_2RuO_4, we performed ultra high resolution angle resolved photoemission (ARPES) experiments on Sr_2RuO_4 with clean surfaces. In the results, we observe kinks in the band dispersions at energies below 10 meV which show strong momentum dependence. To elucidate the origin of these new kinks, we compare ARPES results with inelastic neutron scattering and band calculation results.

9:36AM A23.00009 ARPES lineshapes, coherent to incoherent ratios, and the waterfall self-energy of Bi2212 cuprate superconductors , QIANG WANG, ZHE SUN, TANMOY DAS, ALEXANDER BALATSKY, ELI ROTENBERG, HELMUTH BERGER, HIROSHI EISAKI, YOSHIHIRO AIURA, DANIEL DESSAU — We report a detailed lineshape analysis of ARPES data on Bi2212 in which we separate out the sharp coherent peaks from the higher energy incoherent "background" portions, which includes and makes up the famous waterfall regions. We find that the ratio of the incoherent to coherent weights scales quadratically with the peak energy of the coherent portion of the spectra over a very wide energy range. We show that this behavior, including the waterfalls, can be understood with a simple model electron self-energy, giving a new and powerful experimental tool for determining self-energy effects in correlated electron systems.

9:48AM A23.00010 Effects of a particle-hole asymmetric pseudogap on Bogoliubov quasiparticles in ARPES , J.P.F. LEBLANC, University of Guelph, J.P. CARBOTTE, Mcmaster University, E.J. NICOL, University of Guelph — Motivated by recent angle-resolved photoemission experiments (ARPES) on the underdoped cuprates [1], we show that the particle-hole asymmetry of the pseudogap energy bands acts to reveal new spectral peaks due to Bogoliubov quasiparticles in the superconducting state. With sufficient broadening, the Bogoliubov peaks will merge with existing peaks and will lead to the anomalous observation, seen in experiment, that the carrier spectral density appears to broaden with reduced temperature. Using the resonating valence bond (RVB) spin liquid model [2], we compare with recent experimental data to empirically determine the temperature dependence of the pseudogap. Further, we demonstrate that the d-density wave model cannot explain the same data.

[1] Hashimoto et al. Nature Physics **6** 414.
[2] K.Y Yang, T.M. Rice and F.-C. Zhang, PRB **73** 17541 (2006).

10:00AM A23.00011 Intrinsic Scattering Rates and the "Filling" Gap of Bi2212 , T.J. REBER, N.C. PLUMB, Z. SUN, Y. CAO, Q. WANG, Univ. of Colorado, H. IWASAWA, M. ARITA, HiSor, J.S. WEN, Z.J. XU, G. GU, Brookhaven National Lab, Y. YOSHIDA, H. EISAKI, Aist Tsukuba Central, Y. AIURA, Hiroshima Synchrotron Radiation Center, D.S. DESSAU, Univ. of Colorado — As a direct measure of the electronic interactions in a solid, knowledge of the electronic scattering rates is essential for understanding a material's behavior. Since angle resolved photoemission spectroscopy (ARPES) can probe an individual momentum state, it holds great promise for the most detailed and accurate measurements of the k-dependent electron scattering rates. Unfortunately, the scattering rates determined from ARPES are typically an order of magnitude greater than those obtained from other probes, (e.g. optical spectroscopy). Here we present a new type of spectrum, the ARPES tunneling spectrum (ATS), which resolves this discrepancy, as well as provides a qualitatively different understanding of the gaps and scattering rates along the Fermi surface. Applying this technique to the study of Bi2212, we find that the scattering rates are approximately independent of Fermi surface position but grow exponentially with temperature. Furthermore, we find that this strongly temperature dependent scattering rate is the source of the long observed but not understood "filling" of the superconducting gap in the cuprates.

10:12AM A23.00012 Pairing fluctuations determine low energy electronic spectra in cuprate superconductors , SUMILAN BANERJEE, Department of Physics, Indian Institute of Science, Bangalore-560012, India, TIRUPPATTUR RAMAKRISHNAN, Department of Physics, Banaras Hindu University, Varanasi-221005, India, CHANDAN DASGUPTA, Department of Physics, Indian Institute of Science, Bangalore 560012, India — Over the years, Angle Resolved Photo Emission Spectroscopy (ARPES) has uncovered a number of unusual spectral properties of near Fermi energy electrons with definite in-plane momenta in the hole doped cuprates. We describe here a minimal theory of tight binding electrons moving on the square planar Cu lattice of the cuprates, mixed quantum mechanically with pairs of them (Cooper pairs); superconductivity occurring at T_c is their long range (d-wave symmetry) phase coherence. Fluctuations necessarily associated with incipient long range superconducting order have a generic large distance behavior near T_c. We calculate the spectral density of electrons coupled to such Cooper pair fluctuations and show that properties observed in ARPES above T_c for different cuprates as a function of doping x and temperature T emerge inevitably; e.g. the 'Fermi arcs' with T dependent length and an antinodal pseudogap which fills up linearly as T increases towards the pseudogap temperature T^*. Below T_c, the effects of nonzero superfluid density and thermal fluctuations are calculated and compared successfully with experiment.

10:24AM A23.00013 The0ry 0f Dipolon-Phonom Interaction and Isotope Shift in Superconducting Cuprates , RAM SHARMA, University of Illinois at Chicago — Quite recently we have deduced five principles of photoemission and not only we have explained the observed low energy kink but we have also predicted two more high energy kinks [1,2] in quasiparticle energydistribution which have now been observed experimentally, all by means of the dipolon theory [3,4]. Here, the Hamiltonian for the interaction of dipolons with phonons will be presented.The Hamiltonian requires the evaluation of phonon-generated dynamic polarization fields at the oxygen sites in the $Cu-O_2$-planes. The quasi-dipolons (phonon-dressed dipolons) now play role as mediators of electron-electron pairing. Expression for the change in the transition temprature T_C due to change in oxygen isotopic mass has been derived. We have found a small decrease of about 1 per cent in T_C due to $^{16}O \rightarrow ^{18}O$, in agree ment with experiments [5]. The change in dipolon frequencies owing to the interaction with phonons has been calculated. [1] R. R. Sharma, "Dipolon Theory of Kink Structure.....", in Superconducting Cuprates....", Ed. K. N. Courtlandt, P. 81-100, Nova Sc, Pub., New York, 2009. [2] R. R. Sharma, Physica **C 468**, 190 (2008). [3] R. R. Sharma, Phy. Rev. **B 63**, 054506 (2001). [4] R. R. Sharma, Physica **C 439**, 47 (2006). [5] J. p. Franck in Physical Properties.....IV, Ed. D. M. Ginsberg, P. 189-293,World Scientific, Singopore, 1994.

10:36AM A23.00014 New Fermi Surface Sheets Revealed in Sr2RuO4 Revealed by High Resolution Angle-Resolved Photoemission Spectroscopy , SHANYU LIU, WENTAO ZHANG, LIN ZHAO, HAIYUN LIU, XIAOWEN JIA, DAIXIANG MU, GUODONG LIU, XIAOLI DONG, JUN ZHANG, XIAOYANG WANG, QINJUN PENG, ZHIMIN WANG, SHENJIN ZHANG, FENG YANG, Z. Q. MAO, CHUANGTIAN CHEN, ZUYAN XU, X. J. ZHOU, NATIONAL LABORATORY FOR SUPERCONDUCTIVITY, BEIJING NATIONAL LABORATORY FOR CONDENSED MATTER PHYSICS, TEAM[1], TECHNICAL INSTITUTE OF PHYSICS AND CHEMISTRY, CHINESE ACADEMY OF SCIENCES, BEIJING 100190, CHINA COLLABORATION, DEPARTMENT OF PHYSICS, TULANE UNIVERSITY, NEW ORLEANS, LOUISIANA 70118, USA COLLABORATION — We will present our detailed Fermi surface measurements on Sr2RuO4 by high resolution angle-resolved photoemission spectroscopy (ARPES) including vacuum ultra-violet (VUV) laser-based ARPES. In addition to the three sets of Fermi surface sheets originating from the bulk bands, the surface bands and the shadow bands of the surface bands, we have revealed two new Fermi surface sheets. The origin of these new Fermi surface sheets will be discussed.

[1]Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

10:48AM A23.00015 Anisotropic mass renormalization in Sr2RuO4 , E.J. ROZBICKI, A. TAMAI, P.D.C. KING, Univ. of St Andrews, W. MEEVASANA, Suranaree Univ.of Technology, A. GIBBS, D.G. SLOBINSKY, A.P. MACKENZIE, F. BAUMBERGER, Univ. of St Andrews — The layered perovskite Sr_2RuO_4 continues to attract interest as a model system of a multiband Fermi liquid. Previous dHvA and ARPES studies successfully determined its Fermi surface [1, 2] and reported a large and sheet dependent renormalization of the Fermi velocity due to electron-electron interactions with v_{band}/v_F ranging from ≈ 3 for the $d_{xz/yz}$ derived α and β sheets to ≈ 5.5 for the γ sheet with dominant dxy orbital character [1, 3]. Here, we report new high-resolution ARPES data revealing an additional strong momentum dependence of the renormalization within a single Fermi surface sheet. This effect is most pronounced in the γ band and is larger than expected from the mixing of the orbital composition along individual Fermi surface sheets induced by spin-orbit coupling [4,5]. Our observations therefore provide evidence for a genuinely momentum dependent self-energy in the vicinity of a van Hove singularity.
[1] C. Bergemann et al., Advances in Physics 52, 639 (2003)
[2] A. Damascelli et al., Physical Review Letters 85, 5194 (2000).
[3] K.M. Shen et al., Physical Review Letters 99, 187001 (2007).
[4] M.W. Haverkort et al., Phys Rev Lett. 101, 026406 (2008)
[5] J. Mravlje et al., arXiv:1010.5910v1(2010)

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A24 DCOMP: Computational Methods I: Numerical Methods for Strongly Correlated Systems D167

8:00AM A24.00001 Modeling pump-probe spectroscopy in systems with electron-phonon coupling[1] , ALEXANDER F. KEMPER, BRIAN MORITZ, THOMAS P. DEVEREAUX, Stanford University — In pump-probe experiments, the electronic system is driven out of equilibrium by the application of a strong electric field. Phonons are of critical importance in returning the system to its original state, as they dissipate the energy introduced by the field. Using the non-equilibrium Keldysh formalism, we study how phonons affect the electronic current and energy in the Migdal limit, for both pulsed and continuous fields, and how this affects various spectroscopic measurements. Finally, we consider charge density- wave systems and their behavior in pump-probe experiments.

[1]Supported under DOE Contract No. DE-AC02-76SF00515

8:12AM A24.00002 Pulsed-field pump-probe response in correlated systems[1] , B. MORITZ, T.P. DEVEREAUX, SLAC National Accelerator Laboratory and Stanford University, J.K. FREERICKS, Georgetown University — We describe pump-probe dynamics of the spinless Falicov-Kimball model subject to strong pulsed driving fields. The photoemission response shows a rapid evolution toward a new steady-state following decay of the pump pulse. We characterize the behavior by analyzing the power delivered to the system by the driving field and the corresponding change in the total energy. This prescription allows us to fit the result to an equilibrium response at a higher temperature determined self-consistently. For strong driving fields and correlations on the metallic side of the metal-insulator transition, the response can be described well by that of a system at a higher temperature; however, for correlations on the insulating side of the transition, the response in the nonequilibrium steady-state deviates significantly from that anticipated in quasi-thermal equilibrium.

[1]This work was supported by the U.S. DOE under Contract Nos. DE-AC02-76SF00515, DE-FG02-08ER46542, and DE-FG02-08ER46540.

8:24AM A24.00003 Numerical study of interacting systems driven by a constant electric field , JANEZ BONCA, J. Stefan Institute, 1000 Ljubljana, Slovenia and FMF, University of Ljubljana, 1000 Ljubljana, Slovenia, LEV VIDMAR, J. Stefan Institute, 1000 Ljubljana, Slovenia, MARCIN MIERZEJEWSKI, Institute of Physics, University of Silesia, 40-007 Katowice, Poland, PETER PRELOVSEK, J. Stefan Institute, 1000 Ljubljana, Slovenia and FMF, University of Ljubljana, 1000 Ljubljana, Slovenia, STUART TRUGMAN, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — I will present a fundamental study of a Holstein polaron in one dimension and a single hole in the two dimensional t-J model driven away from the equilibrium by a constant electric field. Taking fully into account quantum effects we follow the time-evolution of systems from their ground state as the constant electric field is switched on at t=0, until they reach a steady state. At small electron phonon coupling (EP) the Holstein polaron experiences damped Bloch oscillations (BO) characteristic for a free electron band. An analytic expression of the steady state current is proposed in terms of EP coupling and electric field. We as well analyze the shape of the phonon tail that forms behind the traveling polaron. In the case of the t-J model we demonstrate that there exist three distinct regimes of the electric field (adiabatic, dissipative and the BO regime) which differ with respect to the real-time response. The d.c. current is shown to be maximal for a finite value of the electric field.

8:36AM A24.00004 Dependence of Condensate Formation in Graphene Bilayers on Relative Layer Orientation , XUEHAO MOU[1], DIPANJAN BASU, LEONARD REGISTER, SANJAY BANERJEE, The University of Texas at Austin — It has been recently predicted that condensates can form between paired n-type and p-type graphene layers separated by a dielectric at room temperature under certain conditions. Recent works by the authors have explored the dependence of the condensate on dielectric thickness, dielectric constant, and charge densities including charge imbalance. However, to date only adjacent layers with the same crystal orientation have been modeled, such that the Dirac cones in each layer are precisely aligned with each other. In practice, obtaining such orientational alignment across a thin dielectric may be problematic. Therefore, the design of experiments to either prove or disprove the theory, and of devices to exploit this room temperature condensation should it exist, may depend critically on orientation dependence. In this work, we will theoretically consider the effects of crystal rotation on the existence and strength of the condensate using mean-field theory much as in the original works on the subject.

[1]Contact:chris_mou@mail.utexas.edu

8:48AM A24.00005 Self-consistent implementation of the multi-band Gutzwiller variational method: Formalism and combination with DFT , NICOLA LANATA', HUGO STRAND, University of Gothenburg, SE-412 96 Gothenburg, Sweden, XI DAI, Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, BO HELLSING, University of Gothenburg, SE-412 96 Gothenburg, Sweden — We have generalized the approach for solving the multi-band Gutzwiller variational problem with density-density interaction to an arbitrary local interaction. The main advantage of our formulation is that it allows for a self-consistent numerical implementation which doesn't require any additional computational effort as compared to the simpler case of density-density interaction. Combined with DFT and the Local Density Approximation (LDA+Gutzwiller) our method allows for ab-initio study of multi-band correlated materials with full (rotationally invariant) Hund's rule coupling. We briefly introduce the method and present applications to several systems of correlated electrons.

9:00AM A24.00006 Hole dynamics in a 2D doped quantum antiferromagnet within the non-crossing approximation , SATYAKI KAR, University of North Florida, EFSTRATIOS MANOUSAKIS, Florida State University; University of Athens, Greece — We study the doping evolution of the hole and magnon spectral functions of the two-dimensional $t-J$ and $t-t'-t''-J$ models by solving the Dyson's equations self-consistently within the non-crossing approximation. The doping dependence of the staggered magnetization and the hole spectral function are calculated for doping concentration where there is antiferromagnetic order for both of these models. We find that the intensity plot of the hole spectral function has characteristics similar to the "waterfall" features observed in the underdoped cuprates by ARPES.

9:12AM A24.00007 Exact quantum dynamics of spin systems using the positive-P representation , RAY NG, ERIK SORENSEN, McMaster University — We discuss a scheme for simulating the exact real time quantum dynamics of interacting quantum spin systems within the positive-P formalism. As model systems we study the transverse field Ising model as well as the Heisenberg model undergoing a quench away from the classical ferromagnetic ordered state. In using the positive-P representation (PPR), the dynamics of the interacting quantum spin system is mapped onto a set of stochastic differential equations (SDEs). The number of which scales linearly with the number of spins, N, compared to an exact solution through diagonalization that in the case of the Heisenberg model would require matrices exponentially large in N. This mapping is exact and can in principle be extended to higher dimensional interacting systems as well as to systems with an explicit coupling to the environment. We compare the results from using a PPR approach based on both the optical coherent states as well as SU(2) Radcliff coherent states.

9:24AM A24.00008 Stochastic evaluation of Bold diagrammatic series for interacting Fermion problems: application to equilibrium and non-equilibrium quantum impurity models[1] , EMANUEL GULL, DAVID R. REICHMAN, ANDREW J. MILLIS, Columbia University — We present the first implementation of a bold expansion, i.e. a numerical sampling of the diagrammatic corrections to an analytic resummation. Our method is based on an expansion around the non-crossing approximation. The method is exact and applicable to both equilibrium and non-equilibrium problems. In equilibrium we show results for the single impurity Anderson model. In the non-equilibrium case we study an interacting quantum dot coupled to two leads and present results for current and occupation numbers for up to three times larger timescales than are reachable using a bare expansion.

[1]David R. Reichman, Andrew J. Millis; NSF-DMR-0705847

9:36AM A24.00009 Non-Local Corrections to the Dynamical Mean Field Theory for the Hubbard Model , HERBERT FOTSO, Department of Physics and Astronomy, Louisiana Sate University, SHUXIANG YANG, KA-MING TAM, JUANA MORENO, MARK JARRELL, Department of Physics and Astronomy, Louisiana State University, HARTMUT HAFERMANN, Centre de Physique Theorique, Ecole Polytechnique, Paris, France, DEPARTMENT OF PHYSICS AND ASTRONOMY, LOUISIANA STATE UNIVERSITY COLLABORATION, CENTRE DE PHYSIQUE THEORIQUE, ECOLE POLYTECHNIQUE, PARIS, FRANCE COLLABORATION — We use the diagrammatic parquet formalism to calculate the non-local corrections to the Dynamical Mean Field Theory ($DMFT$) solution for the two-dimensional Hubbard model. The Dynamical Mean Field Theory vertex and Green's function are used as input to calculate the Feynman diagrams on a finite size cluster. This approach properly addresses the local as well as the short-range correlations, as illustrated by the agreement of the obtained local moment and the Neel critical temperature with Quantum Monte Carlo calculations on a 4x4 cluster.

9:48AM A24.00010 Regularization of Diagrammatic Series with Zero Convergence Radius , BORIS SVISTUNOV, University of Massachusetts, Amherst, LODE POLLET, ETH, Zurich, NIKOLAY PROKOF'EV, University of Massachusetts, Amherst — The divergence of perturbative expansions which occurs for the vast majority of macroscopic systems and follows from Dyson's collapse argument, prevents the direct use of Feynman's diagrammatic technique for controllable studies of strongly interacting systems. We show how the problem of divergence can be solved by replacing the original model with a convergent sequence of successive approximations which have a convergent perturbative series while maintaining the diagrammatic structure. As an instructive model, we consider the zero-dimensional $|\psi|^4$ theory. We believe that this approach opens up an opportunity to utilize Feynman's diagrams as a generic tool to address strongly correlated classical- and quantum-field systems, especially in the context of Diagrammatic Monte Carlo.

10:00AM A24.00011 Discretization of the imaginary-time Greens function , ANDRO SABASHVILI, MATS GRANATH, HUGO STRAND, STELLAN OSTLUND, Gothenburg University — Finite temperature Greens functions are defined on an infinite set of Matsubara frequencies. A well known numerical difficulty is that the discontinuity in the Greens function in the imaginary time domain generates a long tail in the frequency representation which makes truncating a numerical calculation to to finite numbers of frequencies difficult. We have explored a particular "periodization" procedure designed to (1) close the Greens function approximation with a finite and relatively small number of Matsubara frequencies and (2) to be consistent with the Ward-Luttinger-Baym-Kadanoff variational principle. In addition to describing our truncation procedure we will show results of applying the method to standard DMFT calculations. We obtain results that are consistent with other well known but numerically more complex methods.

10:12AM A24.00012 A general method for testing validity of one-particle spectral functions , JUN LIU — Based on the fact that the one-particle spectral function is uniquely extracted from a temperature Green function, a scheme is proposed to test the validity of a one-particle spectral function derived from any temperature Green function of any interacting system under thermal equilibrium. The physical implication of the scheme is discussed. An example is worked out to explicitly show the effectiveness of the scheme.

10:24AM A24.00013 DMRG Study of the $S = 1/2$ Kagome Antiferromagnetic Heisenberg Model , SIMENG YAN, UCI, STEVEN WHITE, DAVID HUSE — Recently we have completed a density matrix renormalization group (DMRG) study of the spin-$\frac{1}{2}$ Kagome antiferromagnetic Heisenberg model. We studied a variety of cylindrical geometries, with widths up to 12 lattice spacings and total sizes up to 400-500 sites. We found a spin liquid ground state with much lower energies than the valence bond crystal found using other approaches. Our energies are variational except for very tiny edge effects, and are comparable to Lanczos energies on 36 or 42 site. The spin liquid can be viewed as a melted valence bond crystal formed from 8 site diamond loops and dimers, with a 12 site unit cell, called the "diamond pattern." In this talk we will focus on the narrowest cylinders, in particular a cylinder with a circumference of 4 lattice spacings which accomodates the diamond pattern, but for which the spin liquid ground state, while metastable in DMRG, is higher in energy than another state with a "topological string" and a resulting "valence bond density wave" broken translational symmetry. We discuss singlet and triplet gaps relative to these two states. The peculiar behavior of this narrow cylinder is presumably due to short resonance loops around the cylinder.

10:36AM A24.00014 DMRG-optimized NRG treatment of sub-ohmic spin-boson model[1] , CHENG GUO, ANDREAS WEICHSELBAUM, Physics Departement of LMU Munich, MATTHIAS VOJTA, Institute for Theoretical Physics, University Cologne, JAN VON DELFT, Physics Departement of LMU Munich — The sub-ohmic spin-boson model exhibits an interesting and much-studied quantum phase transition from a delocalized phase at weak spin-bath coupling to a localized phase at strong coupling. Previous works using NRG to calculate the critical exponents of this model near the phase transition failed partly because it cannot deal with the large number of states per bath oscillator required to describe the localized phase [1]. We show how this problem can be overcome by using DMRG to construct, for each site of the Wilson chain, an optimized boson basis containing only a small number of states, and using the resulting basis for standard NRG calculations. Our results are in good agreement with analytical predictions for this model. The approach presented here should be generalizable to other quantum impurity models with complex baths.

[1] M. Vojta, N.-H. Tong, R. Bulla, Quantum Phase Transitions in the Sub-Ohmic Spin-Boson Model: Failure of the Quantum-Classical Mapping, Phys. Rev. Lett. 94, 070604 (2005); Erratum: Phys. Rev. Lett., 102, 249904 (2009)

[1]We acknowledge support from the CeNS-IDK graduate program, and SFB631 of the DFG.

10:48AM A24.00015 Resonant Inelastic X-ray Scattering in the Falicov-Kimball model[1] , NANDAN PAKHIRA, JAMES FREERICKS, Georgetown University, ANDRIJ SHVAIKA, Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine — We calculate Resonant Inelastic X-ray Scattering (RIXS) spectra in the Falicov-Kimball model. Using Dynamical Mean Field Theory (DMFT) we do a detailed study of the RIXS response as a function of incident photon energy (ω_{in}) or photon energy transfer (Ω) for various photon momentums transfer ($\mathbf{q}$), temperature and other parameters of the model. We also calculate the dynamic structure factor, $S(\mathbf{q}, \Omega)$, for this model and study its possible relation with the RIXS spectra. We find that for large incident photon energy (much larger than the resonant energy) the resonant contribution to RIXS spectra essentially vanishes and $S(\mathbf{q}, \Omega)$ is proportional to the non-resonant part of the response. Finally, time permitting, we will also present Auger life time broadening effects on the RIXS spectra.

[1]Research supported by DOE, CMSN Grant No. DE-FG02-08ER46540 and DOE Grant No. DE-FG02-08ER46542

Monday, March 21, 2011 8:00AM - 10:48AM –
Session A25 DCMP: Superconductivity: Phases and Phase Transitions D166

8:00AM A25.00001 Two-dimensional Quantum Critical Point in Underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$, THOMAS LEMBERGER, JIE YONG, ANDREW MCCRAY, The Ohio State University, MUNTASER NAAMNEH, AMIT KANIGEL, Technion - Israel Inst. of Technology, MOHIT RANDERIA, The Ohio State University — Underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ films with T_c's from 5 to 70 K are fabricated by sputtering and Pulsed Laser Deposition (PLD). Temperature dependences of superfluid densities are measured to study the superconductor-to-insulator quantum phase transition. Sputtered films, which tend have higher dopings, show superfluid densities that are weakly linear in T at low-T and drop dramatically where Kosterlitz-Thouless-Berezinski theory predicts, assuming that individual CuO_2bilayers are uncoupled. However, our PLD films, which are more underdoped than the sputtered films, have superfluid densities that are roughly linear from low T to T_c. Also, There is no indication of thermal critical behavior near T_c. Underdoped YBCO crystals also lack critical behavior, even though critical behavior is strong in optimally doped and moderately underdoped samples. Near the superconductor-to-insulator phase transition, T_c and $n_s(0)$ have a linear relationship that mimics that of ultrathin, two-dimensional films of Ca-doped $YBa_2Cu_3O_{7-\delta}$, thereby indicating a 2-D quantum critical point at low doping.

8:12AM A25.00002 Magnetoresistance Peak in Quench Deposited Ultra-Thin Amorphous Bismuth Films[1] , YEN-HSIANG LIN, ALLEN GOLDMAN, School of Physics and Astronomy, University of Minnesota, SCHOOL OF PHYSICS AND ASTRONOMY, UNIVERSITY OF MINNESOTA TEAM — A magnetoresistance peak in perpendicular magnetic field has been found on the insulating side of the thickness-tuned superconductor-insulator (SI) transition of quench-deposited amorphous bismuth films. The presence of a peak suggests the presence of local superconductivity in these insulating films. Arrhenius type conduction and non-linear I-V characteristics are also observed in the peak regime. The magnitude of this magnetoresistance peak increases substantially with decreasing temperature and with increasing film thickness. The dependence of the peak magnetic field on temperature and thickness may help to explain the underlying mechanism of the magnetoresistance peak.

[1]This work is supported in part by the National Science Foundation under grant NSF/DMR-0854742.

8:24AM A25.00003 Chemical Activity in $YBa_2Cu_3O_{7-\delta}$ Acrosst the Transition to Superconductivity[1] , JUANA V. ACRIVOS, San Jose' State University — Changes in the Gibbs free enthalpy, chemical activity across the transition temperature to superconductivity T_c in $YBa_2Cu_3O_{7-\delta}$ is described by enhanced element X-Ray absorption XAS and diffraction XRD [HKL] reflections. Critical oscillations in the index of refraction within the XAS line width ($\pm$ 2.5eV) at the Ba L2, L3 and Y K-edges observed $\sim$30K above $T_c \approx$93K in [HKL] reflections indicates their activity. Enhanced absorbance A versus T obtains the activation enthalpy and entropy: $\Delta H^{\neq}_{>}$=-220 meV, $\Delta S^{\neq}_{>}$=-2 meV/K ($121 \geq T \geq 93$K) for mixed normal and superconducting phases, which compensates the reported O atom ordering activation energy near T_c by 50 meV. The activation needed to mix differently ordered superconducting phases: $\Delta H^{\neq}_{<}$= -67 meV, $\Delta S^{\neq}_{<}$ = -1 meV/K ($60K \leq T \leq 93$K) indicates lattice ordering persists to 60K. Enhanced XRD scattering induced near the transition to superconductivity in 3D solids indicates that the role of 2D reactive [HKL] planes is similar to the chemical activity of reactive linear bonds in molecular reactions.

[1]Supported by NSF, Dreyfus and DOE Laboratories, SSRL-SLAC and LBL-ALS.

8:36AM A25.00004 Unitarity in periodic potentials and correlated s-wave Cooper pair insulators , PREDRAG NIKOLIC, George Mason University, ZLATKO TESANOVIC, Johns Hopkins University — We explore the emergence of novel universal regimes and correlated states in strongly interacting band insulators. Lattice potentials introduce Cooper, exciton and inter-valley channels for scattering resonances, which can be studied in the BCS-BEC framework. This is revealed by characterizing a large number of renormalization group fixed points. The superfluid-insulator transition is found to be pair-breaking in the weak-coupling BCS limit, while it belongs to the bosonic mean-field or XY universality class in the strong-coupling BEC limit as fermionic excitations remain gapped. The latter leads to correlated bosonic Mott insulators of Cooper pairs, and is the only option in two dimensions. Such an insulator may break lattice symmetries, but even if it doesn't it can be sharply distinguished from the band insulator out of equilibrium. The models we study can be realized with ultra-cold gases of alkali atoms tuned to a broad Feshbach resonance in an optical lattice. We discuss possible consequences for cuprate superconductors, where antinodal pair dynamics has certain features in common with our simple s-wave picture.

8:48AM A25.00005 Cooper pair localization in a-Bi thin films near the superconductor-insulator transition[1] , S.M. HOLLEN, H.Q. NGUYEN, E. RUDISAILE, J. SHAINLINE, Brown University, Department of Physics, G. FERNANDES, J.M. XU, Brown University, Division of Engineering, J.M. VALLES, JR., Brown University, Department of Physics — Ultrathin films near the Superconductor-Insulator Transition (SIT) can exhibit Cooper pair transport in their insulating phase. This Cooper Pair Insulator state is achieved in amorphous Bi films patterned with a nanohoneycomb array of holes. We will present evidence from a number of experiments on these substrates supporting that 1) thickness variations, which result in variations in T_c and Δ, serve to localize the Cooper pairs; 2) the weak links between these superconducting islands control the SIT. Finally, we will discuss our most recent experiments that aim to characterize this Cooper pair insulator state and confirm the role of the thickness variations in the localization of Cooper pairs.

[1]This work was supported by the NSF through No. DMR-0907357, by the AFRL, and by the ONR.

9:00AM A25.00006 Study of granular two-band superconducting films: existence of a zero-temperature metallic phase , BOJUN YAN, TAI-KAI NG — A variational approach is used to study the zero-temperature phase transition of two-band granular superconducting films. For s+(-) superconductors with strong enough disorder, we show the plausible existence of a metallic phase between the superconducting and insulator phases which is absent in normal single band granular superconducting films. We propose that the metallic phase may be observed in granular films of pnictide superconductors. Novel possibilities such as charge 2e metal and "topological metal" are also discussed.

9:12AM A25.00007 Phase diagram of electrostatically doped SrTiO3[1] , YEONBAE LEE, STEVE SNYDER, JACK HELLERSTEDT, COLIN CLEMENT, LAURA KINNISCHTZKE, JOSEPH KINNEY, ALLEN GOLDMAN, School of Physics, University of Minnesota, UNIVERSITY OF MINNESOTA TEAM — We report on the properties of electrostatically doped SrTiO3 over broad ranges of temperature and carrier concentration. Electrostatic doping has been carried out with the use of an electric double layer transistor employing an ionic liquid as a gate dielectric. The result is an apparent carrier-density dependent metal insulator transition that may be associated with the reduction of the density of thermally excited carriers in the conduction band derived from shallow states in the band gap. This results in a phase diagram that is analogous to that found for cuprate superconductors, however, with superconductivity appearing at much lower temperatures. In addition for doping levels short of those inducing superconductivity, an anomalous Hall effect is observed, suggesting the appearance of ferromagnetism near the boundary between the insulating and superconducting regimes of the doping layer.

[1]This work was supported by the National Science Foundation under Grant No. NSF/DMR-0854752

9:24AM A25.00008 Thermodynamic signature for the phase transition at the pseudogap temperature in underdoped YBCO (6.56) , VICTOR FANELLI, National High Magnetic Field Laboratory, Los Alamos National Laboratory, SCOTT RIGGS, ARKADY SHEKHTER, National High Magnetic Field Laboratory, Florida State University, YOKO SUZUKI, JONATHAN BETTS, ALBERT MIGLIORI, National High Magnetic Field Laboratory, Los Alamos National Laboratory, GREG BOEBINGER, National High Magnetic Field Laboratory, Florida State University, BRAD RAMSHAW, RUIXING LIANG, WALTER HARDY, DOUG BONN, Department of Physics and Astronomy, University of British Columbia — The physics of the pseudogap, and its connection to the strange metal phase remain poorly understood. The outstanding problem is whether the apparent crossover between these two regimes is a thermodynamic phase boundary. We performed high precision resonant ultrasound spectroscopy measurement on de-twinned monocrystals of underdoped YBCO (6.56) in a broad temperature range up to 300 K. We find a compelling thermodynamic signature for the phase transition at the pseudogap temperature T = 270 K.

9:36AM A25.00009 Signature of Aslamazov-Larkin fluctuation Hall conductivity in Tantalum Nitride films above their superconducting transition temperature , NICHOLAS BREZNAY, MIHIR TENDULKAR, AHARON KAPITULNIK, Stanford University, KAREN MICHAELI, M.I.T., ALEXANDER FINKEL'STEIN, Texas A&M University — We have studied the Hall effect in superconducting Tantalum Nitride films. We find a large contribution to the Hall conductivity near the superconducting transition, which we can track to temperatures well above Tc and magnetic fields well above the upper critical field, Hc2(0). This contribution arises from Aslamazov-Larkin superconducting fluctuations, and we find quantitative agreement between our data and theoretical analysis based on time dependent Ginzburg-Landau theory. We will also remark on the appearance of a sign change in the Hall effect and on the high field fluctuation conductivity in superconducting Tantalum and Indium Oxide thin films.

9:48AM A25.00010 Magnetic Phase Diagram of the electron-doped high-T_c superconductor $Nd_{2-x}Ce_xCuO_4$, M.K. CHAN[1], E.M. MOTOYAMA[2], G. YU[1], Y. LI[2], J.P. CARLO[3], T.J. WILLIAMS[4], S.K. KIM[3], T. GOKO[3,4], Y.J. UEMURA[3], G.M. LUKE[4], M. GREVEN[1], [1]University of Minnesota, [2]Stanford University, [3]Columbia University, [4]McMaster University — An intriguing issue in high-T_c superconductivity is the phase diagram asymmetry with respect to electron and hole-doping. The antiferromagnetic phase extends further with electron doping and appears to overlap with superconductivity. Our prior results suggested that genuine long-range antiferromagnetic order and superconductivity do not co-exist in $Nd_{2-x}Ce_xCuO_4$ [Motoyama *et al.* Nature 445, 186 (2007)]. However, some uncertainty remained due to Ce concentration inhomogeneity in large single crystals. Here we report neutron scattering and μSR measurements on crystals with improved Ce homogeneity. Inelastic neutron scattering indicates that genuine long-range antiferromagnetic order indeed disappears within a small doping window around x =0.12. Meanwhile, μSR measurements show that static magnetic order persists up to x = 0.14, where bulk superconductivity first unambiguously appears. Our results suggest a possible first-order phase transition in a narrow region of the phase diagram, between x = 0.12 and x =0.14, characterized by clusters of short-range static magnetic order and traces of superconductivity.

10:00AM A25.00011 Multiple Phase Transitions: Phase Diagram with Interacting Phase Boundaries of Different Order , BOHDAN ANDRAKA, PRADEEP KUMAR, University of Florida, AVADH SAXENA, Los Alamos National Laboratory — We present a thermodynamic discussion of the consequences of interacting phase boundaries. The particular focus here is when the superconducting phase boundaries are of different order in a phase diagram in the magnetic field-temperature (H-T) plane. Thus depending on the form of the dominant interaction, we derive thermodynamic observables such as specific heat, superfluid density (as could be measured by lower critical field) and thermal expansion as a function of field and temperature and especially their discontinuities at the phase boundaries. We suggest that these considerations have relevance for the superconducting transition and the phase diagram in PrOs4Sb12.

10:12AM A25.00012 Properties and behavior of superconductors exhibiting a Fulde-Ferrell-Larkin-Ovchinnikov phase[1] , WILLIAM A. CONIGLIO, CHARLES C. AGOSTA, Clark University — The body of data on the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state in 2d organic superconductors has grown to a critical mass where we may begin studying the boundaries of the FFLO phase in detail. In some very clean layered superconductors, when a magnetic field is aligned exactly parallel to the conducting layers, a superconducting phase develops at fields above the Pauli paramagnetic limit H_p and temperatures below about $T_c/3$. The phase is widely ascribed to FFLO behavior. We focus on the superconductors κ-(ET)$_2$Cu(NCS)$_2$, β''-(ET)$_2$SF$_5$CH$_2$CF$_2$SO$_3$, and λ-(BETS)$_2$GaCl$_4$, which have been studied by rf penetration depth and other techniques. We have probed the boundaries of the FFLO phase using alignment angle to tune the amount of spin-orbit scattering and temperature to control the degree of Pauli paramagnetic limiting. Using our data collected in pulsed magnetic fields at low temperature, we have gained new understanding about the behavior of the state and the conditions necessary for it to develop.

[1]We acknowledge Department of Energy support from ER46214.

10:24AM A25.00013 Exploration of the pressure-induced superconducting phase in rare-earth tritellurides (RTe$_3$)[1] , DIEGO A. ZOCCO, JAMES J. HAMLIN, M. BRIAN MAPLE, Department of Physics, University of California, San Diego, JIUN-HAW CHU, IAN R. FISHER, Department of Applied Physics, Geballe Laboratory for Advanced Materials, Stanford University — It has recently been reported that the low-dimensional rare-earth tritellurides RTe$_3$ (R = La-Nd, Sm, Gd-Tm) enter an unidirectional, incommensurate charge-density-wave (CDW) state when cooled below a temperature $T_{CDW1} \sim$ 450 - 250 K, which decreases with increasing rare earth atomic number, due to the effect of chemical pressure. For the heavier R (*i.e.*, Dy-Tm), a second CDW appears at $T_{CDW2} < T_{CDW1}$, orthogonal to the first one. We have recently found that the application of external pressure induces a superconducting (SC) state in TbTe$_3$ at low temperatures, coexisting with the two CDWs and the local moment rare-earth magnetism. In this talk, we present the results of experiments we have performed on these materials at high pressures and very low temperatures, to help develop an understanding of the origin of the superconducting state.

[1]UCSD: NNSA/SSAA DOE DEFG52-06NA26205 - Stanford: DOE DE-AC02-76SF00515

10:36AM A25.00014 Violation of Onsager reciprocity in underdoped cuprates? , VICTOR YAKOVENKO, University of Maryland, CHANDRA VARMA, University of California at Riverside, AHARON KAPITULNIK, Stanford University — One of the canons of condensed matter physics is the Onsager reciprocity principle for systems in which the Hamiltonian commutes with the time-reversal operator. Recent results of measurements of the Nernst coefficient [1] in underdoped $YBa_2Cu_30_{6+x}$, together with the measurements of the anisotropy of conductivity and the inferred anisotropy of the thermopower, imply that this principle is violated [2]. The probable violation and its temperature dependence are shown to be consistent with the loop-current phase which has been directly observed in other experiments. The violation is related directly to the magneto-electric symmetry of such a phase in which an applied electric field generates an effective magnetic field at right angle to it and to the order parameter vector, and vice versa.

[1] R. Daou *et al.*, Nature **463**, 519 (2010).
[2] C. M. Varma, V. M. Yakovenko, A. Kapitulnik, arXiv:1007.1215

Monday, March 21, 2011 8:00AM - 11:00AM –
Session A26 DMP DCOMP: Focus Session: Iron Based Superconductors – Theory D162/164

8:00AM A26.00001 Domain Walls in Normal and Superconducting States of Iron Pnictides , HUAIXIANG HUANG, DEGANG ZHANG, TAO ZHOU, C.S. TING, University of Houston — The electronic and magnetic structures in the normal and superconducting states of iron pnictides are investigated by solving self-consistently the Bogoliubov-de Gennes equation. It is shown that strong electron correlations can induce domain walls, which separate regions with different spin density wave orders. At zero or low electron doping, 90° domain walls are formed while anti-phase domain walls are produced at higher electron doping. On the domain walls, there always exist larger electron densities. The results agree qualitatively with recent observations of scanning tunneling microscopy and superconducting quantum interference device microscopy.

8:12AM A26.00002 Correlation, magnetization and conduction in iron pnictides and iron chalcogenides , ZHIPING YIN, Department of Physics, Rutgers and Stony Brook University, KRISTJAN HAULE, GABRIEL KOTLIAR, Department of Physics, Rutgers University — By combining density functional theory (DFT) and dynamical mean field theory (DMFT), we study the electronic properties of iron pnictides and iron chalcogenides in both the paramagnetic and magnetic states. With ab initio derived realistic Coulomb interaction U and Hund's exchange coupling J, we find detailed agreements bewtween our calculations and many experimental observations in these compounds, including ARPES, magnetic properties, optical conductivity and anisotropy, and so on, WITHOUT any adjustment such as shifting of atomic positions, Fermi level and bands and renormalizations of bands which are commonly needed in DFT calculations in order to compare with experiments. Our theory explains the origin of the different magnetizations in FeTe and other iron pnictides and provides a unique physical picture. We find that in the magnetic phase of the iron pnictides, both the spin and the orbital polarization are strongly energy dependent. The spin polarization becomes weaker around Fermi level when the orbital polarization is stronger and vice verse at high energies. We stress on the role of the Hund's J rather than the Coulomb U and show how the iron pnictides and iron chalcogenides differ from other compounds.

8:24AM A26.00003 Charged Stripes in the Two-Orbital Hubbard Model for Pnictides[1] , DAO-XIN YAO, State Key Lab of Optoelectronic Materials and Technologies, Sun Yat-sen University, QINLONG LUO, Department of Physics and Astronomy, The University of Tennessee, and Materials Science and Technology Division, Oak Ridge National Lab, THOMAS PRESTEL, MARIA DAGHOFER, IFW Dresden, Germany, ADRIANA MOREO, ELBIO DAGOTTO, Department of Physics and Astronomy, The University of Tennessee, and Materials Science and Technology Division, Oak Ridge National Lab — The two-orbital Hubbard model for the pnictides is studied numerically in the real-space Hartree-Fock approximation. Upon electron doping, states with a nonuniform ditribution of charge are stabilized. The patterns observed correspond to charge stripes that run perpendicular to the direction of the spin stripes of the undoped magnetic ground state. These striped states are robust when the undoped state has a gap, although with a decreasing amplitude as the gap decreases. Results for hole doping and implications for recent experiments that reported electronic nematic states and spin incommensurability in the pnictides are also discussed.

[1]This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division (Q.L., A.M., E.D.), the SYSU and NSFC-11074310 (D.X.Y.), the DFG under the Emmy-Noether program (T.P., M.D.).

8:36AM A26.00004 Computational studies of models for the magnetism and superconductivity in iron pnictides

, ADRIANA MOREO, University of Tennessee and Oak Ridge National Lab — The properties of multiorbital electronic model Hamiltonians for the pnictides are explored using a variety of many-body techniques. Via mean-field approximations, a regime where the undoped system develops $(\pi, 0)$ magnetic order while remaining metallic is found at intermediate values of the Hubbard repulsion U. Comparison of our results against ARPES and neutron scattering data allows us to determine a range of realistic values for the parameters in the models [1]. The orbital spectral weight redistribution that occurs near the Fermi surface in the $(\pi, 0)$ magnetic state without long-range orbital order is also discussed [2]. The two-orbital "t-U-J" Hubbard model at intermediate U, with magnetic order and pairing tendencies enhanced by the addition of Heisenberg terms that arise from the strong coupling expansion, is studied via exact diagonalization. At intermediate couplings and considering two extra electrons added to the undoped system, an A_{1g} bound state is found compatible with the "extended s±" pairing discussed in the RPA approximation. Bound states with B_{2g} symmetry, involving intra- and inter-band components, are also stable in portions of the phase diagram, while states with B_{1g} symmetry are close in energy, suggesting that small changes in parameters may render any of the three channels stable [3]. Finally, using the real-space Hartree-Fock approximation on finite clusters the presence of charge stripes at intermediate U is also observed for electron-doped systems. The patterns of charge, spin, and orbital order, as well as the influence of quenched disorder will be discussed [4].

[1] Q. Luo *et al.*, Phys. Rev. B **82**, 104508(2010). See also R. Yu *et al.*, Phys. Rev. B **79**, 104510 (2009).
[2] M. Daghofer *et al.*, Phys. Rev. B **81**, 180514(R) (2010).
[3] A. Nicholson *et al.*, preprint. See also M. Daghofer *et al.*, Phys. Rev. Lett. **101**, 237004 (2008), and A. Moreo *et al.*, Phys. Rev. B **79**, 134502 (2009).
[4] Q. Luo *et al.*, preprint.

9:12AM A26.00005 Order-Parameter Anisotropies in the Pnictides - An Optimization Principle for Multi-Band Superconductivity

, CHRISTIAN PLATT, Institute for Theoretical Physics and Astrophysics, University of Wuerzburg, RONNY THOMALE, Department of Physics, Princeton University, WERNER HANKE, Institute for Theoretical Physics and Astrophysics, University of Wuerzburg — Using general arguments of an optimization taking place between the pair wave function and the repulsive part of the electron-electron interaction, we analyze the superconducting gap in materials with multiple Fermi-surface (FS) pockets, with application to two proto-type (P-based and As-based) ferropnictides. The main point of our work is to show that the SC state, its gap and, in particular, its anisotropy in momentum space is determined by an optimization, which balances the interplay between the attractive interaction in the sign-reversing $s_{\pm}$-channel and the Coulomb repulsion. This Coulomb repulsion, as discussed below, is unavoidable in a multi-band SC situation: it appears because of a kind of frustration in the $s_{\pm}$-channel, when more than two FS-pockets are involved in setting up the pairing interaction. On the basis of functional Renormalization Group (fRG) calculations for a wide parameter span of the bare interactions and for the different FS topologies applying to these two characteristic Fe-based superconductors, we show that the symmetry of the gap and the nodal versus nodeless behavior is driven by this optimization requirement.

9:24AM A26.00006 Electronic Structure of High-T_c Iron-Pnictide Superconductors from the Strong Correlation Limit[1]

, JOSE RODRIGUEZ, California State University at Los Angeles — A two-orbital t-J model for a square lattice of iron (pnictide) atoms that includes magnetic frustration and Hund's rule coupling is studied in the limit where inter-orbital hopping of holes is prohibited. A hidden half-metal phase is predicted at weak enough Hund's rule coupling, where holes move coherently through opposing ferromagnetic spin arrangments that are assigned to each orbital. In particular, two Fermi surface hole pockets centered at zero momentum that have unrenormalized Fermi velocities are predicted. Next, the same model is studied at the quantum critical point that separates the hidden ferromagnet from the commensurate spin-density wave (cSDW), where low-energy spinwaves disperse anisotropically away from cSDW wave numbers. Composite hole-spinwave excitations result in "shadow" hole Fermi surfaces that are centered at cSDW wave numbers. We explore the possibility that these "shadow" bands are intrinsically diffuse enough that they simulate electron bands. Last, determinations of the low-energy spectrum of one hole by numerical exact diagonalization confirms the existence of degenerate ground states at momenta $(0, 0)$ and $(\pi, 0)$ at a quantum critical point.

[1]Research supported in part by AFOSR grant no. FA9550-09-1-0660.

9:36AM A26.00007 Pair hopping mechanism of enhancement in T_c for layered superconductors

, KOICHI KUSAKABE, Osaka University — Two body effective interactions coming from the quantum charge fluctuation may induce pairs tunneling between adjacent layers in high-Tc materials including cuprates, iron-pnictides, MgB_2, and MNX. This mechanism [1] is favored when 1) the one-body Hamiltonian shows negligible inter-layer single electron hopping for the 2D liquid around the Fermi level, and 2) unfilled extended orbitals support the pair tunneling via local two-electron scattering. Localized nature of the 2D liquid is essential. The density functional theory (DFT) can prove this picture in two steps. The Kohn-Sham scheme tells that the single-particle effective Hamiltonian possess these aspects most clearly for the highest T_c material. The multi-reference generalization of DFT allows us to evaluate existence and relevance of the super pair tunneling. A possible mechanism for layered organic superconductors is also discussed.

[1] K. Kusakabe, J. Phys. Soc. Jpn., **78** (2009) 114716.

9:48AM A26.00008 Charge Density Wave Induction by Spin Density Wave in Iron-Based Superconductors[1]

, ALEXANDER BALATSKY, Los Alamos National Laboratory, DMITRI BASOV, UC San Diego, JIAN-XIN ZHU, Los Alamos National Laboratory — We argue that spin density wave (SDW) phase in ferrous superconductors contains charge density wave (CDW) with the modulation momentum that is a double of characteristic momenta of SDW [1]. We discuss symmetry constraints on allowed momenta of CDW generated by coupling to spin modulations. To be specific we considered the CDW that could be realized in Fe-11 (e.g., FeTe) and Fe-122 (e.g., BaFe2As2) compounds. In case of commensurate SDW, the CDW modulation vector is at the Bragg peaks positions and could be revealed by local scanned probes. In case of incommensurate SDW, the CDW is incommensurate and can be seen also by x-ray and elastic neutron scattering. We also discuss observable charge modulation due to CDW formation near defects and twin boundaries.

[1] A. V. Balatsky, D. N. Basov, and Jian-Xin Zhu, PHYSICAL REVIEW B **82**, 144522 (2010).

[1]This work was supported by U.S. Department of Energy through LDRD and BES funds, the National Science Foundation under Grant No. PHY05-51164, and the UCOP- 09-027.

10:00AM A26.00009 Theory of Valley-Density Wave and Hidden Order in Iron-Pnictides[1]

, JIAN KANG, ZLATKO TESANOVIC, Institute for Quantum Matter, Johns Hopkins University, Baltimore, MD 21218 — In the limit of perfect nesting, the physics of iron-pnictides is governed by the density wave formation at the zone-edge vector **M**. At high energies, various spin- (SDW), charge- (CDW), orbital/pocket- (PDW) density waves, and their mutually orthogonal linear combinations, all appear equally likely, unified within the unitary order parameter of the $U(4) \times U(4)$ symmetry. Nesting imperfections and low-energy interactions reduce this symmetry to that of real materials. Nevertheless, the generic ground state preserves a distinct signature of its highly symmetric origins: an SDW along one axis of the square iron lattice is predicted to *coexist* with a PDW along the perpendicular axis, accompanied by a modulated pattern of weak charge currents on inter-iron bonds. This "hidden" order induces the tetragonal-orthorhombic structural transition in our theory, naturally insures $T_s \geq T_N$, and leads to other observable consequences.

[1]Research supported in part by the DOE under Grant No. DE-FG02-08ER46544.

10:12AM A26.00010 Topological and Transport Properties of Dirac Fermions in Antiferromagnetic Metallic Phase of Iron-Based Superconductors , TAKAMI TOHYAMA, TAKAO MORINARI, Yukawa Institute for Theoretical Physics, Kyoto University, EIJI KANESHITA, Sendai National College of Technology, KOUDAI SUGIMOTO, Yukawa Institute for Theoretical Physics, Kyoto University — We investigate Dirac fermions in the antifferomagnetic metallic state of iron-based superconductors [1]. Deriving an effective Hamiltonian for Dirac fermions, we reveal that there exist two Dirac cones carrying the same chirality, contrary to graphene, compensated by a Fermi surface with a quadratic energy dispersion as a consequence of a non-trivial topological property inherent in the band structure. We also find that the presence of the Dirac fermions gives the difference of sign-change temperatures between the Hall coefficient and the thermopower. This is consistent with available experimental data. The Dirac ferimons also contribute to in-plane anisotropy of the optical conductivity [2].

[1] T. Morinari, E. Kaneshita, and T. Tohyama, Phys. Rev. Lett. **105**, 037203 (2010).
[2] K. Sugimoto, E. Kaneshita, and T. Tohyama, submitted to J. Phys. Soc. Jpn.

10:24AM A26.00011 Quasiparticle states around a nonmagnetic impurity in the spin-density-wave state of iron-pnictide superconductors , TAO ZHOU, HUAIXIANG HUANG, YI GAO, University of Houston, JIANXIN ZHU, Los Alamos National Laboratory, C.S. TING, University of Houston — The quasiparticle states around a non-magnetic impurity in the electron doped iron-based superconductors with the presence of spin-density-wave (SDW) ordering will be investigated as a function of doping and for various impurity strengths. We found that In the undoped sample,two resonance peaks are found to approach the Fermi level on the impurity site with the strength of scattering potential increasing from weak to moderate. For doped samples, where the SDW order and the superconducting order coexist, there are two intra-gap resonance peaks for weak scattering potential. For strong scattering potential, one sharp peak appears near fermi energy in underdoped sample and separates to two peaks for larger dopings. For all the cases, the local density of states exhibits clear C_2 symmetry. Our results provide an effective tool to detect the SDW order and probe the coexistence of the SDW and superconducting orders.

10:36AM A26.00012 Renormalization group flow, competing phases, and gap structure in multi-band models of Fe-based superconductors , ANDREY CHUBUKOV, SAURABH MAITI, University of Wisconsin — We perform an analytical renormalization group (RG) study to address the role of Coulomb repulsion, the competition between extended s-wave superconducting order ($s\pm$) and the spin density wave (SDW) order, and the angular dependence of the superconducting gap in multi-pocket models of Fe-based superconductors. Previous analytic RG studies considered a toy 2-pockets model (one hole and one electron). We consider more realistic models of 4 and 5 pockets (2 electron and 2 or 3 hole pockets), and also incorporate angular dependences of the interactions caused by the transformation from orbital to band description. In a toy 2-pocket model, SDW order always wins over $s\pm$ order at perfect nesting; $s\pm$ order only appears when doping is finite and RG flow extends long enough to overcome intra-pocket Coulomb repulsion. In multi-pocket models, there are two new effects. First, the pairing interaction projected onto $s\pm$ channel has an attractive component no matter how strong intra-pocket repulsion is. Second, in 4-pocket model (but not in 5-pocket model), $s\pm$ order wins over SDW order even for perfect nesting, if parquet RG flow extends long enough, suggesting that SDW order is not a necessary pre-condition for the $s\pm$ order. Our analytic results are in full agreement with recent numerical functional RG studies by Thomale et. al.

10:48AM A26.00013 Large D-2 Theory of Superconducting Fluctuations in a Magnetic Field and its Application to Iron Pnictides[1] , JAMES MURRAY, ZLATKO TESANOVIC, Johns Hopkins University — A Ginzburg-Landau approach to fluctuations of a layered superconductor in a magnetic field is used to show that the interlayer coupling can be incorporated within an interacting self-consistent theory of a single layer, in the limit of a large number of neighboring layers [1]. The theory exhibits two phase transitions: a vortex liquid-to-solid transition is followed by a Bose-Einstein condensation into the Abrikosov lattice, illustrating the essential role of interlayer coupling. By using this theory, explicit expressions for magnetization, specific heat, and fluctuation conductivity are derived. We compare our results with recent experimental data on the iron-pnictide superconductors.

[1] J. M. Murray and Z. Tešanović, *Phys. Rev. Lett.* **105**, 037006 (2010).

[1]Supported in part by the Gardner Foundation and the Johns Hopkins-Princeton Institute for Quantum Matter, under Grant No. DE-FG02-08ER46544 by the U.S. Department of Energy, OBES, Division of Materials Sciences and Engineering

Monday, March 21, 2011 8:00AM - 11:00AM –
Session A27 GQI: Focus Session: Quantum Optics with Superconducting Circuits I C155

8:00AM A27.00001 Quantum temperature of a modulated oscillator: spectral signatures , MARK DYKMAN, Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824, MICHAEL MARTHALER, Institut fuer Theoretische Festkoerperphysik and DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institue of Technology, D-76128 Karlsruh, VITTORIO PEANO, Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824 — Relaxation of a quantum system is usually due to emission of excitations of a thermal reservoir. The emission events happen at random. For periodically modulated systems, the corresponding noise leads to a finite-width distribution over the quasi-energy (Floquet) states. It can be characterized by an effective nonzero quantum temperature even where the temperature of the reservoir is zero. We show that, as a result, the spectra of fluctuations and response of a parametrically modulated underdamped nonlinear oscillator can display a fine structure. The form of the spectra sensitively depends on the temperature of the reservoir.

8:12AM A27.00002 Switching in modulated quantum oscillators beyond the rotating wave approximation. , VITTORIO PEANO[1], Albert-Ludwigs University Freiburg, MICHAEL MARTHALER, Karlsruhe University, MARK DYKMAN, Michigan State University — Experiments with Josephson bifurcation amplifiers have reached the regime where the switching between different metastable states is governed by quantum fluctuations [1]. The existing theoretical analysis of the metastable decay relies on the rotating wave approximation (RWA) and gives an exponentially small switching rate [2]. Therefore if corrections to the RWA modify the switching rate, they can become substantial even where they are small. We incorporate them within a semiclassical perturbation theory in the Floquet basis. Our analytical results are corroborated by numerical calculations and suggest a switching mechanism that had been previously overlooked.

[1] R. Vijay et al, Rev. Sci. Instr. 80, 111101 (2009).
[2] M. I. Dykman and V. N. Smelyanskii, Sov. Phys. JETP 67, 1769 (1988); M. Marthaler and M. I. Dykman, Phys. Rev. A 73, 42108 (2006).

[1]from January 2011 Michigan State University

8:24AM A27.00003 Many-body effects of quantum impurity models via circuit QED , PRASENJIT DUTT, MICHEL DEVORET, KARYN LE HUR, Yale University, New Haven, CT. — Circuit QED systems serve as an ideal quantum simulator of condensed matter models, given the great degree of experimental precision and control with which they can be manipulated. Quantum impurity models exhibiting renormalization and confinement ideas reminiscent of QCD, can be realized in circuits comprising superconducting qubits and long transmission lines, which play the role of macroscopic bosonic baths. In particular, it is possible to use such systems to engineer standard low energy many-body Hamiltonians such as the spin-boson or anisotropic Kondo model. We develop a framework combining input-output theory and many-body techniques to study correlated photon transport and specifically the qubit response in such circuits.

8:36AM A27.00004 Autoresonant vs. ladder climbing response in a superconducting Josephson phase circuit , NADAV KATZ, YAARA ROFE, YONI SHALIBO, Hebrew University, RADOSLAW BIALCZAK, JOHN MARTINIS, UCSB, IDO BARTH, LAZAR FRIEDLAND, Hebrew University — Anharmonic oscillators exhibit a unique response to a chirped drive, referred to as either autoresonance or ladder climbing. This typically involves a bifurcation of the oscillation amplitude depending both on the strength of the drive and on the system's anharmonicity. In this parameter space, the threshold of bifurcation exhibits a transition between sequential state excitation (quantum ladder climbing) and the population of coherent-like states (classical autoresonance). Previous attempts to experimentally map this transition have only been possible in either classical or quantum conditions. Superconducting Josephson phase circuits enable us to map these two regimes, including the intermediate regime, due to their tunable anharmonicity. We measure the bifurcation phenomena in this system over the relevant parameter space where the transition is observed. We compare to numerical simulations and theoretical analysis.

8:48AM A27.00005 Quantum Transport of Strongly-Correlated Photons in Waveguide QED , HUAIXIU ZHENG, DANIEL J. GAUTHIER, HAROLD U. BARANGER, Duke University — We present an exact solution of the quantum transport problem of multi-mode photons in a waveguide quantum electrodynamics (QED) system, which may be realized in a variety of circuit-QED, plasmonic, photonic, or cold-atom contexts. The bosonic modes are strongly coupled to a local atomic or qubit system, which can be a two-level, Gamma-type three-level, or N-type four-level system. We show that strong coupling produces dramatic quantum optics effects. In particular, multi-photon bound states emerge in the scattering of two or more photons. Such bound states have a large impact on the transport of coherent-state wave-packets. For a two-level system, the single-photon probability is suppressed while multi-photon probabilities are strongly enhanced, resulting in non-classical statistics. For a three-level system, as one tunes the coupling strength and the control field, the transmitted light can show bunching or antibunching, indicating effective attractive or repulsive interactions. Finally, for a N-type four-level system, we demonstrate that the multi-photon components can be largely suppressed, leading to a potential single-photon filter.

9:00AM A27.00006 Superradiance and Phase Multistability in Circuit Quantum Electrodynamics , MICHAEL DELANTY, STOJAN REBIC, JASON TWAMLEY, Centre for Engineered Quantum Systems, Macquarie University, Sydney, NSW 2109, Australia — By modelling the coupling of multiple superconducting qubits to a single cavity in the circuit-quantum electrodynamics (QED) framework we find that it should be possible to observe superradiance and phase multistability using currently available technology (M. Delanty, S. Rebić and J. Twamley, arxiv:1007.2231). Due to the exceptionally large couplings present in circuit-QED we predict that superradiant microwave pulses should be observable with only a very small number of qubits (just three or four), in the presence of energy relaxation and small differences in the qubit-field coupling strengths. This paves the way for circuit-QED implementations of superradiant state readout and decoherence free subspace state encoding in subradiant states. The system considered here also exhibits phase multistability when driven with large field amplitudes, and this effect may have applications for collective qubit readout and for quantum feedback protocols. Furthermore, we extend our analysis to superradiance and collective effects in multi-resonator circuit-QED systems.

9:12AM A27.00007 Design and Calibration of an Improved Josephson Parametric Amplifier , WILLIAM F. KINDEL, HSIANG-SHENG KU, University of Colorado, FRANCOIS MALLET, JILA, LEILA R. VALE, GENE C. HILTON, KENT D. IRWIN, National Institute of Standards and Technology, KONRAD W. LEHNERT, JILA — Phase sensitive amplifiers are of interested because in principal they can amplify one quadrature of a tone without any added noise, unlike phase insensitive amplifiers which amplify both quadratures but must add half a quanta of noise. In situations where a signal of interest is encoded in the modulation of only one quadrature of a tone, phase sensitive detection is clearly dvantageous. With the goal of creating a microwave-frequency phase-sensitive amplifier that adds no noise, we will present the design and performance of a recently tested Josephson Parametric Amplifier (JPA). Initial measurements indicate that the JPAs added noise is no greater than 0.1 quanta. This is a substantial improvement over a previous design for which the added noise was 0.3 quanta [1]. I will discuss changes made to the design and possible reason for the improvement.

[1] M. A. Castellanos-Beltran et al, Nature Phys. 4 929 (2008). M. A. Castellanos-Beltran

9:24AM A27.00008 Parametric processes in a cavity resonator terminated with a DC-SQUID , FRANCOIS NGUYEN, EVA ZAKKA BAJJANI, NIST Boulder, MINHYEA LEE, University of Colorado, LAFE SPIETZ, LEILA VALE, RAYMOND SIMMONDS, JOSE AUMENTADO, NIST Boulder — The coplanar waveguide resonators with SQUIDs have become common to several recent superconducting quantum information experiments. In this talk, we will present some recent results which demonstrate the manipulation of the internal harmonic modes of a microwave cavity resonator using a flux-driven SQUID as a parametric mode mixing resource.

9:36AM A27.00009 Quantum non-demolition measurement of microwave photons in superconducting circuits using engineered quadratic interactions , CHUNQING DENG, University of Waterloo, JAY GAMBETTA, ADRIAN LUPASCU — We present a quantum electrical circuit with Josephson junctions formed by two anharmonic oscillators coupled with an interaction of the form $g\gamma_1^2\gamma_2^2$ where γ_1 and γ_2 are position-like coordinates. This type of coupling allows the quantum non-demolition measurement of the energy of one oscillator by monitoring the frequency of the second oscillator. We find that the optimized coupling strength g scales as $\sqrt{\omega_1\omega_2}/\sqrt{n_1 n_2}$, with $\omega_{1,2}$ the frequency, and $n_{1,2}$ the maximum photon storage capacity of each resonator. With an optimized coupling, it is possible to achieve high fidelity detection of up to 10 photons over a time of the order of microseconds. We discuss the possibility of observing quantum jumps in the number of photons and related applications. We also present our experimental work on the implementation of this detection scheme. C. Deng, J. M. Gambetta, and A. Lupascu, arXiv:1008.3363 (2010).

9:48AM A27.00010 Lossless on-chip microwave circulator using Josephson parametric converters[1] , BALEEGH ABDO, ARCHANA KAMAL, MICHAEL HATRIDGE, FLAVIUS SCHACKERT, KURTIS GEERLINGS, MICHEL DEVORET, Applied Physics Department, Yale University — Motivated by our recent theoretical work on non-reciprocal parametric devices [1], we propose a novel scheme for realizing a four-port, lossless, on-chip microwave circulator using a compact design of Josephson parametric converters (JPC's) and hybrids. The JPC, which is normally used as a phase-preserving quantum-limited amplifier, is operated here in a pure conversion mode with unity photon gain. The non-reciprocity of the device is induced by a phase shift between the two pump signals feeding two JPC's sharing a common idler port. The non-reciprocity direction can thus be reversed much more rapidly than by changing a magnetic field. Furthermore, since the device consists only of purely dispersive components, the proposed circulator should not add any noise to signals it processes.

[1] A. Kamal, J. Clarke and M.H. Devoret, accepted by Nature Physics, arXiv:1010.1794

[1]Work supported by IARPA, ARO and NSF.

10:00AM A27.00011 Dynamic range and noise of the Josephson parametric converter[1] , FLAVIUS SCHACKERT, BALEEGH ABDO, MICHAEL HATRIDGE, LUIGI FRUNZIO, ROBERT J. SCHOELKOPF, MICHEL H. DEVORET, Yale University — We present recent progress in characterizing key properties of the Josephson parametric converter (JPC): its dynamic range and noise performance. The JPC is a phase-preserving parametric amplifier operating in the microwave regime. It is based on a ring of four Josephson junctions, which provides the non-linearity, coupled to two microwave resonators, which increase the effective interaction between the incoming signal and this non-linearity. The JPC operates with a minimal number of modes, which simplifies its analysis, and is close to the ideal non-degenerate parametric amplifier operating at the quantum limit of noise. Besides having sufficient gain and bandwidth, a practical amplifier useful for e.g. the readout of superconducting qubits will need to exhibit a sufficiently low noise temperature and dynamic range. While dynamic range ensures that an incoming signal does not saturate the amplifier, a low noise temperature is necessary to minimally degrade signal-to-noise ratio.

[1]Work supported by IARPA, ARO and NSF.

10:12AM A27.00012 Microwave Photon Counter Based on Josephson Junctions , Y.-F. CHEN, D. HOVER, S. SENDELBACH, L. MAURER, R. MCDERMOTT, University of Wisconsin, S.T. MERKEL, E.J. PRITCHETT, F.K. WILHELM, Institute for Quantum Computing, University of Waterloo — We describe a microwave photon counter based on current-biased Josephson junctions. The absorption of a single microwave photon causes a junction to switch to the voltage state, producing a large and easily measured classical signal. With a two-junction circuit, we have performed a microwave version of the Hanbury Brown and Twiss experiment at 4 GHz, and demonstrated a clear signature of photon bunching for a thermal source. The design is readily scalable to tens of parallelized junctions, a configuration that would allow number-resolved counting of microwave photons. We discuss possible applications to cavity state readout and to measurement of the counting statistics of microwave photons emitted by mesoscopic conductors.

10:24AM A27.00013 Quantum Limited Amplification and Detection with a Non-Linear Cavity Detector , CATHERINE LAFLAMME, AASHISH CLERK, Department of Physics, McGill University — A variety of recent experiments demonstrate the power of using driven microwave resonators for quantum measurement and amplification. Here, we consider theoretically the use of a driven cavity with a Kerr-type non-linearity to amplify a dispersively coupled signal. We consider the regime where there is no multi-stability in the cavity dynamics; this is similar to recent experiments.[1,2] The amplifier quantum-limit in this case involves the physics of backaction, unlike the more studied 'scattering' mode of operation. We calculate the added noise of this nonlinear cavity amplifier, and show that it exhibits universal scaling in the vicinity of the bifurcation point. We also show that for low frequencies the nonlinear cavity amplifier reaches the fundamental quantum limit on its noise temperature, but has large backaction - imprecision noise correlations. This implies that the non-linear cavity cannot be simply used for QND qubit measurement, but could have interesting applications to non-resonant force sensing. Our results have applications to quantum information processing, electromechanics and optomechanics.

[1]M. Hatridge *et al.*, arXiv:1003.2466v1
[2]F.R. Ong *et al.*, arXiv:1010.6248v1

10:36AM A27.00014 A flux-driven Josephson parametric amplifier for experiments with propagating quantum microwaves[1] , E.P. MENZEL, A. BAUST, F. DEPPE, T. NIEMCZYK, E. HOFFMANN, M. HAEBERLEIN, A. MARX, R. GROSS, Walther-Meissner-Institut and TU Muenchen, Garching, Germany, E. SOLANO, Universidad del Pais Vasco and IKERBASQUE Foundation, Bilbao, Spain, K. INOMATA, RIKEN, Wako-shi, Japan, T. YAMAMOTO, Y. NAKAMURA, NEC, Tsukuba and RIKEN, Wako-shi, Japan — For the detection of propagating quantum microwaves in circuit QED linear amplifiers are key ingredients. Phase sensitive amplifiers [e.g., Josephson parametric amplifiers (JPA)] in principle allow for the amplification of one signal quadrature without adding noise. In practice, however, internal losses often introduce a finite amount of noise. We have recently shown that, despite such a residual noise, signals on the quantum level can be fully characterized using two amplification chains and suitable correlations [E.P. Menzel et al., PRL 105, 100401 (2010)]. In this work, we characterize a flux-driven JPA. At 5.64 GHz the maximum degenerate gain is 25.5 dB and the signal bandwidth is 1.8 MHz. Phase-insensitive measurements yield a noise temperature of 100$\pm$20 mK, which is below the standard quantum limit of 135 mK.

[1]This work is supported by SFB 631, NIM, Basque Government IT4720-10, Spanish MICINN FIS2009-12773-C02-01, and EU project SOLID.

10:48AM A27.00015 Microstrip SQUID amplifiers at gigahertz frequencies[1] , M.P. DEFEO, P. BHUPATHI, M. WARE, B.L.T. PLOURDE, Syracuse University — SQUID amplifiers based on the microstrip resonance formed between the input coil and SQUID washer have demonstrated substantial gain and low noise at frequencies of several hundred MHz. Operation at higher frequencies requires shorter input coils and the corresponding reduced mutual inductance must be compensated with an increased transfer function in order to avoid loss of gain. We have fabricated microstrip SQUID amplifiers using low capacitance Al-AlOx-Al submicron junctions and large resistive shunts to increase the transfer function while keeping the SQUID non-hysteretic. These devices have demonstrated gains beyond 20dB at frequencies in the gigahertz range. Gain and noise measurements as well as applications of these devices in the field of quantum information science will be discussed.

[1]Work supported by DARPA QuEST.

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A28 DMP: Focus Session: Carbon Nanotubes and Related Materials: Fundamentals and Applications C156

8:00AM A28.00001 Carbon nanotube – catalyst composites: from nano-complexes to aerogel functionalization[1] , GORDANA N. OSTOJIC, MARK C. HERSAM, Materials Science and Engineering Department, Northwestern University — Here we present three different strategies to achieve attachment of catalytic nanoparticles to SWNTs and discuss their physical properties. In nano-complex scheme, DNA that solubilizes SWNTs is used as an anchor for Pt nanoparticle growth. Attached platinum strongly influences nanotube phonon and charge carrier distribution. For macroscopic electrodes, no special chemistry is needed. Simple solubilization of both nanoparticles (Pt) and nanotubes in polar surfactants and joint deposition on a porous membrane will result in charge coupled SWNT/Pt electrode. A particularly difficult problem in SWNT research is a task of electrically connecting nanotubes and at the same time keeping the surface available. We present an innovative solution to this problem in which SWNTs are connected through point contacts that leave the majority of the surface free. This method creates self-assembled carbon nanotube aerogel of a record low density that is both luminescent and conductive. Additional value of this material is that it is suitable for subsequent functionalizations. Platinum and titanium dioxide deposition on aerogel suggests that carbon aerogel can be used as a framework for complex structures.

[1]Authors gratefully acknowledge a support of Department of Energy Institute for Catalysis in Energy Processes.

8:12AM A28.00002 Reinforced Epoxy Nanocomposite Sheets Utilizing Large Interfacial Area from a High Surface Area Single-Walled Carbon Nanotube Scaffold , KAZUFUMI KOBASHI, HIDEKAZU NISHINO, TAKEO YAMADA, DON FUTABA, MOTOO YUMURA, KENJI HATA, AIST — We employed single-walled carbon nanotubes (SWNTs) with the available highest specific surface area (more than 1000 m2/g) that provided very large interfacial area for the matrix to fabricate epoxy composite sheets. Through mechanical redirection of the SWNT alignment to horizontal to create a laterally aligned scaffold sheet, into which epoxy resin was impregnated. The SWNT scaffold was engineered in structure to meet the these two nearly mutually exclusive demands, i.e. to have nanometer meso-pores (2-50 nm) to facilitate homogeneous impregnation of the epoxy resin and to have mechanical strength to tolerate the compaction forces generated during impregnation. Through this approach, a SWNT/epoxy composite sheet with a nearly ideal morphology was realized where long and aligned SWNTs were loaded at high weight fraction (33 percent) with an intertube distance approaching the radius of gyration for polymers. The resultant composite showed a Young's modulus of 15.0 GPa and a tensile strength of 104 MPa, thus achieving 5.4 and 2.1 times reinforcement as compared to the neat epoxy resin.

8:24AM A28.00003 Single-walled carbon nanotube buckypaper and mesophase pitch carbon/carbon composites[1] , JIN GYU PARK, NAM GYUN YUN, YOUNG BIN PARK, RICHARD LIANG, LLOYD LUMATA, JAMES BROOKS, CHUCK ZHANG, BEN WANG, HIGH-PERFORMANCE MATERIALS INSTITUTE, FSU COLLABORATION, NATIONAL HIGH MAGNETIC FIELD LABORATORY, FSU COLLABORATION — Carbon/carbon composites consisting of single-walled carbon nanotube (SWCNT) buckypaper (BP) and mesophase pitch resin have been produced through impregnation of BP with pitch using toluene as a solvent. Drying, stabilization and carbonization processes were performed sequentially, and repeated to increase the pitch content. Voids in the carbon/carbon composite samples decreased with increasing impregnation process cycles. Electrical conductivity and density of the composites increased with carbonization by two to three times that of pristine BP. These results indicate that discontinuity and intertube contact barriers of SWCNTs in the BP are partially overcome by the carbonization process of pitch. The temperature dependence of the Raman shift shows that mechanical strain is increased since carbonized pitch matrix surrounds the nanotubes.

[1]High-Performance Materials Institute, NSF DMR-0602859, NSF DMR-0654118

8:36AM A28.00004 Biscrolling nanotube sheets and functional guests into yarns , RAY BAUGHMAN, The University of Texas at Dallas/ Alan G. MacDiarmid NanoTech Institute — Multifunctional applications of textiles have been limited by the inability to spin important materials into yarns. Generically applicable methods are demonstrated for producing weavable yarns comprising up to 95 wt % of otherwise unspinnable particulate or nanofiber powders that remain highly functional. Scrolled 50 nm thick carbon nanotube sheets confine these powders in the galleries of irregular scroll sacks, whose observed complex structures are related to twist-dependent extension of Archimedean spirals, Fermat spirals, or spiral pairs into scrolls. The strength and electronic connectivity of a small weight fraction of scrolled carbon nanotube sheet enables yarn weaving, sewing, knotting, braiding, and charge collection. This technology is used to make yarns of superconductors, Li-ion battery materials, graphene ribbons, catalytic nanofibers for fuel cells, and TiO_2 for photocatalysis.

Work done in collaboration with Shaoli Fang, Xavier Lepro-Chavez, Chihye Lewis, Raquel Ovalle-Robles, Javier Carratero-Gonzalez, Elisabet Castillo-Martinez, Mikhail Kozlov, Jiyoung Oh, Neema Rawat, Carter Haines, Mohammed Haque, Vaishnavi Aare, Stephanie Stoughton, Anvar Zakhidov, and Ray Baughman, The University of Texas at Dallas / Alan G. MacDiarmid NanoTech Institute.

9:12AM A28.00005 Load transfer mechanisms in cross-linked DWNT fibers , T. FILLETER, M. NARAGHI, A. MORAVSKY, R. BERNAL, R.O. LOUTFY, H.D. ESPINOSA — The application of carbon nanotubes (CNT) to macroscopic composite fibers has been limited by weak shear interfaces between adjacent CNT shells and composite matrix elements. A fundamental understanding of load transfer at multiple length-scales is needed to identify how the exceptional mechanical properties of CNTs can be scaled to produce high-performance fibers. Through in-situ electron microscopy tensile testing we have elucidated load transfer mechanisms across multiple scales of cross-linked double-walled nanotube (DWNT) fibers. A low density of polymer cross-links is found to increase the total energy dissipated at failure and ductility of fibers by 5 and 10X, respectively, without reducing strength. This mutiscale approach has identified a need to enhance shear interactions between individual DWNTs within the hierarchical DWNT fiber structures. Through in-situ TEM electron irradiation studies we have shown that load can be effectively transferred to inner DWNTs within bundles by covalently cross-linking the interfaces of adjacent DWNTs and shells. We have observed order of magnitude increases in strength and modulus and identified their dependence on irradiation dose. In future a combined approach of irradiation induced covalent and polymer cross-linking may lead to high-performance DWNT-based fibers and composites with tunable mechanical properties.

9:24AM A28.00006 Aligned Carbon Nanotubes Embedded in Elastic Polymer as Stretchable Conductors , YINGYING ZHANG, Los Alamos National Laboratory, QUANXI JIA, CENTER FOR INTERGRATED NANOTECHNOLOGY TEAM — Stretchable electronics enable new applications in a wide range of fields. Carbon nanotube (CNT) ribbons, composed of bundles of aligned millimeter-long CNTs, represent a unique opportunity for high performance stretchable conductors. In this work, we embedded CNT ribbons in elastic poly(dimethylsiloxane) (PDMS) film (or CNT/PDMS films) and systematically investigated the dependence of film resistance on the tensile strains. The CNT/PDMS films fabricated by this approach are flexible, transparent, and show constant resistance under strains in the range of 0%-100%. We believe that the unique stretchability of CNT ribbons reported here will open new potential applications of CNTs in the next generation intelligent electronics.

9:36AM A28.00007 The Anisotropic Physical Properties of Polyethylene Oxide/Magnetic Carbon Nanotubes Composite Films , IL TAE KIM, ALLEN TANNENBAUM, RINA TANNENBAUM, Georgia Institute of Technology — Magnetic carbon nanotubes (m-CNTs) were synthesized by the tethering of γ-Fe_2O_3 nanoparticles. Subsequently, the m-CNTs were dispersed and aligned in a PEO matrix under a low externally-applied magnetic field ($<$0.3 T). The degree of crystallinity, crystal size, and crystal structure of the composite films were investigated using DSC and XRD. The electrical conductivity of the composite films showed anisotropic characteristics that were correlated to the parallel and perpendicular direction of the applied magnetic field. Young's modulus and tensile strength of the composite films increased with the increasing weight fraction of m-CNT up to 170 % and 157 %, respectively. The elongation at break of the composites improved as well compared to that of the pure-PEO film, due to the lowering of the glass transition temperature (T_g) and was also correlated to m-CNT content and the alignment directions.

9:48AM A28.00008 Changing Carbon Nanostructures by Irradiation[1] , DAVID TOMÁNEK, Michigan State University — Changes in the force field of carbon nanostructures immediately following irradiation by light and electrons may cause important structural changes. Exposure to light may modify the morphology at the apex of carbon nanohorns during Raman spectroscopy observations [1], or exfoliate graphite layer-by-layer upon exposure to specifically shaped femtosecond laser pulses [2]. Irradiation by electrons may significantly improve the structural integrity and mechanical properties of low-quality multi-wall carbon nanotubes grown by Chemical Vapor Deposition [3]. *Ab initio* molecular dynamics calculations in the electronic ground and excited state help to analyze the microscopic mechanisms underlying these structural changes including photo-activated Stone-Wales transformations, cross-linking of nanotube walls at extended defect sites, and charge redistribution causing detachment of graphene monolayers.

[1] T. Fujimori *et al.* (in preparation).
[2] Y. Miyamoto *et al.*, Phys. Rev. Lett. **104**, 208302 (2010).
[3] M. Duchamp *et al.*, J. Appl. Phys. **108**, 084314 (2010).

[1]Supported by NSF NSEC grant EEC-0832785.

10:00AM A28.00009 N-type Doping of Single-walled Carbon Nanotubes: Fundamental Properties, Spectroscopic Signatures, and Transparent Conducting Electrodes , KEVIN MISTRY, BRIAN LARSEN, JEREMY BERGESON, MATTHEW REESE, TERESA BARNES, JEFFREY BLACKBURN, National Renewable Energy Laboratory — Controllable p- and n-type doping of single-walled carbon nanotube (SWNT) films enables technologies such as FETs, LEDs, and solar cells. Because many p-type dopants for SWNTs are environmentally stable, they have been studied in greater detail and used in far more applications than their less stable n-type counterparts. As a result, further studies on n-type SWNTs are needed. We report on the effectiveness of small molecule and polymer amines as n-type dopants on thin film nanotube networks. We find significant doping-induced changes in NMR, XPS, and Raman spectra that can be used in future studies to characterize n-type SWNTs. Moreover, we find that the best amines can produce n-type transparent conducting films with nearly the same sheet resistance (at a given transparency) as p-doped HNO_3 treated films. These results serve both to increase the knowledge base in the community regarding the fundamental properties and spectroscopic signatures of n-type doped SWNTs and to expand the versatility of functional SWNT network electrodes that are typically resigned to p-type SWNTs.

10:12AM A28.00010 From ^{3}He to Xe: adsorption isotherms on the same batch of BuckyPearls^{TM} carbon nanotube bundles[1] , OSCAR VILCHES, EVAN MATTSON, KRISTINE KIM, DAVID COBDEN, University of Washington — We report a study of the adsorption of ^{3}He, ^{4}He, H_2, HD, D_2, Ne, Ar, N_2, Kr and Xe adsorbed on samples of BuckyPearls^{TM}, a form of HiPCo-type^{TM} carbon nanotube bundles, from the same batch used for neutron diffraction studies of the structure of ^{4}He and Ne at low temperatures. For each gas, except ^{3}He and ^{4}He, we have measured three or more isotherms in a range of temperatures where we can observe the completion of both the three-line phase and the first layer. We can correlate the helium and hydrogen isotopes data and the Ne data with previous neutron and/or heat capacity measurements on BuckyPearls and HiPCo bundles. By taking ratios of monolayer completion coverage for the various gases to the N_2 monolayer completion coverage we can compare nanotube adsorption to adsorption on exfoliated graphite. Quantum effects on adsorption can be seen by comparing areas per atom or molecule to Lennard-Jones hard core radii.

[1]Work supported by NSF DMR 0907690

10:24AM A28.00011 Comparative study of small alkane and alkene molecules adsorbed on purified HiPco Single-walled carbon nanotubes[1] , DINESH RAWAT, TOYO FURUHASHI, ALDO MIGONE, Department of Physics, Southern Illinois University, Carbondale, IL-62901 — We have measured adsorption isotherms for ethylene on purified HiPco SWNTs at 11 different temperatures (between 110 and 220K). Our findings for ethylene will be compared to the results of ethane adsorption on the same substrate. Consistent with what we had found for ethane, two groups of distinct binding energy sites are observed for ethylene molecules adsorbed on the nanotube substrate. However, unlike in the case of ethane, no feature suggesting the existence of a phase transition was observed for the ethylene films. In addition, we have determined the coverage dependence of the isosteric heat of adsorption for ethylene on the same substrate. The values of the isosteric heats that we had previously determined for ethane are slightly higher than the ones obtained for ethylene, for the same fractional coverage. Our experimental isosteric heat results will also be compared with simulation results that indicate a similar trend.

[1]This research was supported by NSF through grant # DMR-0705077.

10:36AM A28.00012 Studying of kinetics of rear earth ion (REI) nanoscale complex formation by resonant energy transfer , TETYANA IGNATOVA, Department of Physics, Lehigh University, Bethlehem, PA 18015, DENIS PRISTINSKI, Polymers Division of National Institute of Standards and Technology, Gaithersburg, MD 20899, SLAVA V. ROTKIN, (1) Department of Physics and (2) Center for Advanced Materials and Nanotechnologies, Lehigh University, Bethlehem, PA 18015 — We observed formation of nanoscale complexes between multivalent REIs (Tb and Eu) and negatively charged DNA wrapped SWNTs, ionized in the water solution. Foerster Resonance Energy Transfer (FRET) was found to be an ideal method to confirm the complex formation. Because of its high sensitivity and non-destructive characterization approach FRET can be used to trace the kinetics of the complex formation. Strong dependence of SWNT photoluminescence (PL) on the REI concentration was detected and interpreted as a competition between the REI absorption on the SWNTs and subsequent FRET enhanced PL and the SWNT agglomeration followed by PL quenching. We measured the distance between REI and SWNT which appears to be much shorter than the one from their relative concentration in solution. We speculate that Manning condensation of the REIs on the SWNT/DNA surface happens thereby significantly reducing their spacing and making FRET possible.

10:48AM A28.00013 Attachment of a Genetically Engineered Antibody to a Carbon Nanotube Transistor for Detection of Prostate Cancer Biomarkers , MITCHELL LERNER, JENNIFER DAILEY, BRETT GOLDSMITH, University of Pennsylvania Department of Physics and Astronomy, MATTHEW ROBINSON, Fox Chase Cancer Center, A.T. CHARLIE JOHNSON, University of Pennsylvania Department of Physics and Astronomy — We have developed a novel detection method for osteopontin (OPN) by attaching an engineered single chain variable fragment (scFv) protein with high binding affinity for OPN to a carbon nanotube transistor. Osteopontin is a potential new biomarker for prostate cancer; its presence in humans is already associated with several forms of cancer, arthritis, osteoporosis and stress. Prostate cancer is the most commonly diagnosed cancer and second leading cause of cancer deaths among American men and as such represents a major public health issue. Detection of early-stage cancer often results in successful treatment, with long term disease-free survival in 60-90% of patients. Electronic transport measurements are used to detect the presence of OPN in solution at clinically relevant concentrations.

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A29 GQI: Quantum Communication, Theoretical Entanglement, and Cryptography

8:00AM A29.00001 Intrinsic Quantum Correlations of Weak Coherent States for Quantum Communication , YONG MENG SUA, ERIN SCANLON, TRAVIS BEAULIEU, VIKTOR BOLLEN, KIM FOOK LEE, Michigan Technological University — Intrinsic quantum correlations of weak coherent states are observed between two parties, which can be used as a supplement to the existence decoy-state BB84 and differential phase-shift quantum key distribution protocols. In a proof-of-principle experiment, we generate bi-partite correlations of weak coherent states using weak local oscillator fields in two spatially separated balanced homodyne detections. We employ non-linearity of post-measurement method to obtain the bi-partite correlations from two single-field interferences at individual homodyne measurement. This scheme is then used to demonstrate bits correlations in a transmission fiber over a distance of 10 km. We believe that the scheme can add another physical layer of security to these protocols for quantum key distribution and implement linear optics quantum computing with weak coherent states.

8:12AM A29.00002 Achieving the physical limits of the bounded-storage model , PRABHA MANDAYAM, Caltech, STEPHANIE WEHNER, Centre for Quantum Technologies — The security of most cryptographic systems in use today is based on the premise that certain computational problems are hard to solve for the adversary. However, recent cryptographic models such as the bounded-storage model and the noisy-storage model, are based on more physical assumptions regarding the two parties' resources and allow us to obtain security without relying on any additional hardness results. In the bounded-storage model, where the adversary's quantum storage is limited, it is known that security can be achieved if the adversary can store strictly less then half of the qubits transmitted during the protocol. It has been an open question whether security can still be achieved if the adversary's storage were any larger. Here, we answer this question positively and demonstrate a two-party protocol which is secure as long as the adversary cannot store even a small fraction of the transmitted pulses. This not only settles the question, but also highlights the sharp contrast to classical bounded storage, where it is known that security can only be obtained if the adversary's classical storage is at most quadratic in the storage required by the honest players. In the more general setting of the noisy-storage model, where the adversary's memory is simply assumed to be imperfect, we show that our protocol extends security to a larger class of noisy quantum memories. (Reference: arXiV - quant-ph 1009.1596)

8:24AM A29.00003 High-speed single-photon signaling for daytime QKD , JOSHUA BIENFANG, ALESSANDRO RESTELLI, CHARLES CLARK, NIST/JQI — The distribution of quantum-generated cryptographic key at high throughputs can be critically limited by the performance of the systems' single-photon detectors. While noise and afterpulsing are considerations for all single-photon QKD systems, high-transmission rate systems also have critical detector timing-resolution and recovery time requirements. We present experimental results exploiting the high timing resolution and count-rate stability of modified single-photon avalanche diodes (SPADs) in our GHz QKD system operating over a 1.5 km free-space link that demonstrate the ability to apply extremely short temporal gates, enabling daytime free-space QKD with a 4% QBER.[1] We also discuss recent advances in gating techniques for InGaAs SPADs that are suitable for high-speed fiber-based QKD. We present afterpulse-probability measurements that demonstrate the ability to support single-photon count rates above 100 MHz with low afterpulse probability. These results will benefit the design and characterization of free-space and fiber QKD systems.

[1]A. Restelli, J.C. Bienfang A. Mink, and C.W. Clark, *IEEE J. Sel. Topics in Quant. Electron* **16**, 1084 (2010).

8:36AM A29.00004 Security Proof for QKD Using Qudits and Finite Key Length Analysis of Protocols , LANA SHERIDAN, THINH LE, Centre for Quantum Technologies, National University of Singapore, VALERIO SCARANI, Department of Physics and Centre for Quantum Technologies, National University of Singapore — It is advantageous to use d-dimensional quantum systems for QKD because each signal carries $\log d > 1$ bits, allowing a larger amount of information to be sent per transmission through the channel, and moreover, studies have indicated that the resistance to noise of the protocols increases when the dimension is increased. We provide a security bound against coherent attacks that takes into account finite-key effects for two families of protocols: two-basis protocols, the natural generalization of the Bennett-Brassard 1984 protocol for qubits, and $(d+1)$-basis protocols, the generalization of the six-state protocol for qubits. In the asymptotic limit, our bound vindicates the previous partial results concerning the higher resistance to noise. We also show that for finite key lengths the key rate corrections vary little with d for $2 \leq d \leq 20$ indicating the protocol can be effective in realistic conditions. Finally, we consider some other finite key techniques for more general protocols.

8:48AM A29.00005 Quantum Spread Spectrum Communication , TRAVIS HUMBLE, Oak Ridge National Laboratory — Spread spectrum techniques are widely used in classical contexts, including sensing and communication, for establishing low probability of intercept, resistance to narrowband jamming, and multiuser access protocols. In SS, the spectrum of the signal is spread much larger than the minimal information bandwidth to yield a boost in channel capacity. In this contribution, we apply SS modulation to the transmission and detection of the single-photon spectral probability amplitude (as opposed to SS of the field). We draw upon previous methods for coherently dilating single-photon spectral states to motivate our ideas. Techniques for direct modulation of the spectral amplitude, modulation via pumped single-photon up-conversion, and modulation via spread spectral teleportation are developed as particular modulation schemes for quantum spread spectrum communication. We quantify QSSC performance using the channel capacity and process gain expressed in terms of the spread bandwidth, and we investigate its behavior for a frequency-selective fading model. We conclude by discussing the potential for QSSC to underlie a QKD multiuser access control (MAC) protocol.

9:00AM A29.00006 Remote Semi-State Preparation as SuperDense Quantum Teleportation[1] , HERBERT J. BERNSTEIN, ISIS Institute & School NS, Hampshire College — Recent advances in experimental technique make SuperDense Teleportation (SDT) possible. The effect uses remote state preparation to send more state-specifying parameters per bit than ordinary quantum teleportation (QT) can transmit. SDT uses a maximal entanglement to teleport the relative phases of an **n**-dimensional equimodular state. This means that one can send only **n**-1 of the total (2**n**-2) parameters – comprising the relative phases and amplitudes – of a general state. Nevertheless, for **n**$\geq$ 3, SDT sends more of these state-specifying parameters than QT for a given number of classical bits. In the limit of large **n** the ratio is 2 to 1, hence the nomenclature Bennett suggested, SDT, by analogy with Super Dense Coding. Alice's measurements and Bob's transformations are simpler than in QT. The roles of Charles the state chooser, and Diana who deploys it, are different than in QT. I briefly review possible experimental realizations, including two that are under consideration at the present time by an experimental group leading in higher-dimension entanglement work.

[1]Supported in part by NSF grants PHY97-22614 & 07-58149 & KITP, UCSB, including an ITP Scholar-ship.

9:12AM A29.00007 Entanglment assisted zero-error codes , WILLIAM MATTHEWS, LAURA MANCINSKA, DEBBIE LEUNG, MARIS OZOLS, AIDAN ROY, University of Waterloo — Zero-error information theory studies the transmission of data over noisy communication channels with strictly zero error probability. For classical channels and data, much of the theory can be studied in terms of combinatorial graph properties and is a source of hard open problems in that domain. In recent work, we investigated how entanglement between sender and receiver can be used in this task. We found that entanglement-assisted zero-error codes (which are still naturally studied in terms of graphs) sometimes offer an increased bit rate of zero-error communication even in the large block length limit. The assisted codes that we have constructed are closely related to Kochen-Specker proofs of non-contextuality as studied in the context of foundational physics, and our results on asymptotic rates of assisted zero-error communication yield non-contextuality proofs which are particularly 'strong' in a certain quantitive sense. I will also describe formal connections to the multi-prover games known as pseudo-telepathy games.

9:24AM A29.00008 Extreme Spin Squeezing Beyond Spin-1/2 Ensembles , COLLIN TRAIL, LEIGH NORRIS, IVAN DEUTSCH, University of New Mexico — We consider a protocol for squeezing the collective spin of a cold atomic ensemble through coherent control of the spin and light-polarization interactions. By retro-reflecting a short pulse of light through the ensemble followed by a quantum eraser and phase matching, we achieve exponential scaling of the squeezing with optical density. We show how these results can be extended using state preparation and mapping techniques for s¿1/2 systems, and extend our model of photon-atom scattering to account for decoherence in the higher dimensional case.

9:36AM A29.00009 Engineered optical nonlinearity for a quantum light source , AGATA BRANCZYK, ALESSANDRO FEDRIZZI, TOM STACE, TIM RALPH, ANDREW WHITE, The University of Queensland — Many applications in optical quantum information processing benefit from careful spectral shaping of single-photon wave-packets. By engineering the nonlinearity profile of a poled crystal, we were able to tailor the joint spectral wave-function of photons created in parametric down-conversion. We designed a crystal with an approximately Gaussian nonlinearity profile and confirmed successful wave-packet shaping by two-photon interference experiments. To further explore the underlying spectral correlations in the spectral amplitude, we also measured spatial quantum beating patterns. We numerically show how our method can be applied for attaining one of the currently most important goals of single-photon quantum optics, the creation of pure single photons without spectral correlations.

9:48AM A29.00010 Disappearance of entanglement: a topological point of view[1] , DONG ZHOU, ROBERT JOYNT, GIA-WEI CHERN, JIANJIA FEI, University of Wisconsin-Madison — We give a topological classification of the evolution of entanglement, particularly the different ways the entanglement can disappear. Four categories exhaust all possibilities given the initial quantum state is entangled and the final one is not. Exponential decay of entanglement, entanglement sudden death and sudden birth can all be understood and visualized in the associated geometrical picture - the polarization vector representation. The entanglement evolution categories of any model are determined by the topology of the state space, the limiting state and the memory effect of the environment. Transitions between these types of behaviors as a function of physical parameters are also possible. These transitions are thus of topological nature. We illustrate the general concepts with a visualizable model.

[1]NSF-DMR-0805045, the DARPA QuEST program, and by ARO and LPS W911NF-08-1-0482

10:00AM A29.00011 Optimal Entanglement Transformations Among N-qubit W-Class States[1] , WEI CUI, ERIC CHITAMBAR, HOI-KWONG LO, University of Toronto — We investigate the physically allowed probabilities for transforming one N-partite W-class state to another by means of local operations assisted with classical communication (LOCC). Recently, Kintaş and Turgut have obtained an upper bound for the maximum probability of transforming two such states [1]. Here, we provide a simple sufficient and necessary condition for when this upper bound can be satisfied and thus when optimality of state transformation can be achieved. Our discussion involves obtaining lower bounds for the transformation of arbitrary W-class states and showing precisely when this bound saturates the bound of [1]. Finally, we consider the question of transforming symmetric W-class states and find that in general, the optimal one-shot procedure for converting two symmetric states requires a non-symmetric filter by all the parties.

[1]We thank Benjamin Fortescue for helpful discussions in the development of this work as well as support from the funding agencies CIFAR, CRC, NSERC, and QuantumWorks.

10:12AM A29.00012 Negativity Fonts in Four qubit Maximally Entangled States[1] , SANTOSH SHELLY SHARMA, Depto. de Física, Universidade Estadual de Londrina, Londrina 86051-990, PR Brazil, NARESH KUMAR SHARMA, Depto. de Matemática, Universidade Estadual de Londrina, Londrina 86051-990 PR, Brazil — Recently, we introduced negativity fonts as the basic units of multipartite entanglement in pure states. We show that the relation between global negativity of partial transpose of N- qubit state and linear entropy of reduced single qubit state yields an expression for global negativity in terms of determinants of negativity fonts. Transformation equations for determinants of negativity fonts under local unitaries (LU's) are used to construct N-qubit LU invariant and N-tangle (an entanglement monotone). The difference of squared negativity and N-tangle is an N qubit invariant which contains information on entanglement of the state caused by quantum coherences that are not annihilated by removing a single qubit. Entanglement monotones that detect the entanglement of specific parts of a four qubit state are also constructed. It is shown that these entanglement monotones bring out distinct features of several states which have been proposed to be the maximally entangled four qubit states.

[1]Financial Support from Fundacao araucaria and CNPQ Brazil is acknowledged.

10:24AM A29.00013 ABSTRACT WITHDRAWN —

10:36AM A29.00014 Density matrix renormalization group study of the Kitaev honeycomb lattice model , ZHENYUE ZHU, University of California, Irvine, STEVEN WHITE — The Kitaev model on the honeycomb lattice can be solved exactly through mapping into free majorana fermions with a Z_2 gauge field. As a benchmark for DMRG on this two dimensional system, we have simulated this model with a cylindrical geometry with varying widths. The ground state energy and degeneracy match well with theoretical predictions. The different degenerate ground states exhibit the same short range spin-spin correlation patterns. The von Newmann entanglement entropy and its spectrum are evaluated. We show that the entropy of the Kitaev model satisfies the area law, with the entropy being more specifically proportional to the number of bonds cut at the boundary between the two different regions. The degeneracy of entanglement spectrum can also be determined by the number of dangling majorana fermions at the cut. The above results hold for both the gapped and gapless phase. The non-Abelian phase obtained by applying a magnetic field, which is not exactly solvable, will also be discussed.

10:48AM A29.00015 Towards entanglement of very high orbital angular momentum[1] , ROBERT FICKLER, RADEK LAPKIEWICZ, CHRISTOPH SCHAEFF, PEIZHE LI, SVEN RAMELOW, MARCIN WIESNIAK, ANTON ZEILINGER, University of Vienna, Faculty of Physics, IQOQI Vienna, Austrian Academy of Sciences, Austria — Orbital angular momentum (OAM) of single photons has become an often used tool to realize entanglement in higher dimensions [1,2]. Laguerre-Gaussian modes of light with their helical phase structure carry photonic OAM and thus can be used to define an infinitely dimensional discrete Hilbert. However, the creation of photonic OAM entanglement using the well known spontaneous parametric downconversion process is limited by the strongly reduced efficiency for higher momenta [3]. We investigate novel methods to create this entanglement between two photons with a very high difference in their OAM quantum number and momentum respectively. Furthermore we explore hybrid entanglement of photons in these spatial modes and polarization degree of freedom.

[1] G. Molina-Terriza, J. P. Torres, L Torner, Nature Physics 3, 305 (2007)
[2] A. Mair, A. Vaziri, G. Weihs, A. Zeilinger, Nature 412, 313 (2001)
[3] B. Jack, J. Leach, H. Ritsch, S. M. Barnett, M. J. Padgett, S. Franke-Arnold, NJP 11, 103024 (2009)

[1]Supported by ERC (Advanced Grant QIT4QAD) and the Austrian Science Fund (grant F4007).

Monday, March 21, 2011 8:00AM - 11:00AM –
Session A30 DCMP: Graphene: Growth, Properties and Devices C147/154

8:00AM A30.00001 The effects of copper substrate structure and impurities on the quality of graphene growth , CARL W. MAGNUSON, SHANSHAN CHEN, Univ. of Texas at Austin, LUIGI COLOMBO, Texas Instruments, RICHARD D. PINER, RODNEY S. RUOFF, Univ. of Texas at Austin — Since we discovered growth of mono-layer graphene on Cu substrates, most researchers use the same 99.8% pure foil from Afla-Aesar as sited in our original publication. We have investigated several other copper substrates for their suitability for graphene growth. We find that the purity and thickness of the copper foil have measureable effects on the quality of the graphene and growth parameters needed to obtain large mono-layer coverage. We will present our findings and summarize the effects that we have seen. Our methods for determining graphene quality include SEM, scanning micro-Raman, and AFM.

8:12AM A30.00002 Graphene Films Grown on Insulating Substrates[1] , SIARHEI V. SAMSONAU, College of Staten Island CUNY, Graduate Center CUNY, ANNEMARIE L. EXARHOS, MICHAEL E. TURK, JING CAI, The University of Pennsylvania, YURY DESHKO, College of Staten Island CUNY, Graduate Center CUNY, ANSHEL A. GOROKHOVSKY, College of Staten Island CUNY, JAY M. KIKKAWA, The University of Pennsylvania, ALEXANDER M. ZAITSEV, College of Staten Island CUNY — We report a method of direct CVD growth of carbon films on quartz substrates. The films are grown at temperatures from 650 to 1200 °C in a graphite container filled with methane. Films grown at 1200 °C reveal clear G and 2D Raman bands characteristic of graphene. A combination of Raman, absorption and electrical measurements allows us to conclude that carbon films grown by this method are polycrystalline graphene, large areas of which may be composed of single carbon layer. Sheet resistivity of these graphene films is low enough to make them interesting objects for electronic applications. Advantages of our synthetic approach include simplicity and the ability to deposit films on any insulating substrate, which can stand temperature of at least 650 °C. Thus far, no factors limiting the area of deposition and uniformity of the deposited graphene films have been identified.

[1]US Army Research Office (Grant # 47145-00 01) and PSC-CUNY (Grant # 62323-00-40)

8:24AM A30.00003 Electron Stimulated Decomposition of Acetylene as a Precursor for Graphene , MAHESH KUMAR, National Physical Laboratory, New Delhi, SARA ROTHWELL, PHILIP COHEN, University of Minnesota — We report here on the deposition of carbon via C_2H_2 dissociation by electron beam irradiation and thermal decomposition. The substrates investigated include sapphire, silicon, ALD deposited Al_2O_3/SiO_2, and GaN/sapphire. Raman analyses show that on C-plane sapphire both thermal decomposition and electron beam stimulated dissociation of C_2H_2 deposit carbon successfully. On other substrates these methods were inactive, showing the decomposition of C_2H_2 on sapphire is catalytic. We tested different annealing times and C_2H_2 pressures, gauging absorption saturation with RHEED. Samples exposed to 15 min. C_2H_2 adsorption during 400 eV electron irradiation and then annealed for 2 hr. to above 600°C in high vacuum showed the greatest proportion of sp2 to sp3 bonding by Raman analysis. The Raman spectra also suggest hydrogen adsorption, which may hinder further sp2 bonding. Annealing samples in a hydrogen atmosphere does not change their Raman spectra, suggesting hydrogen saturation. Partial support from the University of Minnesota Institute for Renewable Energy and the Environment

8:36AM A30.00004 Electrical and Raman characterizations of chemical vapor deposited (CVD) graphene grains and grain boundaries , LUIS A. JAUREGUI, HELIN CAO, Purdue University, QINGKAI YU, University of Houston, YONG P. CHEN, Purdue University — We performed Raman spectroscopy and electrical transport studies on graphene grains grown on copper foils by ambient pressure CVD. These grains are found to be hexagonally-shaped with edges macroscopically parallel to zig-zag directions as evidenced by scanning tunneling microscopy and transmission electrical microscopy. After the grains are transferred to SiO_2/Si, Raman spectroscopy and mapping are performed. The intensity of the D peak (I_D) is negligibly small over most grain area with the notable exception of a few isolated spots, attributed mostly as nucleation centers. We show Raman mapping is a convenient tool to identify grain boundaries, which show large I_D. Simultaneous measurements of both intra-grain and inter-grain electronic transport were performed on merged grains. We found the inter-grain resistivity to be always larger than the intra-grain resistivity. Low temperature inter-grain magneto-resistance (R_{xx}(B)) displays a prominent weak localization (WL) feature, which was not observable or was much weaker for intra-grain R_{xx}(B). Our observation indicates that grain boundaries are major sources of intervalley scattering and strongly affect electron transport in polycrystalline CVD graphene.

8:48AM A30.00005 Cyclotron Resonance in Graphene at Ultrahigh Magnetic Fields , L.G. BOOSHEHRI, Rice Univ., LANL, C.H. MIELKE, S.A. CROOKER, LANL, L. REN, E.H. HAROZ, Z. JIN, Z. SUN, Z. YAN, J.M. TOUR, J. KONO, Rice Univ. — To investigate the effects of intentional and unintentional doping on the conduction properties of CVD-grown large-area graphene, we have performed high-field cyclotron resonance (CR) measurements on graphene. We accessed ultrahigh magnetic fields using the Single-Turn Coil System at NHMFL-Los Alamos, which can produce peak fields over 300 T in $\sim$2.5 μs pulses. We investigated magneto-infrared transmission at 10.6 μm in pulsed ultrahigh magnetic fields up to 170 T for a variety of graphene samples on KRS-5 substrates with different levels of doping. Circularly polarized CO_2 light was used to determine the carrier type of the doping, and temperature-dependent measurements were also performed. We observed a clear CR peak at $\sim$50 T corresponding to the n = 1 to n = 2 Landau level transition, which indicates that the Fermi energy measured from the Dirac point has to be $\sim$250-400 meV.

9:00AM A30.00006 Measurement of nanomechanical properties of suspended graphene membranes , JI WON SUK, CARL W. MAGNUSON, RICHARD D. PINER, RODNEY S. RUOFF, Univ. of Texas at Austin — Since graphene was first isolated from graphite, its unique properties have been intensively investigated in various ways. Recently, a method to grow large-area, uniform monolayer graphene has been realized by chemical vapor deposition (CVD) on metal substrates. In this respect various properties of CVD-grown graphene need to be studied and compared with those measured from mechanically exfoliated graphene. In this talk we report mechanical measurement of suspended graphene membranes made by CVD on copper foils. Monolayer graphene was transferred onto through holes to make suspended graphene membranes. Bulge testing with uniform pressure was done on those membranes to extract the mechanical properties of CVD-grown monolayer graphene. Moreover, nanoindentation was performed on those suspended graphene membranes and the result is compared with that obtained by bulge testing.

9:12AM A30.00007 Thermal Conductivity of CVD grown graphene , ANTON SIDOROV, DANIEL BENJAMIN, CHRISTOPHER FOY, ZHIGANG JIANG, Georgia Institute of Tecnology, QINGKAI YU, HELIN CAO, WEI WU, ZHIHONG LIU, JIMING BAO, STEVEN PEI, University of Houston, YONG CHEN, Purdue University — When suspended, CVD grown graphene has a high thermal conductivity (k) of 2,500$\pm$1100 W/mK near 350 K. But for practical applications, graphene would be attached to a substrate. Previously it was reported that the CVD grown graphene supported on Si/SiO2 has a k value as low as 370+650/-320 W/mK in ambient. We find that the k of CVD grown graphene on glass varies in a range of 1100 - 2000 W/mK and depends on the growth parameters. The k of graphene is measured by a differential thermocouple technique and compared with that obtained by scanning thermal microscopy. Moreover, the samples grown in ambient pressure have shown higher k compared to the graphene grown at low pressure.

9:24AM A30.00008 Electrochemistry of individual monolayer graphene sheets , WAN LI, CEN TAN, MICHAEL A. LOWE, HÉCTOR D. ABRUÑA, D.C. RALPH, Cornell University — We report on the fabrication and measurement of devices designed to study the electrochemical behavior of individual monolayer graphene sheets. We have examined both mechanically exfoliated and chemical vapor deposited (CVD) graphene. The effective device areas, determined from cyclic voltammetric measurements, show good agreement with the geometric area of the graphene, indicating that the redox reactions occur on relatively clean graphene surfaces. The electron transfer rates of ferrocenemethanol at both types of graphene electrodes were found to be more than 10-fold faster than at the basal plane of bulk graphite, which we ascribe to corrugations in the graphene sheets. We also demonstrate real-time electrochemical detection of molecular desorption from graphene surfaces. Our results show that electrochemistry can provide a powerful means of investigating the kinetics of interactions between molecules and graphene.

9:36AM A30.00009 Mechanical and Electrical Properties of Polycrystalline Graphene , CARLOS RUIZ-VARGAS, AREND VAN DER ZANDE, PINSHANE HUANG, WILLIAM WHITNEY, MARK LEVENDORF, JOSHUA KEVEK, SHIVANK GARG, JONATHAN ALDEN, DAVID MULLER, PAUL MCEUEN, JIWOONG PARK, Cornell University — Graphene grown by chemical vapor deposition (CVD) has enabled large scale fabrication of graphene-based devices [1]. We apply transmission electron microscopy and AFM techniques to identify individual grain boundaries [2]. This further allows the direct investigation of mechanical and electrical properties of polycrystalline graphene in correlation with its grain structure. We used atomic force microscopy in order to induce and image tearing along individual grain boundaries and find a decreased mechanical strength in CVD graphene compared with pristine exfoliated graphene [3]. Our electrical measurements of CVD graphene devices show that charge mobility is sensitive to different growth conditions. However, we found that average grain size is not directly correlated with the charge mobility, suggesting that grain boundaries are not necessarily a dominating factor.

[1]. Li, X. *et al. Science* **2009**, 1312-1314.
[2]. Huang, P *et al. arxiv* **2010,** 1009.4714v1.
[3]. Lee, C. *et al. Science* **2008**, 385-388.

9:48AM A30.00010 Transparent and Flexible Large-scale Graphene-based Heater , JUNMO KANG, SKKU Advanced Institute of Nanotechnology (SAINT) and Center of Human Interface Nano Technology (HINT), Sungkyunkwan University, CHANGGU LEE, YOUNG-JIN KIM, JAE-BOONG CHOI, School of Mechanical Engineering, Sungkyunkwan University, BYUNG HEE HONG, Department of Chemistry, Sungkyunkwan University — We report the application of transparent and flexible heater with high optical transmittance and low sheet resistance using graphene films, showing outstanding thermal and electrical properties. The large-scale graphene films were grown on Cu foil by chemical vapor deposition methods, and transferred to transparent substrates by multiple stacking. The wet chemical doping process enhanced the electrical properties, showing a sheet resistance as low as 35 ohm/sq with 88.5 % transmittance. The temperature response usually depends on the dimension and the sheet resistance of the graphene-based heater. We show that a 4x4 cm^2 heater can reach 80 °C within 40 seconds and large-scale (9x9 cm^2) heater shows uniformly heating performance, which was measured using thermocouple and infra-red camera. These heaters would be very useful for defogging systems and smart windows.

10:00AM A30.00011 Large Area Chemical Vapor Deposition Graphene Photodetectors[1] , ALLEN HSU, MIT, HAN WANG, KI KANG KIM, JING KONG, TOMAS PALACIOS — We investigate large area graphene photodetectors based on graphene grown by Chemical Vapor Deposition on Cu foils and then transferred to SiO_2/Si wafers. Through scanning photocurrent microscopy (SPM) at 532 nm, we compare the performance of CVD fabricated devices using Ti/Pd/Au, Au, and Pt graphene metal junctions with those from literature fabricated through mechanical exfoliation. Our initial experiments show that photocurrent from CVD graphene is about an order of magnitude smaller than devices in literature. Non-idealities related to material properties, defects, and transfer related inhomogenities are believed to be the cause of the discrepancy. These effects are studied through concurrent registration of atomic force microscopy, optical microscopy, Raman Microscopy, and SPM. In addition to intrinsic material property effects, fabrication related issues of graphene-metal junctions are also explored.

[1]ONR Gate Muri, MSD Focus Center, ISN

10:12AM A30.00012 Solution-gated Field Effect Transistors based on CVD grown Graphene for chemical and bio sensing applications , BENJAMIN MAILLY GIACCHETTI, ALLEN HSU, HAN WANG, KI KANG KIM, JING KONG, TOMAS PALACIOS, MIT — Graphene holds great potential for bioelectronic applications and, more specifically, for fast high-sensitivity pH measurements and biosensing. Its monolayer structure (just one carbon atom thick) in combination with its very high carrier mobility enable very high transconductance, low noise and biocompatibility which are key parameters for chemical sensors with electronic readout. In fact, single molecule detection has already been demonstrated in graphene gas sensors. In this paper we report on the fabrication and characterization of solution-gated field effect transistors (SGFET) arrays based on CVD grown graphene films on copper that can operate in various liquid environments. These devices exhibit transconductances around 20 μSiemens, which highlights their excellent sensitivity. We also performed some pH sensing experiments and demonstrated that the transfer characteristics of the GFET are pH dependent with a pH sensitivity of 14 mV/pH. These results drive the way for chemical and bio-sensing by functionalized graphene, which is the aim of our future work.

10:24AM A30.00013 PECVD silicon nitride gate dielectrics and band-gap engineering in graphene devices , WENJUAN ZHU, DEBORAH NEUMAYER, VASILI PEREBEINOS, PHAEDON AVOURIS, IBM - T.J. Watson Research Center — We found that silicon nitride can provide excellent coverage of graphene in field-effect transistors while preserving its good carrier mobilities, without the need of a seed layer. Moreover, the silicon nitride film has the advantage of higher dielectric constant and higher surface polar optical phonon energy (i.e. less remote phonon scattering in the graphene channel) compared to silicon oxide. The breakdown strength in silicon nitride is high as well. The effect of a perpendicular electric field on the band-structure of different numbers of graphene layers used as channels of the transistor was also studied and the induced band-gap or band-overlap was obtained accounting for the effects of the variation of the surface potential near the Dirac/neutrality point.

10:36AM A30.00014 Graphene: Atomically thin protective coating , DHIRAJ PRASAI, KIRILL BOLOTIN, Department of Physics and Astronomy, Vanderbilt University, JUAN TUBERQUIA, ROBERT HARL, KANE JENNINGS, Chemical and Biomolecular Engineering, Vanderbilt University — We explore the properties of graphene as a cathodic coating to protect copper substrates from oxidation and further corrosion. High-quality and large area graphene films are grown on copper substrates by chemical vapor deposition. Samples were thermally oxidized in an oxygen-rich environment. X-ray photoelectron spectroscopy (XPS) characterization of a Graphene/copper and bare copper samples reveals the absence of oxidized copper at the graphene/copper interface indicating that the graphene monolayer protects the underlying copper. We also determine the protective properties of graphene in aqueous media using electrochemical characterization techniques. First, we use Electrochemical Impedance Spectroscopy (EIS) to show that graphene coated substrates lower frequencies (1Hz) exhibit impedance values 2 orders of magnitude higher compared to bare Cu substrates. Cyclic voltammetry also shows that a monolayer of graphene significantly reduces the oxygen reduction, thus exhibiting little charge transfer at the solid-liquid interface. Finally, we use Tafel analysis to estimate that the corrosion rate exhibited by Graphene/Cu is ~ 7 times lower than that of bare Cu substrates.

10:48AM A30.00015 Ordered carbon nanotube growth on graphene and few-layer graphene , D. PATRICK HUNLEY, STEPHEN JOHNSON, JOSEPH STIEHA, ABHISHEK SUNDARARAJAN, AARON MEACHAM, DOUGLAS STRACHAN, University of Kentucky — Carbon nanotubes are grown on graphene and few-layer graphene films through chemical vapor deposition. The nanotube growth is found to depend on the thickness of the few-layer graphene films. The thinnest films show significant alignment of the nanotubes with the crystallographic axes of the graphene. This alignment is compared to the orientation of the crystallographic etch tracks, permitting the orientation of the nanotubes to be determined. Related nanotube/graphene structures will also be presented and discussed. Supported in part by NSF Award No. DMR-0805136, the Kentucky NSF EPSCoR program, the University of Kentucky Center for Advanced Materials, and the University of Kentucky Center for Nanoscale Science and Engineering.

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A31 DMP: Focus Session: van der Waals Bonding in Advanced Materials: Fundamentals and Simple Systems C145

8:00AM A31.00001 Cohesive Properties of Graphitics and the Random Phase Approximation[1] , JOHN DOBSON, Micro and Nano Technology Centre, Griffith University, Australia — The van der Waals-dominated cohesive energetics of graphitic systems is important in the assembly of many graphene-based nanostructures of current technological interest. In 2006 an unusual power law E = - cD^{-3} was predicted [1] for the van der Waals (vdW, dispersion) interaction energy between parallel graphene sheets at large separations D. By contrast, a conventional sum of pairwise R^{-6} contributions yields E = .- kD^{-4}. The unexpected D^{-3} result came from the electronic correlation energy within the Random Phase Approximation (RPA), which can be solved analytically in the distant regime D .→ .∞. In keeping with other unusual properties of graphene, in this distant non-overlapping regime the relevant response function of a graphene sheet is dominated by the gapless electronic transitions near the Dirac points in the Brillouin Zone where the .π_z and .π_z Bloch bands touch. The D·$^{-3}$ result corresponds to a severe failure of pairwise additivity of the vdW interaction between local spatial regions of the sheets, and so could have implications for the most-used nanoscale energy functionals (e.g. [2,3]); these embody pairwise additivity at various levels. It has remained unclear what this result might imply for the interaction between graphene sheets at smaller spacings near to the equilibrium separation, where the response is sampled at shorter wavelengths so that analytic results cannot be obtained. Very recently, numerically well-converged exact-exchange and RPA correlation energies have been obtained for stretched graphite at a wide range of inter-layer spacings down to the equilibrium distance. These results and their implications will be discussed.

[1]Support is acknowledged from FAST, Egide and the Australian Research Council.

8:36AM A31.00002 Self-consistent calculations of correlation energies within the random phase approximation[1] , STEFANO DE GIRONCOLI, NGOC LINH NGUYEN, SISSA and CNR-IOM DEMOCRITOS,Trieste, Italy, VIET HUY NGUYEN, GIULIA GALLI, University of California, Davis, USA — Calculations of correlation energies within the the formally exact Adiabatic Connection Fluctuation-Dissipation (ACFD) formalism, within the Random Phase Approximation (RPA) for the exchange-correlation kernel, have been recently carried out for a number of isolated and condensed systems. The efficiency of such calculations has been greatly improved by exploiting iterative algorithms to diagonalize RPA dielectric matrices [1]. Unfortunately, for several systems, it has been found that RPA correlation energies may significantly depend about the choice of input single particle wavefunctions [2]. In this work, we derive an expression of the RPA self-consistent potential based on Density Functional Perturbation theory and we present self-consistent RPA calculations for weakly bound molecular dimers, including the controversial case of the Beryllium dimer.

[1] H.-V. Nguyen and S. de Gironcoli, Phys. Rev. B 79, 205114 (2009); H. F. Wilson, F. Gygi, and G. Galli, Phys. Rev. B 78, 113303 (2008).
[2] Huy-Viet Nguyen and G.Galli, J. Chem.Phys. 132, 044109 (2010).

[1]Work partly supported by DOE-scidac-e DE-FC02-06ER25777.

8:48AM A31.00003 Beyond RPA correlation energies: Evaluation of model exchange-correlation kernels , DEYU LU, Center for Functional Nanomaterials, Brookhaven National Laboratory, GIULIA GALLI, Department of Chemistry and Department of Physics, University of California, Davis — The description of van der Waals dispersion interactions using the so called EXX/RPA method has recently attracted a widespread interest. Overall, equilibrium distances and cohesive energies of weakly bound molecular systems exhibit a significant improvement over the the results of semi-local Density Functional Theory calculations [1,2], due to the proper inclusion of long-range correlation effects. However, cohesive energies still result to be underestimated with respect to experiments in several cases. This is mainly due to the neglect of the exchange-correlation kernel in evaluating response functions entering the correlation energy expression. In this work, we study the effect of several model exchange-correlation kernels and evaluate their performance for molecular systems.

[1] D. Lu, Y. Li, D. Rocca and G. Galli, Phys. Rev. Lett. 102, 206411 (2009)
[2] Y. Li, D. Lu, H-V Nguyen and G. Galli, J. Phys. Chem. A, 114, 1944-1952 (2010) and D. Lu, H-V Nguyen, and G. Galli, J. Chem. Phys. 133, 154110 (2010)

9:00AM A31.00004 Van der Waals interactions in complex materials: Beyond the pairwise approximation , ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG, ROBERT A. DISTASIO, JR., ROBERTO CAR, Princeton University, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG — Despite the well-known fact that van der Waals (vdW) interactions are many-body in nature and the polarizability is a non-local function, popular vdW-DF [1] and DFT+vdW [2] methods are based on (semi)-local approximations for the polarizability and only model the pairwise part of vdW interactions. Here we show how to go beyond the pairwise (semi)-local approximation to vdW interactions by coupling the recently developed TS scheme [2] with the Fluctuating-Coupled-Dipole Model (CFDM) [3]. The TS scheme provides parameter-free input atomic polarizability distributions and the CFDM allows to model both polarizing and depolarizing local fields, and captures the many-body nature of vdW interactions. Results are presented for small and medium-size molecules, as well as solids. We find that the many-body screening plays a major role in modifying the polarizability of large systems. Our results for vdW coefficients in semiconductor clusters and solids are in excellent agreement with TDDFT calculations. [1] M. Dion *et al.*, Phys. Rev. Lett., **92**, 246401 (2004); [2] A. Tkatchenko and M. Scheffler, Phys. Rev. Lett., **102**, 073005 (2009); [3] M. W. Cole *et al.*, Mol. Simul. **35**, 849 (2009).

9:12AM A31.00005 Van der Waals materials: what is the origin of the disagreement between ab initio calculations and experiments? , LOREDANA VALENZANO, WARREN PERGER, JACKSON CRISWELL, WILLIAM SLOUGH, Michigan Tech Univ — The robust prediction of accurate physical properties for molecular solids from first-principles calculations continues to present a significant challenge across a wide variety of scientific disciplines. Comparison between computed and experimental values for physical properties derived from differences between states is often promising (such as bulk modulus), however the result is disappointing for absolute values (such as density). Accurate ab initio calculations describe physics occurring at zero Kelvin; but, properties evaluated experimentally are mostly reported at room temperature. Therefore it should hardly be surprising that ab initio results differ dramatically from experimentally measured values. We show how the results from a calculation at zero Kelvin may be compared to experimental values at higher temperatures, helping to foster a stronger linkage between computational and experimental work on systems such as energetic and pharmaceutical materials and metal-organic frameworks in interaction with guest molecules. Among others, investigated behavior comprises mechanical (elastic constants) and vibrational (infrared and Raman spectra) properties. The computational approach adopted, takes into account van der Waals long-range dispersion interaction through an empirical "a posteriori" approach, appropriately fitted to investigate solid materials.

9:24AM A31.00006 Van der Waals interactions in semiconductor solids , GUO-XU ZHANG, ALEXANDRE TKATCHENKO, JOACHIM PAIER, HEIKO APPEL, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft — The binding in semiconductor solids arises mainly from the covalent hybridization of atomic orbitals. Hence, it is typically assumed that van der Waals (vdW) interactions play a minor role for their cohesion. In order to probe this conventional wisdom we develop a method to calculate accurate long-range vdW coefficients for ions and atoms in crystals. We first assess the validity of the Clausius-Mossotti relation between the polarizability and dielectric function for bulk semiconductors by comparing periodic TDDFT calculations to direct extrapolation of the frequency-dependent TDDFT polarizability for finite clusters. We find a good agreement between these two approaches for computing vdW $C_6(V)$ coefficients for a broad variation in the unit cell volume V for diamond, Si, and Ge crystals. When using TDDFT@HSE with the Nanoquanta kernel, the volume-dependent dielectric constant of Si and Ge is in excellent agreement with experimental data. The crystal-field screening reduces the vdW coefficients by a factor of two compared to corresponding free-atom and effective hybridized $C_6[n(r)]$ values [1]. The use of accurate $C_6(V)$ coefficients in the PBE+vdW method [1] improves cohesive properties of Si and Ge in comparison to experimental data. [1] A. Tkatchenko and M. Scheffler, Phys. Rev. Lett. **102**, 073005 (2009).

9:36AM A31.00007 Van der Waals density functionals applied to solids , JIRI KLIMES, London Centre for Nanotechnology, University College London, DAVID BOWLER, London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, ANGELOS MICHAELIDES, London Centre for Nanotechnology, University College London — Dispersion interactions are ubiquitous in nature and contribute to the binding in biomolecules or to the adsorption of molecules on surfaces. However, due to their non-local nature they are difficult to describe accurately with electronic structure methods. It is now well established that standard density functional theory functionals give misleading results for systems where dispersion is important. The van der Waals density functional (vdW-DF) of Dion et al. [Dion et al., Phys. Rev. Lett. 92, 246401 (2004)] is one of several promising approaches for accounting for dispersion. We have shown that with an improved treatment of the exchange part it can offer much better than chemical accuracy for a range of weakly interacting molecular systems [Klimeš et al., J. Phys.: Cond. Matt. 22, 022201 (2010)]. Here we extend this work beyond the weakly bonded regime and report results for lattice constants of solids (metals, semiconductors, ionic solids) and geometries and atomization energies of molecules. This extensive and rigorous test of vdW-DF shows how to a large extent such properties are dependent on its underlying exchange functional. We use this new insight to discuss prospects for further improvement of the method.

9:48AM A31.00008 Application of van der Waals Density Functionals to Extended Systems[1] , KYUHO LEE, DAVID C. LANGRETH, Rutgers University — Recently we proposed[2] a second version of a van der Waals density functional[3] and showed its accuracy for small molecular duplexes as well as a few extended systems. As further applications to extended systems, we present results for molecular adsorptions on surfaces, molecular crystals, and organic ferroelectrics. A comparison with experiments is also given for different functionals.

[1]Work supported by NSF grant DMR-0801343.

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

[3]M. Dion, H. Rydberg, E. Schröder, D. C. Langreth, and B. I. Lundqvist, Phys. Rev. Lett. **92**, 246401 (2004); T. Thonhauser, V. R. Cooper, S. Li, A. Puzder, P. Hyldgaard, and D. C. Langreth, Phys. Rev. B **76**, 125112 (2007).

10:00AM A31.00009 An Efficient Real-Space Implementation of the van der Waals Energy and Analytical Forces in Plane-Wave Ab Initio Molecular Dynamics , ROBERT DISTASIO, ZHAOFENG LI, ULRICH ASCHAUER, Princeton University, XIFAN WU, Temple University, ROBERTO CAR, Princeton University — In this work, we present an efficient algorithmic implementation of the energy and analytical forces of the recent density functional based van der Waals (vdW) correction proposed by Tkatchenko and Scheffler (PRL 102, 073005 (2009)) within the framework of plane-wave based ab initio molecular dynamics. The algorithm presented herein is a highly parallelizable, order (N) formulation that allows for accurate treatment of large molecular systems with a computational cost that is negligible with respect to the underlying evaluation of the exchange-correlation functional. The computational resources and performance of our algorithm, which utilizes a real-space implementation of the molecular pro-density, will be analyzed and compared against a reciprocal-space formulation of the Hirshfeld volume based on a spherical wave expansion of the underlying plane-wave basis. The effects of this vdW correction are demonstrated within the context of the oxygen-oxygen and oxygen-hydrogen radial distribution functions obtained via highly accurate PBE0-based liquid water simulations.

10:12AM A31.00010 Comparison of methods for inclusion of van der Waals interactions: the case of physisorption of nucleobases on graphene[1] , DUY LE, ABDELKADER KARA, TALAT S. RAHMAN, University of Central Florida — The physisorption of the nucleobases adenine (A), cytosine (C), guanine (G), thymine (T), and uracil (U) on graphene is studied using many flavors of density functional theory (DFT): the generalized gradient approximation (GGA) with the inclusion of van der Waals (vdW) interaction based on the TS approach [A. Tkatchenko and M. Scheffler, *PRL* **102**, 073005 (2009)], our simplified version of this approach, the vdW density functional (vdW-DF) [M. Dion *et al.*, *PRL* **92**, 246401 (2004)], and the vdW-DF2 [K. Lee *et al.*, *PRB* **82**, 081101 (2010)] methods. The binding energies of nucleobases on graphene lie in the range of 496962 meV and are found to be in the following order G>A>T>C>U within vdW-DF, vdW-DF2 and our method and G>A>T∼C>U in the TS approach. The binding separations lie between 3.293.53 Å and are found to be about 0.1 0.2 Å shorter in DFT-D, as compared to vdW-DF approaches. We comment on the efficiency of combining the DFT-D and vdW-DF methods to study vdW interactions in molecular adsorption.

[1]Work supported by DOE Grant No. DE-FG02-07ER15842.

10:24AM A31.00011 Spinodal de-wetting of thin films in the presence of oscillatory Casimir forces

, LEONARDO GOLUBOVIC, ADI CONSTANTINESCU, West Virginia University — Long range de-wetting forces, e.g., van der Waals interactions, may drive the formation of large clusters in thin films of polymeric materials, and in liquid and solid metals films. We elucidate film de-wetting in the presence of spatially oscillatory Casimir forces, such as the fermionic Casimir forces mediated by conducting electrons in metal films. What happens with interfaces of a liquid metal film in the presence of the spatially oscillating forces? Is the film going to exhibit spinodal de-wetting instability yielding the formation of clusters ? We find that, at low temperatures, the film interface pins to the minima of the oscillatory Casimir force potential. This suppresses the spinodal de-wetting. However, at elevated temperatures, the interface efficiently hops between the minima of the oscillatory potential, and the film quickly de-wets and structures into clusters. The spinodal de-wetting is governed by an effective non-oscillatory de-wetting potential that entropically emerges from a coarse-graining of the oscillatory Casimir force potential.

10:36AM A31.00012 Dynamic Precision Measurement of the Casimir Force Using Gold Surface

, CHIA-CHENG CHANG, UC Riverside Physics Dept., UMAR MOHIDEEN — High precision dynamic Casimir force measurements between a gold coated sphere and plate are performed in UHV with short coherence length light source interferometer will be presented. A comparison to the theory using generalized Plasma and Drude model at room temperature will be discussed.

10:48AM A31.00013 Inelastic Helium Atom Scattering from the Commensurate Monolayer Solid H_2/NaCl(001)

, L.W. BRUCH, Department of Physics, University of Wisconsin-Madison, F.Y. HANSEN, Department of Chemistry, Technical University of Denmark — A calculation of inelastic low energy helium atomic scattering by a monolayer with one-phonon creation[1] is reported for the dilated quantum monolayer solid H_2/NaCl(001). The shear horizontal phonon mode again is accessed for small misalignment of the scattering plane relative to the monolayer axes. Qualitative agreement for the systematic trends in the inelastic scattering experiments[2] is achieved. Two monolayer phonon branches are identified. The role of the Debye-Waller attenuation in diffraction intensities is discussed.

[1]F. Y. Hansen and L. W. Bruch, J. Chem. Phys. **127**, 204708 (2007)
[2]F. Traeger and J. P. Toennies, J. Phys. Chem. B **108**, 14710 (2004)

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A32 DMP: Focus Session: Optical Properties of Nanostructures and Metamaterials I

C144

8:00AM A32.00001 Ultra-low Damping of Surface Plasmon Polaritons in Atomically Smooth Epitaxial Ag Films: An Extraordinary Optical Transmission Study

, CHARLOTTE E. SANDERS, UT Austin, B.H. LI, Chinese Academy of Sciences, Institute of Physics, Beijing, JAMES MCILHARGEY, S. HOSSEIN MOUSAVI, ALEXANDER B. KHANIKAEV, UT Austin, X.G. QIU, Chinese Academy of Sciences, Institute of Physics, Beijing, GENNADY SHVETS, C.K. SHIH, UT Austin — When an electro-magnetic radiation field couples strongly to surface plasmons, a surface plasmon polariton (SPP) is formed. In recent years, studies of SPPs in metal films perforated with hole lattices have revealed broad technological implications ranging from exotic metamaterials for sub-wavelength resolution microscopy to ultra-compact plasmonic waveguides for optical interconnects, as well as many other exciting technological applications. Thus far, most investigations have employed dielectric/metal hybrid structures with granular polycrystalline metal films. Although many conceptual devices have been demonstrated, one factor significantly limits their technological potential: the strong damping of SPP propagation. By using atomically smooth, epitaxial Ag films we show that such a damping effect can be mostly eliminated, resulting in nearly ideal extraordinary optical transmission (EOT) through sub-wavelength hole arrays in the mid-infrared range. This also allows us to map out very detailed SPP band structure, with analogy to the electronic band structure in solids.

8:12AM A32.00002 Visualization of Coherent Processes in Plasmonic Interference Transparency

, ZILIANG YE, SHUANG ZHANG, YUAN WANG, YONG-SHIK PARK, XIAOBO YIN, THOMAS ZENTGRAF, GUY BARTAL, XIANG ZHANG[1], University of California, Berkeley — Recently, optical analogs that mimic the dynamics of atomic EIT are attracting attention since they could maintain coherence at room temperature and are easier to fabricate as well as to integrate. However, the understanding of the relationship between atomic EIT and its classical counterparts still remains on the spectroscopic level, which strongly limits the applicability of the analogy. As the coherent evolution of a quantum system is characterized by the oscillatory population transferring between the states, here, we map the coherent oscillation strength of a plamonic interference transparency (PIT) structure and show that there is a deeper resemblance embedded in the analogy: both systems are populated in the 'dark' state at the transparency point.

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8:24AM A32.00003 Polarization-sensitive optical response of plasmonic metasurfaces[1]

, PAUL G. THOMPSON, CLAUDIU G. BIRIS, EDWARD J. OSLEY, University College London, RICHARD M. OSGOOD, JR., Columbia University, NICOLAE C. PANOIU, PAUL A. WARBURTON, University College London — We have fabricated arrays of nanoscale asymmetric cruciform apertures that support localized surface-plasmon polaritons (LSPPs) in the lower mid-infrared. The cruciform apertures were created by focussed ion beam milling into a gold film on a CaF_2 substrate. The measured transmission spectra of these arrays show two distinct maxima that correspond to the excitation of LSPPs, the magnitude of which can be tuned by varying the in-plane electric-field polarization of the incident photons. These findings are further validated by simulations based on the rigorous coupled-wave analysis method, namely, the maxima of the transmission spectra correspond to hybridized localized surface plasmon resonances in the two arms of the cruciform aperture. More generally speaking, it is demonstrated that the planar distribution of polarization-dependent LSPPs can be viewed to form a polarization-sensitive plasmonic metasurface. We will discuss possible applications of these plasmonic arrays in biosensing.

[1]Supported by NSF/EPSRC Materials World Network

8:36AM A32.00004 Designer plasmonic structures and metamaterials for subwavelength photonics , FEDERICO CAPASSO, Harvard University — Plasmonic structures and metamaterials have opened up new opportunities for manipulating light at subwavelength scales thus opening up new frontiers in optical materials design and photonics in such areas as imaging, sensing and new optical sources. In this talk I will present recent research from our group in this area. Through innovative use of plasmonic structures we have demonstrated how one can design the far field and near field of state of the art semiconductor lasers and optical fibers. Examples are plasmonic laser antennas creating ultrahigh intense near field nanospots in the near infrared, mid-infrared semiconductor lasers with very low divergence and control of polarization (linear/circular) as well as multibeam lasers. Metamaterials have created unique opportunities for nanophotonics. Recently we have shown that by patterning the facet of Terahertz quantum cascade lasers with subwavelength periodic structures one can dramatically modify the surface plasmon dispersion curve which leads to a highly collimated THz beam with divergence reduced from 180 deg to 5 deg. I will also discuss work on new clusters of colloidal core-shell metallic nanoparticles using self-assembly techniques. Magnetic activity in trimers at near infrared wavelengths and strikingly pronounced Fano-like resonances in heptamers are among the exciting new findings from light scattering experiments. Such building blocks are an important stepping stone towards novel designer metamaterials synthesized bottom up. Finally experiments with gold plasmonic nanocavity gratings have shown that the latter can dramatically enhance surface nonlinear optical processes. The four-wave mixing signal was enhanced by a factor up to 2000, two orders of magnitude higher than previously reported.

9:12AM A32.00005 Experimental demonstration of gradient index plasmonics , MAIKEN H. MIKKELSEN, THOMAS ZENTGRAF, YONGMIN LIU, JASON VALENTINE, XIANG ZHANG, NSF Nanoscale Science and Engineering Center, University of California, Berkeley — Plasmonics is an emerging field essential for bridging nanoelectronics and diffraction-limited photonics. One central objective of plasmonics research is modifying the propagation of surface plasmon polaritons (SPPs) in order to implement diverse functionalities in the context of two-dimensional optics. Here, we demonstrate an effective approach to manipulate SPPs by adiabatically tailoring the topology of a dielectric layer adjacent to a metal surface using grey-scale lithography. In such a way, we are able to continuously modify the propagation constant of SPPs, analogous to traditional gradient index optics. Applying this method, we design and experimentally demonstrate two different devices: a plasmonic Luneburg lens to focus SPPs and a plasmonic Eaton lens to bend SPPs.[1] Our approach has the potential to achieve low-loss functional plasmonic elements and provides a scheme to realize more complex structures using transformation optics.

[1]T. Zentgraf*, Y. Liu*, M. H. Mikkelsen*, J. Valentine, X. Zhang, *Submitted*, (2010)

9:24AM A32.00006 Propagation of surface plasmons on highly anisotropic dielectric substrates[1] , NAGARAJ NAGARAJ, ARKADII KROKHIN, University of North Texas — We calculate the propagation length of surface plasmons in dielectric-metal-dielectric structures with anisotropic substrates. We show that the proper orientation of the optical axis of the crystal with respect to the metal surface minimizes Joule losses enhancing the propagation length of surface plasmons. The propagation length in a wide range of frequencies including the telecommunications region is analyzed. A simple Kronig-Penney model for anisotropic plasmonic crystal where the substrate is a periodic sequence of dielectric delta-peaks is also proposed. In this model the dispersion relation for surface plasmon has a band structure where the band width tends to zero when the frequency approaches the resonant frequency.

[1]This work was supported by the US Department of Energy through Grant No. DE-FG02-06ER46312.

9:36AM A32.00007 Metal-less Plasmonics: Surface Electromagnetic Waves in Dielectric Mulitlayers , WILLIAM ROBERTSON, Department of Physics & Astronomy and Computational Science Program, Middle Tennessee State University — The use of suitably designed dielectric multilayers is demonstrated as an alternative to metal films for the generation of surface-bound electromagnetic waves. The growing field of plasmonics invokes the sub-wavelength resolution, resonant optical coupling, and high surface fields of surface plasmons for applications such as high-resolution lithography, biosensing, optical circuits, and enhanced non-linear optic phenomena. Surface electromagnetic waves with characteristics similar to surface plasmons can be generated in dielectric multilayer stacks. The dielectric loss in multilayers is much less than for surface plasmons in metal films leading to sharper coupling resonances, higher surface fields, and longer propagation distances than for surface plasmons. These features are advantageous for current and projected applications in plasmonics. Additionally, the wavelength of coupling and the dispersion of the surface electromagnetic waves can be engineered by the multilayer design. Examples of the use of surface electromagnetic waves in multilayers for bio-sensing will be presented.

9:48AM A32.00008 Dispersion and Mirage of Surface Plasmon Waves in Metallic Photonic Crystals[1] , CHEUNG WAI CHAU, YUN SAN CHAN, MING JIE ZHENG[2], KIN WAH YU, The Chinese University of Hong Kong — We have studied the dispersion and propagation of surface plasmon (SP) waves in a one-dimensional metallic photonic crystal composed of metal-dielectric multilayered films by a transfer matrix method. By virtue of Bloch theorem, we are able to obtain the dispersion (frequency-wavevector) relation for arbitrary oblique propagation of SP waves for various non-zero transverse wavevectors. Model calculations are performed for alternative gold and MgF_2 films to obtain the photonic band-gap structure. For a progressively decreasing gold film thickness, the band (gap) width increases (decreases), rendering a precise and feasible tunability of photonic band gaps. Moreover, by imposing a gradual variation in the thickness of dielectric along the multilayers, it is possible to alter the dispersion relation locally, allowing us to study the bending of SP wave at various incident angles. We use Hamiltonian optics approach to obtain the trajectories of propagation. As the transverse wavevector is a constant of motion for a certain incident angle, we obtain different mirage at various oblique incidence. The results are useful for achieving superbending of SP waves.

[1]Supported by the General Research Fund of the HKSAR Government.
[2]Now in University of Wisconsin - Madison

10:00AM A32.00009 Plasmonic Forces in Nanoscale Metal Clusters , PHILIP BATSON, Rutgers University, USA, ALEJANDRO REYES-CORONADO, Donostia International Physics Center, Spain, RUBEN BARRERA, Universidad Nacional Autonoma de Mexico, Mexico, PEDRO ECHENIQUE, JAVIER AIZPURUA, Donostia International Physics Center, Spain — Passage of keV-energy electrons near nanometer-sized metal clusters is known to transfer energy from the electron to the clusters by excitation of surface plasmons. In groups of clusters, these plasmon modes couple, producing inter-cluster forces which favor coalescence. A single cluster is also expected to experience a smaller, attractive, force in the presence of a passing electron from simple image charge considerations. Detailed calculations that evaluate the Maxwell Force Tensor for plasmonic modes confirm this for large impact parameters, but for small impact parameters, comparable or less than the cluster diameter, the plasmonic force becomes repulsive. We have verified this behavior experimentally, using a sub-Angstrom electron beam at 120 KeV to move nano-scale Au clusters, discovering a weak attractive motion for large impact parameters and a stronger, repulsive motion for small impact parameters. We will present this finding and suggest physical reasons for this non-intuitive behavior.

10:12AM A32.00010 Optical properties of subwavelength plasmonic structures , ZHU YONGYUAN, Nanjing University — Some recent progress achieved in our group will be reported here, focusing on the optical properties of subwavelength holes and metallic particles. By dressing the periodic holes with the metallic components, new transmission features, such as the enhanced transmission due to the magnetic resonance, the peak splitting due to the hole symmetry breaking etc. can be obtained. With the multilayer slit gratings, the transmission resonance associated with the longitudinal interference effect as well as the tuning of spectrum by the temperature control have been realized. In addition, the plasmon resonance of isolated gold nanorod particles and the plasmonic waveguiding using a linear chain of nanorod particles have been studied. In addition, due to the strong coupling between the incident light and vibrations of free electrons, a bulk polariton mode can be induced in a plasmonic crystal composed of gold nanorod particles. The fundamental equations governing the coupling have been developed and the long-wavelength optical properties of the crystal have been suggested.

10:24AM A32.00011 Screening effect on the polaron by surface plasmons[1] , XIAOYING XU, XIAOSHAN XU, Oak Ridge National Lab, KATYAYANI SEAL, HANGWEN GUO, Oak Ridge National Lab; The University of Tennessee, JIAN SHEN, Fudan University; The University of Tennessee, LOW DIMENSIONAL MATERIALS PHYSICS, OAK RIDGE NATIONAL LAB TEAM, THE UNIVERSITY OF TENNESSEE TEAM, PHYSICS DEPARTMENT, FUDAN UNIVERSITY TEAM — Surface plasmons occur when the conduction electrons at a metal/dielectric interface resonantly interact with external electromagnetic fields. While surface plasmons in vicinity of a polaron in the dielectric material, a strong screening effect on polaron characteristics is introduced. In this work, we observed the reduction of polarons in multiferroic LuFe2O4, which is mainly contributed by surface plasmons.

[1]Research sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U. S. Department of Energy.

10:36AM A32.00012 Surface Plasmon Polaritons: Geometric Resonance at Singularities , YUN-SHAN WANG, University of Notre Dame, Department of Chemical and Biomolecular Engineering, Graduate Student, HSUEH-CHIA CHANG, University of Notre Dame, Department of Chemical and Biomolecular Engineering, Professor — Unlike planar plasmonic waves, the electric field of radially confined surface plasmon polariton (SPP) at a geometric singularity does not decay from the interface, but rather interacts around the singularity. A discrete SPP spectral theory for solid and hollow cones/wedges shows that the resulting azimuthal optical capacitor produces an infra-red shift of the classical planar plasmonic resonant frequency with a larger bandwidth at small angles. An analysis of the conformal map between the complex spectral space and the complex permittivity space shows the resonant SPPs can be sustained by materials with positive permittivity, although negative permittivity provides higher intensification. Asymptotic analysis of the SPP dispersion relationship also provides a closed-form estimate of the optimum angle due to enhanced conductive loss at small angles and also a prediction of optimal frequency. Experimental confirmation with transmission and scattering measurements will also be reported.

10:48AM A32.00013 ABSTRACT WITHDRAWN –

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A33 DMP DCOMP: Focus Session: Dielectric, Ferroelectric, and Piezoelectric Oxides: Piezoelectrics, Oxides on Semiconductors, and Applications C143/149

8:00AM A33.00001 High-Throughput Density Functional Theory Categorization of Ferroelectric Ternary Perovskite Oxides for Use as High-Performance Piezoelectrics , RICKARD ARMIENTO, Massachusetts Institute of Technology, BORIS KOZINSKY, Bosch Research and Technology Center, MARCO FORNARI, Central Michigan University, GERBRAND CEDER, Massachusetts Institute of Technology — We present a nearly exhaustive density functional theory (DFT) survey over the chemical space of perovskite compounds on ABO3 form, with the aim of identifying alloy end points for new piezoelectric materials. Our screening criteria on the DFT results selects 85 relevant compounds, among which all well known alloy end points for high performance piezoelectrics are present. We analyze the compounds with respect to macroscopic polarization, born effective charges, and energy differences between different structure distortions. We discuss the energy features that cause the high piezoelectric performance of the well known piezoelectric lead zirconate titanate (PZT), and to what extent these features are rare among the found compounds. The results are used to discuss relevant isovalent alloys of the selected compounds.

8:12AM A33.00002 Searching for ferroelectricity and piezoelectricity in Heusler compounds using first-principles calculations , ANINDYA ROY, JOSEPH BENNETT, KARIN M. RABE, DAVID VANDERBILT, Rutgers University — Hundreds of half Heusler (HH) and full Heusler (FH) compounds have been synthesized, and they exhibit a multitude of properties. However, we are unaware of any Heusler compounds showing ferroelectricity (FE), or for which the piezoelectricity (PzE) has been measured. Determining these polar properties would be of theoretical interest as well as having practical importance for the design of new functional materials. In this *ab initio* study, we search a large set of HH and FH compounds, both known and hypothetical, for FE/PzE. We screen the zone-center phonons, computed with first-principles density-functional-theory methods, for unstable polar modes that would drive a distortion to a ferroelectric phase, and calculate PzE coefficients of compounds in the $F\bar{4}3m$ space group, which includes all HH and many FH, using density-functional perturbation theory. Preliminary results from our calculations confirm that the Heusler compounds are very robust against FE instabilities. However, we found several HH compounds having e_{14} coefficients in the range of 0.5-1.0 C/m^2, comparable to that of some well-known piezoelectric materials such as ZnO. We also investigate the effects of epitaxial constraints on these properties, both for bulk materials and for superlattices built of Heusler materials.

8:24AM A33.00003 Origin of the anomalous piezoelectric response in wurtzite $Sc_xAl_{1-x}N$ alloys[1] , FERENC TASNADI, BJORN ALLING, CARINA HOGLUND, GUNILLA WINGQVIST, JENS BIRCH, LARS HULTMAN, IGOR A. ABRIKOSOV[2], Department of Physics, Chemistry and Biology (IFM), Linkoping University, Sweden, IFM COLLABORATION — We present the theory that reveals the origin of the observed anomalous enhancement of piezoelectric response in wurtzite $Sc_xAl_{1-x}N$ alloys [1]. Our first-principles calculations confirm that the 400% increase of the piezoelectric constant is an intrinsic alloying effect. The energy surface topology is found to be strongly influenced by the alloying, being elongated around the global minimum along c=a direction. This leads to the large elastic softening along the crystal parameter c, and raises significantly the intrinsic sensitivity to axial strain resulting in the highly increased piezoelectric constant. The effect is particularly accentuated at intermediate compositions where the elongated double-minimum energy landscape is flattened due to the energy proximity of the wurtzite and so far experimentally unknown hexagonal phases of these alloys. Our observation provides a route for the design of materials with high piezoelectric response.

[1] F. Tasnadi, *et al.,* Phys. Rev. Lett. **104**, 137601 (2010).

[1]The Swedish Foundation for Strategic Research (SSF) is acknowledged.

[2]Presenting author

8:36AM A33.00004 Giant piezoelectricity on Si for hyper-active MEMS , CHANG-BEOM EOM, University of Wisconsin-Madison — Smart materials that can sense, manipulate, and position are crucial to the functionality of micro- and nano-machines. Integration of single crystal piezoelectric films on silicon offers the opportunity of high performance piezoelectric microelectromechanical systems (MEMS) incorporating all the advantages of large scale integration on silicon substrates with on-board electronic circuits, improving performance and eliminating common failure points associated with heterogeneous integration. We have fabricated oxide heterostructures with the highest piezoelectric coefficients and figure of merit for piezoelectric energy harvesting system ever realized on silicon substrates by synthesizing epitaxial thin films of $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$(PMN-PT) on vicinal (001) Si wafers using an epitaxial (001) $SrTiO_3$ template layer. We have also demonstrated fabrication of PMN-PT cantilevers, whose mechanical behavior is consistent with theoretical calculations using the material constants of a bulk PMN-PT single crystal. These epitaxial heterostructures with giant piezoelectricity can be used for MEMS or NEMS devices that function with low drive voltage such as transducers for ultrasound medical imaging, micro-fluidic control and energy harvesting. Beyond electromechanical devices, our approach will open a new avenue to tune and modulate the properties of other multifunctional materials by dynamic strain control. This work was done in collaboration with S. H. Baek, J. Park, D. M. Kim, V. Aksyuk, R. R. Das, S. D. Bu, D. A. Felker, J. Lettieri, V. Vaithyanathan, S. S. N. Bharadwaja, N. Bassiri-Gharb, Y. B. Chen, H. P. Sun, H. W. Jang, D. J. Kreft, S. K. Streiffer, R. Ramesh, X. Q. Pan, S. Trolier-McKinstry, D. G. Schlom, M. S. Rzchowski, R. Blick. This work was supported by the National Science Foundation through grants ECCS-0708759.

9:12AM A33.00005 Monolayer modification of interface dipoles between a-Al_2O_3 and silicon , STEPHANIE FERNANDEZ-PEÑA, University of Geneva, A.M. KOLPAK, S. ISMAIL-BEIGI, C.H. AHN, F.J. WALKER, Center for Research on Interface Structures and Phenomena, Yale University, New Haven, Connecticut — Interface dipoles occurring at high-k oxide-silicon interfaces play an important role in the function of electronic devices. The magnitude and sign of the dipole depend sensitively on the chemistry of the first few atomic planes around the interface. In this work, we control the dipole between a-Al_2O_3 and silicon by monolayer modifications of interface chemistry. The interface composition ranges from a clean 2×1 Si (001) surface prepared by SiO desorption in ultra high vacuum to surfaces having thicknesses of SiO_x as thin as 1 monolayer. In these materials, we observe using x-ray photoelectron spectroscopy band-offset changes induced by a modified interface dipole as large as 0.4 eV. From the capacitance-voltage behavior of metal oxide semiconductor (MOS) devices, we find that this dipole responds to an applied electric field in a non-linear way. We understand this non- linear behavior using first principles theory of complex oxide- electrode interfaces.

9:24AM A33.00006 Alloyed Hf-La High-k Oxide Film Grown by Remote Plasma Atomic Layer Deposition[1] , FU TANG, CHIYU ZHU, ROBERT NEMANICH, Arizona State University — The growth of alloyed Hf-La oxide was investigated using remote plasma atomic layer deposition (RPALD) at low temperatures ranging from 80 to 250C. The low temperature process is particularly important for the applications in thin film transistors, where the device is very often fabricated on flexible plastic substrate. Alloyed oxide films were deposited with 1-3 cycles of La oxide between two adjacent Hf oxide cycles. The atomic bonding structure was determined by in situ XPS. AFM and TEM were used to characterize the morphology and crystalline structure. The XPS results indicated that the percentages of Hf and La components in the alloyed films can be controlled by the ratio of the number of Hf and La cycles. In addition, carbon residue in the alloyed film is reduced compared with that of a pure La oxide film. This is attributed to the role of Hf in preventing formation of La carbonate. The AFM and TEM images indicated that the periodic alloying has suppressed the crystallization of HfO2 and led to improvement of the morphology compared with the roughness of the pure Hf oxide film. The IV curves show that the alloyed Hf-La oxide film has a break down voltage of 3 MV/cm.

[1]Supported through US Army Cooperative Agreement W911NF-04-2-0005 (FDC-10-4.6)

9:36AM A33.00007 Linking the Electronic and Atomic Structure of Epitaxial Complex Oxides on Semiconductors , DIVINE KUMAH, JAMES REINER, JOSEPH NGAI, YARON SEGAL, ALEXIE KOLPAK, DIANA QIU, SOHRAB ISMAIL-BEIGI, CHARLES AHN, FRED WALKER, Department of Applied Physics, Yale University, DONG SU, YI ZHU, Brookhaven National Laboratory, ZHAN ZHANG, Argonne National Laboratory — Understanding the interfacial coupling between materials with different electronic properties is critical to achieve the integration of epitaxial complex oxides with semiconductors. Using a combination of synchrotron x-ray diffraction and first principles calculations, we show that the electronic properties and atomic structure of epitaxial $SrTiO_3$ films on Si, and $BaTiO_3$ films on Ge are directly linked to the chemical composition at their respective interfaces. Sub-angstrom [001] cation-anion displacements observed in the $SrTiO_3$/Si system, lead to a positively polarized film. The polar distortions are found to arise from an interplay between compressive strain and localized interface states. In contrast to $SrTiO_3$/Si, we find that the $BaTiO_3$/Ge interface has a 2x1 structure that drives an in-plane polarization.

9:48AM A33.00008 Piezoelectric force microscopy of crystalline oxide-semiconductor heterostructures[1] , MATTHEW S.J. MARSHALL, JAMES W. REINER, DIVINE KUMAH, CRISP, Dept. of Applied Physics, Yale University, PETER MAKSYMOVYCH, ART P. BADDORF, CNMS, Oak Ridge National Lab, CHARLES AHN, FRED J. WALKER, CRISP, Dept. of Applied Physics, Yale University — Coupling the properties of a ferroelectric material to a semiconductor has been pursued for decades. Epitaxial, coherently strained thin films of ferroelectric BaTiO3 can be grown on germanium with out-of-plane polarization using molecular beam epitaxy (MBE). Similarly, epitaxial thin films of SrTiO3 can be grown on Si with some indication that these films can be ferroelectric. In this work, we use oxide MBE to grow epitaxial films of SrTiO3 and BaTiO3 on Si and Ge, respectively, and we use both ambient and ultrahigh vacuum (UHV) piezoelectric force microscopy (PFM) to study the question of ferroelectricity in these systems. We find that the modulation of the PFM amplitude for thin films of SrTiO3 (6 uc. and 25 uc) on Si is the result of an electrostatic mechanism that can be traced back to tip-induced or as-grown defects in the film. These results are compared to results on thin films of BaTiO3 on Ge.

[1]A portion of this research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Scientific User Facilities Division, U.S. Dept. of Energy.

10:00AM A33.00009 Molecular Beam Epitaxy of YInO3 on GaN , CAMERON KEENAN, FELIO PEREZ, DAVID LEDERMAN, West Virginia University — Novel non-volatile ferroelectric materials are of significant interest in the field of materials science as devices and integrated circuits approach smaller dimensions and broader use. Materials and device structures incorporating GaN are also of particular interest as devices transition away from relying solely on silicon. Oxide materials, such as YMnO3 on GaN, have been researched in an effort to fill this niche, but problems associated with lattice mismatch and interfacial degradation have limited sample quality and utility. YInO3 is another material that may provide an avenue for oxide device integration with GaN. YInO3 thin films were prepared on metal organic chemical vapor deposition GaN templates via molecular beam epitaxy. Atomic force microscopy was used to determine surface roughness and morphology. X-ray reflectivity and x-ray diffraction were implemented in order to determine the thickness, crystallinity, and crystal structure of the films. Results for structural analysis, as well as, ferroelectric measurements will be presented and discussed.

10:12AM A33.00010 Electrocaloric and Pyroelectric Properties of Ferroelectric Films , JIALAN ZHANG, GEORGE ROSSETTI, PAMIR ALPAY, University of Connecticut — We use a non-linear thermodynamic model to investigate the electrocaloric and pyroelectric response of thin film perovskite ferroelectrics under the influence of differing electrical, thermal and mechanical boundary conditions including bias and driving field, temperature, lateral clamping, and misfit strain. A comparison of ferroelectric solid solutions comprised of $BaTiO_3$, $PbTiO_3$ and/or $SrTiO_3$ illustrates the influence of composition and lateral clamping effect on the electrocaloric properties. The theoretical analysis of a variety of ferroelectric thin films on IC-friendly substrates such as Si and sapphire shows that the room temperature dielectric and electrothermal responses of these films depend strongly on the synthesis/processing temperature. These combined results provide insights concerning how the deposition temperature, substrate material and composition can be adjusted to obtain desired electrothermal properties.

10:24AM A33.00011 Polarization switching in Ferroelectric capacitors , ASIF KHAN, UC Berkleey, RAMAMOORTHY RAMESH, SALAHUDDIN SAYEEF, UC Berkeley — A capacitor is an electrical circuit element that stores energy in the form of electric field. A ferroelectric is essentially analogous to an ordinary capacitor with an electrically switchable built-in polarization. The properties of ferroelectrics had been well described by Landau's phenomenological framework. However, during polarization switching in realistic ferroelectrics, switching occurs via "non-ideal" defect mediated domain nucleation and domain wall movement. It can be argued that, within the framework of nucleation based models of FE switching, energy injected into the FE is not stored in the form of electric field, which makes capacitor like description of FE during switching "unclear." In this talk, we will revisit the different switching based models of ferroelectrics and discus the properties of FE as a circuit element during switching.

10:36AM A33.00012 Synthesis and characterization of novel high energy density capacitors for green energy , VENKATA S. PULI, ASHOK KUMAR, RAM S. KATIYAR, Department of Physics and Institute for Functional Nanomaterials, University of Puerto Rico, San Juan, Puerto Rico 00931-3343, USA — We have developed lead free high energy density capacitor materials, $\{Ba(Zr_{0.2}Ti_{0.8})O_3\}_{(1-x)}$ $\{(Ba_{0.7}Ca_{0.3})TiO_3\}x$ [x = 0.10,0.15,0.20 ($BZT_{(1-x)}BCT_x$] with high dielectric constant and moderate breakdown voltage. The ceramic materials were prepared using high energy ball milling for 4 hours at 400 rpm. The ball milled powders were calcined at 1250^{o}C for 10hrs. Ceramic pellets having 13mm diameter were prepared using hydraulic press (2 ton) and sintered at 1400^{o}C-1500^{o}C for 4 hrs. X-ray diffraction studies of the sintered pellets revealed the rhombohedral/pseudo cubic crystal structure. The crystal structure was further confirmed by Raman spectra and TEM analysis. High dielectric constant and moderate polarization ($\sim P_s \sim$ 15-25 μC/cm^2) were obtained in the sintered pellets. The SEM images revealed monolithic grain growth in samples sintered at 1500^{o}C. Preliminary data show moderate breakdown field $\sim$ 15-20 kV/cm and energy density of 0.12-0.3 J/cm^3 for all compositions. Details of the results will be presented.

10:48AM A33.00013 Capacitance response and strain sensing properties of barium titanate thin film[1] , SATREERAT HODAK, PAVARIT PROMSENA, Department of Physics, Faculty of Science, Chulalongkorn University, ANURAT WISITTSORAAT, Nanoelectronics and MEMS Laboratory, National Electronics and Computer Technology Center, JOSE HODAK, Department of Inorganic Analytic and Physical Chemistry, Faculty of Exact and Natural Sciences, University of Buenos Aires — Strain gauges are devices that convert mechanical stress into an electronic signal. In this research, barium titanate ($BaTiO_3$) films were deposited on flexible borosilicate glasses using a sol-gel method. Interdigitated electrodes were patterned on the films to fabricate a strain gauge. The strain gauge comprised of an array of individual coplanar capacitors on a 1.2x0.4 cm rectangular borosilicate glass of 0.16 mm thickness. A parallelogram clamp and a mechanically amplified piezoelectric actuator were used for supporting the device under test and for the application of the strain, respectively. Measurements of the strain were carried out on a cantilever beam by monitoring the changes in device capacitance and the frequency shift of an oscillator circuit. We obtained the frequency change per unit stress equal to 0.00163 MHz/MPa and the frequency change per unit strain equal to 1.038x10^{-4} MHz/unit strain, respectively.

[1]Acknowlegement: Asahi, TRF, CIN, A1B1 and SP2

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A34 DMP: Focus Session: Interfaces in Complex Oxides - LaAlO3/SrTiO3 Transport

C141

8:00AM A34.00001 Tailoring a two-dimensional electron gas at the $LaAlO_3/SrTiO_3$ (001) interface by epitaxial strain , DAVID FELKER, C.W. BARK, University of Wisconsin, Y. WANG, University of Nebraska, Y. ZHANG, University of Michigan, H.W. JANG, C.M. FOLKMAN, J.W. PARK, S.H. BAEK, University of Wisconsin, X.Q. PAN, University of Michigan, E.Y. TSYMBAL, University of Nebraska, M.S. RZCHOWSKI, C.B. EOM, University of Wisconsin — Recently a two-dimensional electron gas (2DEG) was discovered at the interface between insulating oxides $LaAlO_3$ and $SrTiO_3$. Properties of this 2DEG have attracted interest due to its potential applications in nanoelectronics. Control over the carrier density and mobility is essential for applications of these novel systems, and may be achieved by epitaxial strain. The relationship between the strain and electrical properties of this 2DEG remains largely unexplored. We use different lattice constant single crystal substrates to produce $LaAlO_3/SrTiO_3$ interfaces with controlled levels of biaxial epitaxial strain. We have found that tensile strained $SrTiO_3$ destroys the conducting 2DEG, while compressively strained $SrTiO_3$ retains the 2DEG, but with a carrier concentration reduced in comparison to the unstrained $LaAlO_3/SrTiO_3$ interface. We have also found that the critical $LaAlO_3$ overlayer thickness for 2DEG formation increases with $SrTiO_3$ compressive strain. Our first-principles calculations suggest that a strain-induced electric polarization in the $SrTiO_3$ layer is responsible for this behavior.

8:12AM A34.00002 The effect of epitaxial strain and R^{3+} magnetism on interfaces between $RAlO_3$ and $SrTiO_3$, MARK C. MONTI, SHIRIN MOZAFFARI, JOHN T. MARKERT, Department of Physics, The University of Texas at Austin — We have embarked on a systematic study of novel charge states at oxide interfaces. We have performed pulsed laser deposition (PLD) growth of epitaxial oxide thin films on single crystal oxide substrates. We are studying the effects of epitaxial strain and rare-earth composition of the metal oxide thin films. We have successfully created TiO_2 terminated $SrTiO_3$ (STO) substrates and have grown epitaxial thin films of $LaAlO_3$ (LAO), $LaGaO_3$ (LGO), and $EuAlO_3$ (EAO) on STO using a KrF pulsed excimer laser. Current work emphasizes the importance of understanding the effect of both epitaxial strain and R^{3+} magnetism on the interface between $RAlO_3$ and STO. We have demonstrated that the interfaces between LAO/STO and LGO/STO are metallic with carrier concentrations of 1.1 x 10^{14} cm^{-2} and 4.5 x 10^{14} cm^{-2}, respectively. Surprisingly, we find that even good epitaxial interfaces between EAO/STO are insulating. We will investigate the effect of strain by growing $La_xY_{1-x}AlO_3$ on STO: for example $La_{0.4}Y_{0.6}AlO_3$ mimics the lattice size of EAO. We will systematically vary the magnetism of the $RAlO_3$ thin films for R = Ce, Pr, Nd, Sm, Eu, Gd, Tb, La_xEu_{1-x}, ect. This work was supported by: Texas Advanced Research Program 003658-0126, The Robert A. Welch Foundation F-1191, and the National Science Foundation DMR-0605828.

8:24AM A34.00003 High mobility interface electron gas by defect engineering in a modulation doped oxide heterostructure , GUUS RIJNDERS, MARK HUIJBEN, University of Twente/MESA+ Institute for Nanotechnology, GERTJAN KOSTER, HAJO MOLEGRAAF, SANDER WENDERICH, JOSEE KLEIBEUKER, ALEXANDER BRINKMAN, HANS HILGENKAMP, DAVE BLANK, MICHELLE KRUIZE, University of Twente/MESA+ Institute for Nanotechnology, A. MCCOLLAM, V.K. GUDURU, ULI ZEITLER, JAN CEES MAAN, Radboud University, High Field Magnet Laboratory, UNIVERSITY OF TWENTE/MESA+ INSTITUTE FOR NANOTECHNOLOGY TEAM, RADBOUD UNIVERSITY, HIGH FIELD MAGNET LABORATORY TEAM — The manifestation of quantum behavior in two dimensional electron gases in semiconducting heterostructures and their progressive complexity towards fractional quantum Hall effect went hand-in-hand with the efforts to remove the effect of impurity scattering. For oxide materials, history is repeating itself and to date sample quality is reaching levels where quantum behavior starts to become accessible. To really understand the ground state of two dimensional electron gases in oxide systems, where electron-electron correlation effects seem more important, a step towards modulation doping is necessary, removing dopants away from a conduction channel. We will show that the impurity scattering of a 2DEG at the LaAlO3/SrTiO3 interfaces can be significantly suppressed by defect engineering, allowing the observation of quantum transport in a modulation doped oxide system.

8:36AM A34.00004 Effect of stoichiometry on the interface conductivity of MBE-grown $LaAlO_3/SrTiO_3$ heterostructures , M.P. WARUSAWITHANA, J. LUDWIG, P. ROY, A.A. PAWLICKI, Department of Physics and NHMFL, Florida State University, T. HEEG, D.G. SCHLOM, Department of Materials Science and Engineering, Cornell University, C. RICHTER, S. PAETEL, J. MANNHART, Experimentalphysik VI, University of Augsburg, L. FITTING KOURKOUTIS, J. MUNDY, D.A. MULLER, School of Applied and Engineering Physics, Cornell University, M. ZHENG, B. MULCAHY, J.N. ECKSTEIN, Department of Physics, University of Illinois at Urbana - Champaign, W. ZANDER, J. SCHUBERT, Inst. of Bio and Nanosystems IBN1-IT and JARA-FIT, Research Centre Jülich — Through careful control of the stoichiometry in molecular-beam epitaxy grown $LaAlO_3/SrTiO_3$ samples, we find that a 2-dimensional electron gas occurs at the interface between the two insulating oxides as reported in samples grown by pulsed-laser deposition. In this talk, I will discuss the controlled experiments that we have carried out, which effectively eliminate the extrinsic effects that have been suggested as possible mechanisms of conductivity, for the conductivity observed in our MBE-grown samples. We find that the cation stoichiometry of the $La_{(1-x)}Al_{(1+x)}O_3$ layer is key to the existence of the interface 2-dimensional electron gas and that a La/Al ratio, (1-x)/(1+x) less than or equal to 0.97 $\pm$ 0.03 is a necessary condition to obtain a conducting interface in this system.

8:48AM A34.00005 Importance of defects and stoichiometry in the interfacial metal-insulator transition in LaAlO3 thin films on SrTiO3 , C. STEPHEN HELLBERG, Naval Research Lab — The observed metal-insulator transition in thin films of LaAlO3 on SrTiO3 depends critically on the stoichiometry of the film: metallic interfaces are found for Al-rich films, while growing even slightly La-rich results in insulating interfaces. Using first-principles density functional calculations, we examine the effects of changing the stoichiometry of the films. We find that Al will substitute for La, but La will not substitute for Al. Instead, Al-vacancy structures occur in La-rich films. The Al vacancies can migrate to the interface, screening the potential divergence and preventing a metallic interface from forming.

9:00AM A34.00006 Interfacial superconductivity and its magnetic field dependence in MBE-grown $LaAlO_3/SrTiO_3$ heterostructures , P. ROY, J. LUDWIG, E. STEVEN, A. KISWANDHI, A.A. PAWLICKI, J. BROOKS, M.P. WARUSAWITHANA, Department of Physics and NHMFL, Florida State University, D.G. SCHLOM, Department of Materials Science and Engineering, Cornell University, C. RICHTER, J. MANNHART, Experimentalphysik VI, University of Augsburg — In our MBE-grown $LaAlO_3/SrTiO_3$ samples we find the interface to be conducting and sometimes even superconducting when the La/Al ratio is less than or equal to 0.97 $\pm$ 0.03. Here, we report on the superconducting behavior observed in some samples with La/Al ratio above 0.84 $\pm$ 0.03 and below 0.97 $\pm$ 0.03. The superconducting critical temperature is found to be between 160 – 235 mK on different samples. We measure the magnetic field dependence of superconductivity and find that the critical magnetic field required to quench superconductivity depends on the direction of the applied magnetic field. The strong anisotropy in the critical field suggests that the superconductivity in these MBE-grown samples is confined to a thin layer at the interface.

9:12AM A34.00007 Low temperature, high magnetic field magnetoresistance and Hall measurements on MBE-Grown $LaAlO_3/SrTiO_3$ interfaces , J. LUDWIG, P. ROY, E. STEVEN, A. KISWANDHI, A.A. PAWLICKI, J. BROOKS, M.P. WARUSAWITHANA, Department of Physics and NHMFL, Florida State University, D.G. SCHLOM, Department of Materials Science and Engineering, Cornell University, C. RICHTER, J. MANNHART, Experimentalphysik VI, University of Augsburg — We have measured MBE-grown $LaAlO_3/SrTiO_3$ samples at temperatures ranging from room temperature to 20mK and at magnetic fields up to 18 Tesla. The $La_{(1-x)}Al_{(1+x)}O_3$ films studied were grown with a stoichiometry gradient (varying x). We report on the low-temperature sheet carrier density and mobility of the conducting samples – samples with La/Al ratio less than or equal to 0.97 $\pm$ 0.03. We discuss the dependence of sheet carrier density and mobility on stoichiometry by using samples grown on the same substrate and then isolated by using a wire saw. In the devices we measured, the low-temperature sheet carrier densities are on the order of $1x10^{13}$ cm^{-2} with an approximate variation of $2x10^{12} cm^{-2}$ form device to device. The mobilities observed are on the order of $1x10^3$ $cm^2V^{-1}s^{-1}$.

9:24AM A34.00008 Two-dimensional quantum oscillations of the conductance at the $LaAlO_3/SrTiO_3$ interface , ANDREA CAVIGLIA, STEFANO GARIGLIO, NICOLAS REYREN, CLAUDIA CANCELLIERI, ALEXANDRE FETE, BENJAMIN SACEPE, DPMC University of Geneva, MARC GABAY, University of Paris, ALBERTO MORPURGO, JEAN-MARC TRISCONE, DPMC University of Geneva, DPMC UNIVERSITY OF GENEVA TEAM, LABORATOIRE DE PHYSIQUE DES SOLIDES, UNIVERSITÉ PARIS-SUD TEAM — Electronic states with unusual properties can be promoted at interfaces between complex oxides. A striking example is the interface between the band insulators $LaAlO_3$ and $SrTiO_3$, which displays conductivity with high mobility and 2D superconductivity. We report on a study of magnetotransport in $LaAlO_3/SrTiO_3$ interfaces characterized by mobilities of the order of several thousands cm^2/Vs. We observe Shubnikov-de Haas oscillations whose period depends only on the perpendicular component of the magnetic field. This observation directly indicates that the electron gas is two-dimensional and originates from quantum confinement at the interface. From the temperature dependence of the oscillation amplitude we extract an effective carrier mass $m* \simeq 1.45 m_e$. We discuss the relevance of spin effects on the observed phenomenology.

9:36AM A34.00009 Direct Magnetization Measurement of the $LaAlO_3/SrTiO_3$ heterostructure , LU LI, Massachusetts Institute of Technology, CHRISTOPH RICHTER, JOCHEN MANNHART, Univ. Augsburg, RAY ASHOORI, Masschusetts Institute of Technology — The $LaAlO_3/SrTiO_3$ heterostructure is a potential candidate for a high mobility two-dimensional electron system with novel electronic and magnetic properties. Although $LaAlO_3$ and $SrTiO_3$ are both large-gap band insulators, the interface is conductive and even superconducts below 200 mK. Magnetic ordering has been proposed to arise from the polarization-driven charge transfer, but the magnetization of this system has not previously been studied, likely due to the small volume of the interface. Using torque magnetometry, we detect directly the magnetic moment of the interface system. Control experiments with samples without $LaAlO_3$ display a background signal two orders of magnitude smaller, indicating that the observed magnetic moment arises from the deposition of $LaAlO_3$. The measured equilibrium $M - H$ curve resembles that of a soft ferromagnet. Our results indicate the existence of a magnetic ordering at the two-dimensional conductive interface.

9:48AM A34.00010 Quantum Oscillations at the $LaAlO_3/SrTiO_3$ Interface , A. MCCOLLAM, V.K. GUDURU, U. ZEITLER, J.C. MAAN, High Field Magnet Laboratory, Radboud University Nijmegen, Netherlands, M.K. KRUIZE, S. WENDERICH, H. HILGENKAMP, D.H.A. BLANK, MESA+ Institute for Nanotechnology, University of Twente, Netherlands — Under certain growth and preparation conditions, the interface between the perovskite oxides $LaAlO_3$ and $SrTiO_3$ can support a 2-dimensional electron gas (2deg) with diverse and remarkable electronic properties. When the mobility of this 2deg becomes high enough, quantum oscillations appear in the magnetoresistance and provide important information about the origin of the electronic behavior. Here we present an angle-dependent magnetotransport study of a high mobility $LaAlO_3/SrTiO_3$ interface, at millikelvin temperatures and in magnetic fields of up to 30 T. Large quantum oscillations are observed, with a complex dependence on the applied magnetic field and its orientation with respect to the plane of the interface. We propose that the unusual properties of the oscillations have their origin in the multi-subband character of the 2deg, and present a simple model, based on two-dimensional conductivity, which supports the scenario that several spin-split subbands, with field and angle-dependent occupancy, are contributing to the quantum transport in this system.

10:00AM A34.00011 Magnetotransport in the 2DEG at Interface Between $LaAlO_3$ and Thin Film $SrTiO_3$[1] , T. HERNANDEZ, D.A. FELKER, C.W. BARK, C.B. EOM, M.S. RZCHOWSKI, University of Wisconsin-Madison — Transport properties of the 2DEG formed at the heterointerface between $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) grown on Si and $(LaAlO_3)_{0.3}$-$(Sr_2AlTaO_3)_{0.7}$ (LSAT) were compared to those of the LAO on single crystal STO interface. The STO layer on Si was grown by molecular beam epitaxy and on LSAT by pulsed laser deposition (PLD). In all cases, the LAO overlayers were grown using PLD. Mobility, carrier concentration, and magnetoresistance (MR) were measured over the range 3-300K and magnetic fields of 0-8T. The transport properties were similar at room temperature for the different structures. However, at low temperatures, the structures on single crystal STO showed metallic behavior and positive MR, constant in temperature in the 3-20K regime, whereas the ones on Si and LSAT substrates showed a temperature dependence consistent with Mott-type variable range hopping and negative MR with power law behavior in temperature.

[1]Funded by National Science Foundation.

10:12AM A34.00012 Hysteretic magneto-resistance at the $LaAlO_3$-$SrTiO_3$ interface - interplay between superconducting and ferromagnetic properties[1] , MANAN MEHTA, DIMITRY DIKIN, Northwestern University, CHUNG WUNG BARK, CHAD FOLKMAN, CHANG-BEOM EOM, University of Wisconsin-Madison, VENKAT CHANDRASEKHAR, Northwestern University — The conducting interface formed between $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) has been shown to have both magnetic and superconducting properties. The behaviour can be tuned from one to the other by changing the applied gate voltage, thus changing the density of carriers at the interface. We will present magneto-transport data on a Hall-bar geometry patterned LAO/STO interface, with 10 unit cells LAO thickness. The longitudinal magneto-resistance shows strong hysteretic behaviour, indicating a ferromagnetic state, at negative gate voltages; the transverse magneto-resistance being linear. However, the hysteresis survives even into the superconducting state, and also shows up in the transverse magneto-resistance. This suggests an interplay between the superconducting and ferromagnetic order parameters of this system.

[1]Funded by the DOE through grant number DE-FG02-06ER46346

10:24AM A34.00013 Oxygen vacancies at the $LaAlO_3/SrTiO_3$ interface: formation energies and metal-insulator transition , HANGHUI CHEN, Department of Physics, Yale University, ALEXIE KOLPAK, Department of Material Science and Engineering, MIT, SOHRAB ISMAIL-BEIGI, Department of Applied Physics, Yale University — The intriguing transport properties observed at the $LaAlO_3/SrTiO_3$ interface have stimulated numerous studies in the past few years. However, the microscopic mechanism that leads to the formation of the two-dimensional conducting electron gas at the interface remains elusive, partly due to the fact that both intrinsic and extrinsic factors can contribute. We report first principles results on the formation energies of oxygen vacancies on the $LaAlO_3$ thin film surface as a function of coverage and film thickness. In addition to electrostatic contributions to the formation energy due to the polar field in $LaAlO_3$, structural distortions also play an important role in the energetics. We build a simple analytical model to describe our findings which allows us to determine the critical thickness for an oxygen vacancy-induced metal-insulator transition. We discuss the relation of these predictions to the experimental results on this interfacial system.

10:36AM A34.00014 Electronic Phase Separation at the $LaAlO_3/SrTiO_3$ Interface , A. ARIANDO, X. WANG, Z.Q. LIU, J.B. YI, A. ANNADI, A. ROY BARMAN, A. RUSYDI, S. DHAR, Y.P. FENG, J. DING, T. VENKATESAN, National University of Singapore, Singapore, G. BASKARAN, The Institute of Mathematical Sciences, India, J. HUIJBEN, H. HILGENKAMP, University of Twente, The Netherlands — Among the wealth of electronic and magnetic properties exhibited by complex oxides, electronic phase separation (EPS) is one of those whose presence can be linked to many types of exotic behavior, such as colossal magnetoresistance, metal- insulator transition and high-temperature superconductivity. Recently, the oxide community has once again been energized by the observation of a variety of new and unusual electronic phases at the interfaces between the complex oxides, in particular between two nonmagnetic insulators $LaAlO_3$ and $SrTiO_3$. However, no EPS has been observed thus far in this system despite a theoretical prediction. Here, we will show the observation of a ferromagnetic phase and its coexistence with a paramagnetic or a giant diamagnetic phase below 60 K at the interface between $LaAlO_3$ and $SrTiO_3$. The ferromagnetic phase persists even above room-temperature. The coexistence of these multiple magnetic phases along with the interface quasi- 2D electron gas suggests that EPS exists in this system, which can be explained on the basis of selective occupancy of interface sub-bands derived from the nearly degenerate t_{2g}- orbitals of Ti $3d$-states in the $SrTiO_3$.

10:48AM A34.00015 Electronic Phases and Phase Separation in the Hubbard-Holstein Model of a Polar Interface[1] , BIRABAR NANDA, SASHI SATPATHY, University of Missouri — From a mean-field solution of the Hubbard-Holstein model, we show that a rich variety of different electronic phases can result at the interface between two polar materials such as $LaAlO_3/SrTiO_3$. Depending on the strengths of the various competing interactions, viz., electronic kinetic energy, electron-phonon interaction, Coulomb energy, and electronic screening strength, the electrons could (i) either be strongly confined to the interface forming a 2D metallic or an insulating phase, (ii) spread deeper into the bulk making a 3D phase, or (iii) become localized at individual sites forming a Jahn-Teller polaronic phase. In the polaronic phase, the Coulomb interaction could lead to unpaired electrons resulting in magnetic Kondo centers. Under appropriate conditions, electronic phase separation may also occur resulting in the coexistence of metallic and insulating regions at the interface.

[1]Work supported by the US Department of Energy

Monday, March 21, 2011 8:00AM - 10:48AM –
Session A35 DCMP: Topological Insulators: Growth C140

8:00AM A35.00001 Epitaxial Growth of Bi2Se3 Topological Insulator Thin Films on Si (111) , LIANG HE, FAXIAN XIU, Dept. of Elec. Eng., UCLA, YONG WANG, The University of Queensland, ALEXEI V. FEDOROV, Lawrence Berkeley National Laboratory, GUAN HUANG, XUFENG KOU, Dept. of Elec. Eng., UCLA, WARD P. BEYERMANN, Dept. of Phys., UCR, JIN ZOU, University of Queensland, KANG L. WANG, Dept. of Elec. Eng., UCLA, DEPT. OF ELEC. ENG., UCLA TEAM, MATERIAS ENGINEERING, THE UNIVERSITY OF QUEENSLAND COLLABORATION, ADVANCED LIGHT SOURCE DIVISION, LAWRENCE BERKELEY NATIONA LABORATORY COLLABORATION, DEPT. OF PHYS., UCR COLLABORATION — We report the studies of Bi2Se3 epitaxial films on Si(111) substrate using molecular beam epitaxial techniques. The structural properties of as-grown films have been investigated by AFM, STM and TEM, which exhibit good crystalline quality and terrace-like quintuple layers on the surfaces. Single-Dirac-cone-like surface states with a linear (E-K) dispersion have been observed through ARPES. Temperature- and thickness-dependent magneto-transport measurements indicate a combination of shallow impurity band hopping and surface-state electron conductions. More significantly, a very high surface contribution up to 50% can be estimated in these ultrathin films, promising a potential applications in nanoelectornics and spintronics.

8:12AM A35.00002 Topological insulator Bi2Se3 thin film growth by MBE , SHUANG LI, YIJIE HUO, DONG LIANG, Stanford University, THORSTEN HESJEDAL, University of Waterloo, JAMES HARRIS, Stanford University — Single crystalline high quality Bi2Se3 thin films were growth by molecular beam epitaxy (MBE) on sapphire c-plain substrate in UHV environment. X-ray diffraction (XRD) proved single crystal growth is achieved. Atomic ratio was measured by x-ray photoelectron spectroscopy (XPS) and Auger electron spectroscopy. The growth parameters, including substrate temperatures ranging from room temperature to 400°C, growth rate ranging from 0.5 nm/minute to 10 nm/minute and bismuth and selenium flux ratio, were optimized based on the results from scanning electron microscope (SEM), atomic force microscopy (AFM), XRD, and Raman spectroscopy. Triangle and hexagonal single crystals were preferred in the beginning of the growth at high temperature. More Bi2Se3 growth mechanisms will be discussed in the conference.

8:24AM A35.00003 Crystal growth and physical property of Bi-Sb-Te-Se topological insulator materials[1] , GENDA GU, ZHIJUN XU, WEIDONG SI, ZHIHUI PAN, TONICA VALLA, JOHN TRANQUADA, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory — The discovery of 3D topological insulator materials opens up a new research field in the condensed matter physics. In order to exploit the novel surface properties of these topological insulators, it is crucial to achieve a bulk-insulating state in these topological insulator crystals. Unfortunately, all available topological insulator crystals are not bulk-insulating. We have grown a number of Bi-Se, Bi-Te, Sb-Te-Se, Bi-Sb-Se and Bi-Sb-Te-Se topological insulator single crystals by using 5N and 6N pure elements. We have measured the physical properties on these single crystals. We have studied the effect of growth condition and impurity on the bulk electrical conductivity of these single crystals. We try to answer two questions if it is possible to grow the bulk-insulating topological insulator single crystals and Which maximum resistivity of these topological insulator single crystals we can grow.

[1]The work was supported by the DOE under contract No. DE-AC02-98CH10886.

8:36AM A35.00004 MBE growth of topological insulator Bi2Se3 and Bi2Te3 films , TONG ZHANG, 1. Center for Nanoscale Science and Technology, NIST, Gaithersburg, MD, 2. Maryland NanoCenter, UMD, College Park, MD, NIV LEVY, YOUNG JAE SONG, JUNGSEOK CHAE, JOSEPH A. STROSCIO, Center for Nanoscale Science and Technology, NIST, Gaithersburg, MD — Three-dimensional (3D) topological insulators are a new state of quantum matter with a band gap in bulk but gapless states on the surface. The surface states with spin helicity can be the host of many striking quantum phenomena. In this work, we use ultrahigh vacuum molecular beam epitaxy to grow atomically flat topological insulator (TI) Bi2Se3 and Bi2Te3 films. High quality TI films were obtained using epitaxial graphene on SiC as a substrate for TI growth. The growth dynamics was characterized by real time reflection high-energy electron diffraction (RHEED). The growth condition was optimized by adjusting for proper flux rate and substrate temperature while monitoring the RHEED patterns. In situ Auger spectroscopy and scanning tunneling microscopy (STM) measurements at 5K are used to study the as-grown films for their stoichiometry and defect density. We expect these MBE grown samples will provide a good candidate for studying the topological surface states and related phenomena, which will be studied using scanning tunneling spectroscopy at millikelvin temperatures [1]. 1. Y. J. Song et al., Nature 467, 185 [2010].

8:48AM A35.00005 Growth of the topological insulator Bi2Se3 on Al2O3 by molecular beam epitaxy , PHILLIP TABOR, CAMERON KEENAN, DAVID LEDERMAN, SERGEI URAZHDIN, West Viginia University Department of Physics — We report the growth of single crystalline Bi_2Se_3 on Al_2O_3 (110) by molecular beam epitaxy. Previous studies utilizing silicon as a substrate demonstrate favorable structural, optical and transport properties, although this can include contributions from the substrate-film interface. In contrast, growth on Al_2O_3 may influence substrate-film interfacial contributions to structural and electronic properties. Films grown under a range of temperatures and relative selenium to bismuth deposition rates were characterized by ex-situ XPS, XRD, and Hall measurements and will be compared to previous measurements using silicon as a substrate.

9:00AM A35.00006 Growth of topological insulator Bi2Se3 thin films by the van-der-Waals epitaxy on vicinal Si(111) substrate , Z.Y. WANG, Physics Department, The University of Hong Kong, Pokfulam Road, Hong Kong, China, H.D. LI, Physics Department, The University of Hong Kong, Pokfulam Road, Hong Kong, China; and Department of Physics, Beijing Jiaotong University, Beijing, X. KAN, X. GUO, Physics Department, The University of Hong Kong, Pokfulam Road, Hong Kong, China, H.T. HE, Z. WANG, J.N. WANG, T.L. WONG, N. WANG, Physics Department, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, People's Republic of China, M.H. XIE, Physics Department, The University of Hong Kong, Pokfulam Road, Hong Kong, China — Thin films of Bi2Se3, a three-dimensional topological insulator, have been synthesized by molecular-beam epitaxy with varying thicknesses. Their surface, structural and transport properties have been characterized. For the purpose of lowering the structural defects in film, van-der-Waals epitaxy (vdWe) was adopted in a "two-step" growth process, where the initial low-temperature seed layer is followed by a crystalline layer grown at elevated temperatures. Employing vicinal Si(111) substrates, the crystallinity and surface morphology of the epiflm is further improved. Relatively high magnetoresistance along with its linear dependence on the magnetic field at high fields have been observed in the vicinal samples.

9:12AM A35.00007 Coherent heteroepitaxy of Bi_2Se_3 on GaAs and ZnSe , A. RICHARDELLA, D.M. ZHANG, J.S. LEE, A. KOSER, N. SAMARTH, Physics Dept., Penn State University, University Park PA 16802, A. YEATS, B.B. BUCKLEY, D.D. AWSCHALOM, Physics Dept., University of California, Santa Barbara CA 93106 — Bi_2Se_3 is considered to be one to the most promising topological insulator candidate materials currently known because of its 0.3eV bandgap and mid-gap Dirac point. We use molecular beam epitaxy to deposit high quality c-axis oriented single crystal thin films of Bi_2Se_3 on (111) surfaces of GaAs after the growth of either GaAs or ZnSe buffer layers. Atomic force microscopy reveals films with large single quintuple layer terraces hundreds of nanometers wide. Transmission electron microscopy shows an atomically sharp interface at the heterostructure and narrow X-ray diffraction rocking curves indicate good quality single crystalline growth. We discuss the variation in carrier density, mobility and magnetoresistance with growth conditions. Spatially- and temporally-resolved Kerr spectroscopy allows us to explore coherent electron spin dynamics at the interface between this promising topological insulator and conventional semiconductor heterostructures. Supported by NSF and ONR.

9:24AM A35.00008 MBE growth of topological insulator Bi_2Se_3 on epitaxial graphene on 6H-SiC(0001) , Y. LIU, University of Wisconsin-Milwaukee, M. WEINERT, L. LI — In this work, we report results on the MBE growth of Bi_2Se_3, a prototypical topological insulator, on epitaxial graphene on 6H-SiC(0001). Step flow growth is observed, characterized by atomically smooth terraces that are 10 to 50 nm in width and separated by steps of 1-2 quintuple-layer in height. Two characteristic peaks at 130.21 and 171.48 cm^{-1} are observed by Raman spectroscopy, corresponding to the in-plane E_g^2 and out-of-plane A_{1g}^2 vibrational modes, respectively. The close resemblance of the positions and line shapes of both peaks to that of bulk Bi_2Se_3 demonstrates the very high quality of the film. Oscillations are also observed near the steps in dI/dV imaging, attesting to the metallic nature of the surface states of the topological insulator Bi_2Se_3.

9:36AM A35.00009 Transition-metal impurities and intercalation in Bi_2Se_3 , M. WEINERT, Y. LIU, L. LI, U. Wisconsin-Milwaukee — The prototype topological insulator Bi_2Se_3 consists of 5-layer (QL) units. Using first-principles calculations, we show that even for large (20%) elongations along the c-axis, the in-plane lattice constant remains essential unchanged and the nearest neighbor bond lengths within a QL vary by only $\sim$0.02 Å. These results suggest that impurities may preferentially intercalate between the QLs, possibly leading to δ-doped topological insulator superlattices. For Cu-intercalated Bi_2Se_3, the calculated separation between QLs slightly contracts ($\sim$2%), and the Cu intercalation layer provides the internal surfaces necessary for the material to exhibit a Dirac cone. The competition between substitutional impurities and intercalation layers for Cu and Mn will be discussed and compared to experiment.

9:48AM A35.00010 Epitaxial Bi_2Se_3 films on Si (111) with atomically sharp interface , ELIAV EDREY, YONG SEUNG KIM, NAMRATA BANSAL, YOICHI HORIBE, SEONGSHIK OH, Rutgers University, OH GROUP TEAM — Atomically sharp epitaxial growth of Bi_2Se_3 films has been achieved on Si (111) substrate with MBE. The growth was self-limited; that is, growth rate was determined completely by Bi flux with excess Se species around. The Bi:Se flux ratio, measured by QCM, was kept $\sim$1:15. Two step growth temperatures were a key to achieving second-phase-free high quality Bi_2Se_3 films on Si substrates. With single-step high temperature growth, second phase, presumably $SiSe_2$ clusters, was formed at the early stage of growth. On the other hand, with low temperature growth, crystalline quality of the films was poor even if second phase was absent. With low temperature initial growth followed by high temperature growth, second-phase-free atomically sharp interface was obtained between Bi_2Se_3 and Si substrate, as verified by RHEED, TEM and XRD. The lattice constant of Bi_2Se_3 relaxed to its bulk value during the first quintuple layer based on the RHEED analysis, implying the absence of strain from the substrate. Single-crystalline XRD peaks of Bi_2Se_3 were observed in films as thin as 4 QL. TEM shows full epitaxial structure of Bi_2Se_3film down to the first quintuple layer without any second phases. This growth method was used to grow high quality epitaxial Bi_2Se_3 films from 3 QL to 3600 QL.

10:00AM A35.00011 Robust surface state and bulk carrier density in transport properties of Bi2Se3 films grown with MBE , YONG SEUNG KIM, Sejong University, NAMRATA BANSAL, ELIAV EDREY, MATHEW BRAHLEK, GARY A. KAPILEVICH, SANG-WOOK CHEONG, SEONGSHIK OH, Rutgers University — One of the main predictions of 3D topological insulators (TI) is the existence of a surface metallic state, independent of the sample thickness. However, so far this simple prediction has never been experimentally verified because of significant parallel bulk conduction. Here, we report observation of a robust 2D surface state for MBE-grown thin films in their magneto-transport properties. We also observed that volume carrier density tends to decrease as film gets thicker. Even if a robust 2D surface state exists, its topological protection seems to degrade in thin films due to interference with the bulk carriers, and thus this bulk carrier problem will be the most important next step to solve in order to implement the full topological protection on this surface state.

10:12AM A35.00012 Controlling the topological states of Bi_2Se_3 by silver atom intercalation , M. YE, K. KURODA, M. NAKATAKE, S. KIM, Y. YAMADA, A. KIMURA, K. MIYAMOTO, M. ARITA, T. OKUDA, K. SHIMADA, Hiroshima University, Y. UEDA, Kure National College of Technology, H. NAMATAME, M. TANIGUCHI, Hiroshima University — Among the known topological insulators, the layered material, Bi_2Se_3, is one of the most promising candidates for potential applications to ultra-low power consumption quantum devices that can work stably at room temperature due to a sufficiently large energy gap in the bulk. The realization of quantum devices generally requires the exposure of the materials to ambient conditions, which significantly disturbs the topological properties through absorption. While intercalation of impurities into layered materials might be thought to be usually detrimental, we show here that that intercalation of Ag into Bi_2Se_3 has a benefit. After depositing silver atoms on the surface of Bi_2Se_3, massive electrons can be formed on the surface due to the decoupling of the layer-structure by silver intercalation. The newly formed massive electron observed on the surface serves as an evidence of an extremely weak interaction between the decoupled layers and the bulk TI crystal. These results strongly suggest the existence of a new non-trivial boundary state, which opens a pathway to realizing topological insulator-based electronic and spintronic devices, and fault tolerant quantum computation.

10:24AM A35.00013 Magnetically doped nanoplate crystals of topological insulators Sb_2Te_3 and Bi_2Te_3[1] , LUKAS ZHAO, LIN BO, LIMIN HUANG, ALISA AGAFONOVA, SIMON DIVILOV, STEPHEN O'BRIEN, MYRIAM SARACHIK, LIA KRUSIN-ELBAUM, CCNY — The surface states of topological insulators are robustly protected by time-reversal symmetry. Introducing magnetic impurities should open a gap in the otherwise gapless surface states. Recent first-principle calculations predict that when topological insulators are doped with transition metal elements, such as Cr or Fe, a *magnetically ordered* insulating state will form, a state distinctly different from the conventional dilute magnetic semiconductors. In thin (quasi-2D) samples, this magnetic order gives rise to a topological electronic structure, with the quantized Hall conductance. Here we report synthesis and electrical and magnetic characterization of Fe and Cr doped *thin* nanoplates of topological insulators Sb_2Te_3 and Bi_2Te_3. Nanoplate crystals were grown by catalyst-free vapor-liquid-solid method and were doped using the *in situ* exchange of sources. Low-temperature magnetic, in-plane resistivity, and Hall measurements were performed in magnetic fields up to 9 T fields. The effects of magnetic dopant concentration on susceptibility and charge transport will be discussed.

[1]Supported in part by CCNY Center for Exploitation of Nanostructures in Sensors and Energy Systems (CENSES) and by NSF-DMR-0451605

10:36AM A35.00014 Atmospheric Doping Affects on the Transport Properties of the Topological Insulator Bismuth Selenide (Bi_2Se_3) Grown By MBE , MATTHEW BRAHLEK, YONG SEUNG KIM, NAMRATA BANSAL, ELIAV EDREY, SEONGSHIK OH, Rutgers University — During the last five years much experimental work has been done to determine if the theoretical prediction of topological insulting (TI) states truly exist. Angle resolved photo emission spectroscopy (ARPES) measurements have shown that a Dirac type linear dispersion does exist for a variety of materials, and the surface states have been observed by direct transport measurements. The next challenge is to isolate the surface electrons by removing the bulk conduction. This not trivial because bismuth selenide's Fermi energy sits in the conduction band, and most of the measured carriers are due to these bulk states. The prediction is that the surface states are robust under perturbation, but like standard semiconductors, Bi_2Se_3's bulk states are sensitive to doping. I will report on our work done on how the transport properties of MBE grown Bi_2Se_3 thin films are affected by atmospheric dopants such as oxygen and water vapor. Future prospects for studying TIs such Bi_2Se_3 and ultimately building a device depend on being able to tune the Fermi level into the gap thereby isolating the surface states, and then passivating the surface against contamination due to atmospheric oxygen and water vapor.

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A36 DMP GERA: Focus Session: Scalable Technologies for Terawatt Photovoltaics

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8:00AM A36.00001 Film Si photovoltaics from high quality c-Si layers on inexpensive substrates[1] , PAUL STRADINS, National Renewable Energy Laboratory — We develop crystalline silicon film photovoltaic (PV) technology to approach the efficiency of wafer silicon PV at thin-film manufacturing costs. Epitaxial c-Si layers can be grown by a fast, scalable hot-wire CVD technique at rates that exceed those of amorphous and nanocrystalline thin film PV by factor of 20, with quality approaching that of the crystalline Si wafer. This approach greatly reduces the absorber material costs that today account for about half the cost of a Si wafer PV module while bypassing the low growth-rate bottleneck that dominates thin film Si PV economics. As part of this equation, devices must also be fabricated on inexpensive substrates. To this end, we explore homo- and hetero-epitaxy at display glass-compatible temperatures as well as collaborate with several groups on promising high crystal quality seed layer technology. In the talk, we discuss key physics issues associated with film Si PV and describe recent experimental results, including: 1) device physics showing feasibility of 2 -10 microns thick c-Si PV absorber layers and their relative tolerance to defects and impurities; 2) demonstration of epitaxial cells on Si wafers with open-circuit voltages up to 600 mV; 3) understanding of high-rate, high-quality epitaxial growth in the temperature range 620 to 760C; 4) growth on seed layers on display glass and metal foils; 5) novel light trapping schemes that result in improved spectral response without texturing the growth template or etching away valuable absorber layer material.

[1]This work is supported by the U.S. Department of Energy Solar Energy Technology Program under Contract No. DE-AC36-99GO10337.

8:36AM A36.00002 CdTe Solar Cells Scaling to Grid Parity , DAVID EAGLESHAM, First Solar — CdTe thin-film solar cells are leading the technology race to deliver low-cost and sustainable photovoltaics. The technology has an inherent cost advantage over c-Si, and has achieved volume manufacturing ahead of any other thin-film technology. TF-CdTe is also more sustainable than other approaches, with a lower carbon-footprint and far faster energy-payback than c-Si. Having achieved the long-standing target of $1/W module and well over 1GW/year in volume, the technology is continuing to drive down costs towards a levelised cost of electricity comparable to fossil fuels.

9:12AM A36.00003 Challenges to Scaling CIGS Photovoltaics , B.J. STANBERY, HelioVolt — The challenges of scaling any photovoltaic technology to terawatts of global capacity are arguably more economic than technological or resource constraints. All commercial thin-film PV technologies are based on direct bandgap semiconductors whose absorption coefficient and bandgap alignment with the solar spectrum enable micron-thick coatings in lieu to hundreds of microns required using indirect-bandgap c-Si. Although thin-film PV reduces semiconductor materials cost, its manufacture is more capital intensive than c-Si production, and proportional to deposition rate. Only when combined with sufficient efficiency and cost of capital does this tradeoff yield lower manufacturing cost. CIGS has the potential to become the first thin film technology to achieve the terawatt benchmark because of its superior conversion efficiency, making it the only commercial thin film technology which demonstrably delivers performance comparable to the dominant incumbent, c-Si. Since module performance leverages total systems cost, this competitive advantage bears directly on CIGS' potential to displace c-Si and attract the requisite capital to finance the tens of gigawatts of annual production capacity needed to manufacture terawatts of PV modules apace with global demand growth.

9:48AM A36.00004 CZTSSe: Materials and Physics Challenges[1] , OKI GUNAWAN, IBM T J Watson Research Center — Thin-film photovoltaic (PV) technologies led by CdTe and Cu(In,Ga)Se_2 (CIGS) are enjoying growing market share, due to their high performance and cost competitiveness, in the quest for renewable energy for the future. However the reliance on non-earth abundant elements tellurium and indium in these technologies presents a potential obstacle to ultimate terawatt deployment. We recently demonstrated kesterite $Cu_2ZnSn(Se,S)_4$ (CZTSSe) solar cells, comprised of the earth abundant metals copper, zinc and tin, with world record efficiency of 9.7%. In this talk we present a comprehensive device characterization study that pinpoints the key performance bottlenecks in these cells. We find strong buffer-absorber interface recombination and low minority carrier lifetimes that limit the open circuit voltage and a high and diverging device series resistance at lower temperature that suggests a blocking back contact that may limit the fill factor. These findings help to identify key areas for improvement for these CZTSSe cells in the pursuit of a high performance terawatt-scalable PV technology.

[1]In collaboration with Teodor K. Todorov, Aaron Barkhouse, Kejia Wang, David B. Mitzi, Supratik Guha, IBM T J Watson Research Center.

10:24AM A36.00005 Screening of inorganic wide-bandgap p-type semiconductors for high performance hole transport layers in organic photovoltaic devices , DAVID GINLEY, ANDRIY ZAKUTAYEV, ANDREAS GARCIA, NICODEMUS WIDJONARKO, PAUL NDIONE, AJAYA SIGDEL, PHILLIP PARILLA, DANA OLSON, JOHN PERKINS, JOSEPH BERRY, National Renewable Energy Laboratory — We will report on the development of novel inorganic hole transport layers (HTL) for organic photovoltaics (OPV). All the studied materials belong to the general class of wide-bandgap p-type oxide semiconductors. Potential candidates suitable for HTL applications include SnO, NiO, Cu2O (and related CuAlO2, CuCrO2, SrCu2O4 etc) and Co3O4 (and related ZnCo2O4, NiCo2O4, MgCo2O4 etc.). Materials have been optimized by high-throughput combinatorial approaches. The thin films were deposited by RF sputtering and pulsed laser deposition at ambient and elevated temperatures. Performance of the inorganic HTLs and that of the reference organic PEDOT:PSS HTL were compared by measuring the power conversion efficiencies and spectral responses of the P3HT/PCBM- and PCDTBT/PCBM-based OPV devices. Preliminary results indicate that Co3O4-based HTLs have performance comparable to that of our previously reported NiOs and PEDOT:PSS HTLs, leading to a power conversion efficiency of about 4 percent. The effect of composition and work function of the ternary materials on their performance in OPV devices is under investigation.

10:36AM A36.00006 A New Paradigm for Multijunction Solar Cells , MARINA LEITE, CALTECH, ROBYN WOO, Spectrolab Inc., EMILY WARMANN, Caltech, DANIEL LAW, Spectrolab Inc., HARRY ATWATER, Caltech — We propose an approach for a multijunction solar cell (MJSC) based on direct band gap InAlAs/InGaP/InGaAsP/InGaAs alloys. Device simulations indicate that the proposed design can achieve over 50 % efficiency at 100-suns illumination by using an alloy combination with lattice parameter of 5.80 Å. For that, we created a virtual substrate for epitaxial growth. By relieving 40nm thick coherently-strained $In_xGa_{1-x}As$ films from InP substrates, full relaxation occurs preserving the crystalline quality of the films, as confirmed by X-ray diffraction, transmission electron microscpy and photoluminescence measurements. Once these films are transferred to a cheap support they can be used as a template for epitaxial growth with specifically chosen lattice parameter and therefore band gap energy. Our realization demonstrates the ability to control the lattice parameter and energy band structure of single layer crystalline alloy semiconductors in an unprecedented way. For the top subcell, we fabricated InAlAs solar cells with efficiencies > 14 % and Voc $= 1$ V. These results indicate that the novel MJSC design is feasible. Future directions and subcells performance will be presented.

10:48AM A36.00007 Resonant TCO nanostructures for improved light trapping in thin-film photovoltaics , ALOK VASUDEV, MARK BRONGERSMA, Stanford University — The desire for widespread photovoltaic (PV) adoption has motivated many recent efforts in advanced photon management in thin-film solar cells. Approaches to enhance PV optical absorption by exploiting surface plasmon resonances in metallic nanostructures, in particular, have been extensively studied. Here we present an alternative means to improve light trapping in thin-film solar cells using resonant transparent conductive oxide (TCO) nanostructures. Dielectric nanowires support leaky mode resonances, which, in poorly absorbing media, can scatter light efficiently. This resonant scattering can enhance optical absorption in a nearby photoabsorber. Using finite difference frequency domain (FDFD) techniques we show that an optimized planar solar cell's performance is improved by patterning the TCO into resonant scatters. Unlike their plasmonic counterparts, these resonators do not suffer large absorption losses, depend strongly on polarization or force a radical change in processing. We will discuss scalability, future improvements and application to a variety of solar cell configurations.

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A37 DMP: Focus Session: Graphene: Growth, Characterization and Devices: Theory and Transport C146

8:00AM A37.00001 Engineering gate-controlled potential barrier and nano-constriction in bi-layer graphene , CHING-TZU CHEN, IBM TJ Watson Research Center, HSIN-YING CHIU, DAVID DIVINCENZO, SIYURANGA KOSWATTA — Graphene, as a material with zero net nuclear spin and a small spin-orbit coupling, is a natural candidate for building quantum-dot-based spin qubits, since electron spin coherence time can potentially be much longer compared to the prevailing GaAs-based systems. To date, graphene quantum dots have largely been realized using etch-defined nanoribbons or nano-islands. Due to fabrication-related edge defects or channel doping inhomogeneity, these etch-defined nanostructures generally suffer from randomly distributed incidental dots, causing undesirable resonance peaks in transport. To eliminate the disorder-induced localized states, we explore the possibility of electron confinement by using electric-field-controlled band gap opening in bilayer graphene. In this talk, we discuss various nanostructure designs towards this aim. We will present the transport characteristics of the dual-gated and side-gated devices, compare their performance, and analyze the gate tunability in various configurations. We will also comment on their use in quantum dots and other device applications.

8:12AM A37.00002 First Principle Simulations of Dual Gate Bilayer Graphene Field Effect Nanotransistors , J.E. PADILHA, M.P. LIMA, A.J.R. DA SILVA, A. FAZZIO, University of São Paulo — In this work we present, via first principle calculations, a study of bilayer graphene dual-gate field effect nanotransistor. We show the $I_{ds} \times V_{ds}$ curves as a function of the channel length, back(V_{bg})/top(V_{tg}) gate voltages, temperature and charge excess on the system. For this study we use Landauer-Büttiker model with Hamiltonian generated through ab initio Density Functional Theory coupled with non-equilibrium Green's Function formalism. To investigate finite gates we implement a multigrig real space Poisson solver. Our results shows that the current can be tuned varying the strength of the electric field by setting different values of $V_{bg}(V_{tg})$ as well as modifying the channel length. We also show that the current depends on the amount of net charge in the system, controlled by the $V_{bg}(V_{tg})$ values, and the minimum of flowing current occurs when the system is neutral (charge neutrality point) only for gate lengths bigger than $4nm$. In all calculations we find a finite current due to a temperature effect associated with the Fermi-Dirac distribution. Decreasing the temperature from $300K$ to $4.5K$ the current diminishes one order of magnitude. Our study predicts that bilayer graphene dual gate field effect nanotransistors with small channel lengths ($< 5nm$) presents a upper limit for the ON/OFF current ratio of 10 for $300K$ and 100 for $4.5K$. This ratio can be increased using larger channel lengths.

8:24AM A37.00003 Charge transport in dual-gated bilayer-graphene Corbino-disk[1] , JUN YAN, MICHAEL FUHRER, Center for Nanophysics and Advanced Materials, University of Maryland, College Park, MD 20742-4111, USA — We use the Corbino-disk geometry to study the electron transport behavior of dual-gated bilayer graphene devices. Experimental exclusion of the edge states enables us to probe the bulk of bilayer graphene and its electronic properties. The temperature dependence of the maximum resistivity is found to be well described by simple thermal activation at high temperatures and variable range hopping at low temperatures, consistent with other transport studies. The electric-field-dependent band gap extracted from thermal activation is found to be in good agreement with infrared spectroscopic studies (Zhang et al. Nature 459, 820 (2009)). The similarity of our data to those of conventional dual-gated bilayer graphene devices with edges suggests that edges do not play a significant role in such devices at least for temperatures above 5 K, and points to the importance of reducing bulk disorder for improving device performance.

[1]This work is supported by the U.S. ONR MURI, the NSF-UMD-MRSEC Grant No.DMR05-20471, and an NRI-MRSEC supplement grant.

8:36AM A37.00004 Theory of the electronic and transport properties of epitaxial graphene[1] , MARCO BUONGIORNO NARDELLI, North Carolina State University — Advances in the epitaxial growth of graphene films on SiC have the potential to open new classes of device applications that may revolutionize the semiconductor roadmap for future decades. However, this progress will require an in-depth understanding and utilization of the electronic processes that take place at the nanoscale. In this talk I will review our recent results on the electronic and transport properties of epitaxial graphene on SiC. Using calculations from first principles, I will discuss the the role of the interface buffer layer in the tuning of the band alignment and the magnetic doping at the heterojunction; I will describe the effect of electron-phonon interactions in mono- and bi-layer graphene in determining the intrinsic carrier-phonon scattering properties of this material and thus the ultimate limit of any electronic device; finally, I will briefly discuss the thermal properties of the graphene/SiC interface, since understanding of the heat transfer properties is essential for optimal thermal management and heat removal in device applications.

[1]Work done in collaboration with K.W. Kim, T. Jayasekera, J. Mullen, K. Borysenko, S. Xu, X. Li and B.D. Kong

9:12AM A37.00005 Strong Enhancement of Doping in Graphene via Substrate , BING HUANG, SU-HUAI WEI, National Renewable Energy Lab — Controlling the type and density of charge carriers by doping is the key step for developing graphene electronics. Based on first-principles calculations, we demonstrate that doping could be strongly enhanced in epitaxial graphene on silicon carbide (SiC) substrate. Compared to free- standing graphene, the formation energies of dopants decrease dramatically by 2 $\sim$ 8 eV. The dopants prefer to stay in the interface buffer layer between epitaxial graphene and substrate, which could tune the interface dipoles evidently. The type and density of charge carriers of epitaxial graphene layer can be effectively manipulated by suitable dopants and surface passivation. Contrasting to the direct doping of graphene, the charge carriers in epitaxial graphene layer are weakly scattered by dopants due to the spatial separation between dopants and conducting channel, in the spirit of modulation doping, which takes advantages in maintaining the high carrier mobility of graphene. Beyond controlling the charge carriers via buffer layer doping, we find that the reconstructed vacancy in the interface buffer layer breaks the spin symmetry of epitaxial graphene, which induces a half-metallic state without magnetic impurities doping.

9:24AM A37.00006 Magnetic impurities in graphene with defects , FEIMING HU, RISTO NIEMINEN, COMP/Department of Applied Physics, School of Science and Technology, Aalto University, Finland — We theoretically study magnetic impurities in graphene with defects. The defects are described by vacancies which can be realized in graphene experimentally. The occupancy number, local moment and spin susceptibility of the impurities are calculated by quantum Monte Carlo simulations. When the Fermi energy of the system is changed by gate voltage, it is found that the behaviors of these physical quantities are very different from those in perfect graphene. The spectral density of the impurity is also studied by maximum entropy methods to explain these unusual behaviors.

9:36AM A37.00007 Carrier Transport in Epitaxial Multi-layer Graphene , YU-MING LIN, CHRISTOS DIMITRAKOPOULOS, DAMON FARMER, SHU-JEN HAN, YANQING WU, WENJUAN ZHU, IBM, D. KURT GASKILL, JOSEPH TEDESCO, RACHAEL MYERS-WARD, CHARLES EDDY, JR., NRL, ALFRED GRILL, PHAEDON AVOURIS, IBM, IBM TEAM, NRL TEAM — Significant attention has been focused recently on the electrical properties of graphene grown epitaxially on SiC substrates, because it offers an ideal platform for carbon-based electronics using conventional top-down lithography techniques. The transport properties of graphene are usually studied via Hall effect measurements, which provide information on the carrier mobility and density. Hall measurements performed at a single magnetic field yield a weighted average of carrier mobility and density, and are strictly applicable to homogeneous samples. In this study, we performed variable-field Hall and resistivity measurements on epitaxial graphene, and the results were analyzed with a multi-carrier model. Good agreements were obtained between experimental data and the model, providing further evidence of multi-carrier transport in the C-face grown MLG. This work is supported by DARPA under contract FA8650-08-C-7838 through the CERA program and by the Office of Naval Research.

9:48AM A37.00008 Hole-channel conductivity in epitaxial graphene determined by terahertz optical Hall-effect and midinfrared ellipsometry[1] , T. HOFMANN, A. BOOSALIS, P. KÜHNE, University of Nebraska-Lincoln, J.L. TEDESCO, D.K. GASKILL, U.S. Naval Research Laboratory, C.M. HERZINGER, J.A. Woollam Co. Inc., Lincoln, NE, J.A. WOOLLAM, M. SCHUBERT, University of Nebraska-Lincoln — We report non-contact, optical determination of free-charge carrier mobility, sheet density, and effective mass parameters in epitaxial graphene at room temperature using terahertz and midinfrared ellipsometry and optical Hall-effect (generalized ellipsometry in magnetic fields) measurements. The graphene layers are grown on Si- and C-terminated semi-insulating 6H silicon carbide polar surfaces. Data analysis using classical Drude functions and multilayer modeling render the existence of a p-type channel with different sheet densities and effective mass parameters for the two polar surfaces. The optically obtained parameters are in excellent agreement with results from electrical Hall effect measurements.

[1]ARO (W911NF-09-C-0097), NSF (MRSEC DMR-0820521, MRI DMR-0922937, DMR-0907475), and Office of Naval Research

10:00AM A37.00009 Quantum corrections to the conductivity in graphene , ALEKSEY KOZIKOV, University of Exeter, FEDOR TIKHONENKO, University of Southampton, ALEX SAVCHENKO, University of Exeter, BORIS NAROZHNY, Karlsruhe Institute of Technology, ANDREI SHYTOV, University of Exeter — The low-temperature conductivity in electron systems is determined by two quantum corrections. They originate from the interference of electron waves scattered by impurities (weak localisation, WL) and electron-electron interaction (EEI) in the presence of disorder. In graphene, due to the chirality of charged carriers, the quantum interference is sensitive not only to inelastic, dephasing, scattering, but also to elastic, inter- and intra-valley, scattering processes. It was theoretically predicted that depending on the scattering rates of such processes, weak antilocalisation (WAL) is possible in graphene. In this work we study both magnetoresistance and the temperature dependence of the conductivity and observe a transition from WL to WAL by tuning the carrier density and temperature. We show that quantum interference in graphene can survive at temperatures up to 200 K due to weak electron-phonon scattering. We also investigate the EEI correction, which is separated from the WL correction by two methods, and show that it is also affected by intra-valley scattering. This scattering leads to a new temperature regime of EEI. We find the Fermi liquid constant to be small, -0.1, and discuss the origin of this value.

10:12AM A37.00010 First-principles Theory of Nonlocal Screening in Graphene[1] , MARK VAN SCHILFGAARDE, Arizona State University, MIKHAIL KATSNELSON, Radboud University Nijmegen — Using the quasiparticle self-consistent *GW* (QS*GW*) and local-density (LD) approximations, we calculate the q-dependent static dielectric function, and derive an effective 2D dielectric function corresponding to screening of point charges. In the $q\rightarrow 0$ limit, the 2D dielectric constant is found to scale approximately as the square root of the macroscopic dielectric function. Its value is $\simeq 4$, in agreement with the predictions of Dirac model. At the same time, in contrast with the Dirac model, the dielectric function is strongly dependent on q. The QS*GW* approximation is shown to describe QP levels very well, with small systematic errors analogous to bulk sp semiconductors. Local-field effects are rather more important in graphene than in bulk semiconductors.

[1]Supported by NSF

10:24AM A37.00011 First-Principles Investigation of Polymer Binding to Graphene and Carbon Nanotubes[1] , OGUZ GULSEREN, AYJAMAL ABDURAHMAN, Bilkent University — The interactions between a polymer (Poly[(phenylene)-co-(9,9- bis-(6-bromohexyl)uorene)]) and graphene and carbon nanotubes are investigated by using pseudopotential planewave calculations based on density functional theory (DFT). In the quest of searching the most favorable binding configurations, the monomer under investigation is placed at different orientations on graphene. In order to obtain further insight into the binding interactions of polymer-graphene system, we also calculated the binding energy for the structure in which the polymer is attached to graphene sheet via atomic oxygen. Considering the graphene impurity, we have also further investigated the polymer approaching from the chain side onto graphene with a vacancy. However, our results demonstrated that the interaction between the (Poly[(phenylene)-co-(9,9-bis-(6-bromohexyl) uorene)]) polymer and graphene is weak, mostly dispersive, but this interaction is slightly stronger when the graphene has structural defects, like vacancies. The implications of these results to the polymer and carbon nanotube interactions also are discussed.

[1]This project is supported by TUBITAK (Grant No: TBAG-107T892) and European Union 7. Framework project Unam-Regpot (Grant no: 203953).

10:36AM A37.00012 Spectral and optical properties of doped graphene with charged impurities in the self-consistent Born approximation , FERNANDO DE JUAN, Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), EUYHEON H. HWANG, Condensed Matter Theory Center, Physics Department, University of Maryland, MARIA A. H. VOZMEDIANO, Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC) — Spectral and transport properties of doped (or gated) graphene with long range charged impurities are discussed within the self-consistent Born approximation. It is shown how, for impurity concentrations greater than the electron concentration, $n_{imp} \geq n$, a finite DOS appears at the Dirac point, the one-particle lifetime no longer scales linearly with the Fermi momentum, and the lineshapes in the spectral function become non-lorentzian. These behaviors are different from the results calculated within the Born approximation. We also calculate the optical conductivity from the Kubo formula by using the self-consistently calculated spectral function in the presence of charged impurities.

10:48AM A37.00013 ABSTRACT WITHDRAWN –

Monday, March 21, 2011 8:00AM - 10:24AM –
Session A38 DCP: Focus Session: Ultrafast Dynamics and Imaging I A130/131

8:00AM A38.00001 Attosecond Physics: Time-dependent electronic dynamics in atoms, molecules, and solids[1] , JOACHIM BURGDOERFER, Institute for Theoretícal Physics, Vienna University of Technology — With the advent of sub-femtosecond ultrashort XUV pulses and of phase-stabilized IR pulses with sub-cycle time resolution, novel pathways have been opened up for studying time-resolved electronic quantum dynamics on the attosecond scale. These experiments pose challenges for theory: How do short pulses interact with matter? Which novel information can be extracted from time-resolved spectroscopies that cannot be gained from precision experiments in the spectral domain? In this talk, these issues will be addressed with the help of a few examples. Attosecond streaking allows a direct look at electronic correlations and rearrangement processes. Photoemissions from solid surfaces reveal an attosecond time delay between conduction electrons and core electrons and provide time-resolved information on electron transport, plasmon excitation, and dissipation. Attosecond pulses allow not only to probe but also to control and manipulate electronic dynamics which we will illustrate for two-electron emission from atoms and molecular break-up.

[1]In collaboration with J. Feist, S. Graefe, C. Lemell, S. Nagele, R. Pazourek, F. Krausz, V. Yakovlev, L. Collins, and B. Schneider, work supported by FWF-SFB 016 ADLIS.

8:36AM A38.00002 Simulation of Transmission Electron Microscopy in Time Domain[1] , JIA-AN YAN, Department of Physics, Georgia Southern University, J. DRISCOLL, KALMAN VARGA, S.T. PANTELIDES, Department of Physics, Vanderbilt University — Based on the time-dependent Schrodinger equation, a new method of simulating transmission electron microscope (TEM) images by directly propagating an electron wave packet in real time and real space is presented. Compared to other widely used methods, the new technique yields an accurate description of the electron scattering in solid thin films for both low-energy and the high-energy electrons. We demonstrate the method by simulating TEM images for silicon crystalline films and low-energy-electron diffraction (LEED) images of Si surfaces and graphene. The time-dependent simulations described here could be useful for studying ultrafast electron dynamics in solids.

[1]This work was supported in part by DOE grant DE-FG02-09ER46554.

8:48AM A38.00003 Ultrafast imaging of nanoclusters with intense x-ray laser pulses , CHRISTOPH BOSTEDT, Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, CA 94025 — Ultrafast x-ray scattering opens the door for unprecedented insight into the structure and dynamics of matter with atomic resolution. Any sample in an x-ray laser flash, however, will be converted into a highly excited, non-equilibrium plasma during the pulse. The scatter signal itself is sensitive to changes in the electronic structure of the sample leading to distortions of the signal intensities with respect to the ground state configuration. On the other hand, the information about the electronic structure carried by the scatter signal can be exploited to gain insight into transient electronic states on the femtosecond time scale of the x-ray pulse. We have performed single shot – single particle scattering experiments on clusters to investigate the interplay between excitation and scattering in nanoscale objects with x-ray pulses from both, the FLASH and LCLS free electron lasers. Atomic clusters have been proven ideal to investigate the interaction between intense light pulses and matter in a wide spectral regime from the infrared to x-rays due to their finite size and simple electronic structure. Spectroscopy data recorded in coincidence with the scattering patterns revealed strong power-density dependent ionization dynamics of the clusters. The scattering patterns themselves provide information on the 2-dim as well as 3-dim structure of clusters and of cluster ensembles. Modeling the scattering patterns indicates that the optical constants of the clusters, which are inherently coupled to its electronic structure and thus charge states, change during the femtosecond pulse. Time resolved experiments with pump – probe techniques have started which allow following the time evolution of cluster ionization up to several ps.

9:24AM A38.00004 Thermal transport in thin films measured by time-resolved grazing-incidence x-ray diffraction[1] , D.A. WALKO, Advanced Photon Source, Argonne National Laboratory, Y.-M. SHEU, University of Michigan, M. TRIGO, D.A. REIS, SLAC National Accelerator Laboratory and Stanford University — Depth- and time-resolved x-ray diffraction were used to study thermal transport across single crystal Bi films grown on sapphire, to determine the thermal conductivity of the films and the Kapitza conductance of the interfaces. Ultrafast Ti:sapphire laser pulses heated the films; x-ray diffraction measured the subsequent lattice expansion. Use of grazing incidence geometry provided depth sensitivity with the x-ray angle of incidence near the critical angle, in contrast to symmetric Bragg geometries which only measure the average temperature of the film. The shift of the film's Bragg peak position with time was used to determine the film temperature, averaged over an x-ray penetration depth that could be selected by choice of the angle of incidence. Films that were thick compared to the laser penetration depth exhibited a large temperature gradient at early times; in this case, measurements with the incident angle below and above the critical angle were more sensitive to the film conductivity and Kapitza conductance, respectively. For thinner films, however, cooling was dominated by the Kapitza conductance on all accessible time scales.

[1]APS supported by U. S. DOE under Contract DE-AC02-06CH11357.

9:36AM A38.00005 Probing electron correlations by laser-induced tunnel ionization , ANDRÉ STAUDTE, National Research Council of Canada — Pairwise electron correlation has been intensely studied by projecting two electrons to the continuum simultaneously via a well controlled perturbation, e.g. a collision with an energetic electron, a fast ion or a single XUV photon. Electron correlation studies using multiphoton ionization remain an exception. One reason may be that recollision aside, studies in rare gas atoms have largely suggested that multiphoton multiple ionization in the tunneling limit proceeds sequentially - each successive ionization stage loosing memory of previous electronic correlations. On the other hand, laser tunnel ionization has been known to access multiple electronic states. Recent evidence, corroborating the notion that tunneling can prepare these correlated multielectron states in a coherent superposition, suggests that sequential multiple ionization may provide insight into dynamical correlations in the parent ion. Here, we demonstrate how dynamics of electron correlation can be investigated using laser-induced tunnel ionization by interrogating valence shell electrons in rare gas atoms with intense laser pulses. We find a strong spatial propensity in the sequential double tunnel ionization regime. For instantaneous emission, we find that the two electrons are preferentially emitted in perpendicular directions. Applying laser scanning tunneling microscopy in a pump-probe scheme we directly observe the periodic charge redistribution in the valence shell of singly charged noble gas atoms that was predicted by Santra and coworkers and recently inferred in an attosecond pump-probe experiment using XUV probe pulses. In contrast to single photon ionization, tunneling is highly directional. Here, we exploit that property of tunnel ionization to remove an electron from a rare gas atom along a specific spatial direction. We then probe the correlation by ionizing a second electron via a laser-induced tunneling gate. Since our tunneling gates are optically controlled, the second gate can be opened at any angle and at any time relative to the first. Hence, not only spatial but also temporal variations of the correlation can be probed. We demonstrate the generality of this concept by extending our measurements to a small molecule (HCl).

10:12AM A38.00006 2D Fano-resonances in momentum space , WAI-LUN CHAN, JOHN TRITSCH, ANDREI DOLOCAN, XIAOYANG ZHU, University of Texas at Austin — Using the model system of molecular quantum wells and image potential states at the C_{60}/Au(111) interface and the experimental technique of time- and angle-resolved two photon photoemission spectroscopy, we probe many body interaction in coupled two-dimensional (2D) systems. Transiently populated 2D bands with different effective masses are found to intersect with each other in the reciprocal space. At the points of intersection, we observe strong modulations in the photoemission intensity as a function of parallel momentum vector. The intensity modulation in the reciprocal space can be explained by the well-known Fano resonances – the interference between different quantum mechanical pathways in optical excitation. The experimental results agree semi-quantitatively with simulation based on optical Bloch's equations. Differing from conventional Fano resonances in energy space, our observation establishes the existence of 2D Fano resonance in momentum space.

Monday, March 21, 2011 8:00AM - 10:00AM –

Session A39 DBP: Focus Session: Energy Future: Biological and Biometric Systems A124/127

8:00AM A39.00001 Energy conversion in photosynthesis[1] , GARY BRUDVIG, Yale University — Photosystem II (PSII) uses light energy to split water into protons, electrons and O_2 [1]. In this reaction, Nature has solved the difficult chemical problem of efficient four-electron oxidation of water to yield O_2 without significant side reactions. In order to use Nature's solution for the design of materials that split water for solar fuel production, it is important to understand the mechanism of the reaction. The X ray crystal structures of cyanobacterial PSII provide information on the structure of the Mn and Ca ions, the redox-active tyrosine called Y_Z, and the surrounding amino acids that comprise the O_2 evolving complex (OEC) [2,3]. We have used computational studies used to refine the structure of the OEC to obtain a complete structural model of the OEC that is in agreement with spectroscopic data [4,5]. The structure of the OEC and the mechanism of water oxidation by PSII will be discussed in the light of biophysical and computational studies, inorganic chemistry and X-ray crystallographic information.

[1] J.P. McEvoy and G.W. Brudvig, Chem. Rev. (2006) 106, 4455-4483.
[2] K.N. Ferreira et al., Science (2004) 303, 1831-1838.
[3] B. Loll et al., Nature (2006) 438, 1040-1044.
[4] E.M. Sproviero et al., J. Am. Chem. Soc. (2008) 130, 6728-6730.
[5] E.M. Sproviero et al., J. Am. Chem. Soc. (2008) 130, 3428-3442.

[1]Supported by NIH GM32715.

8:36AM A39.00002 Engineered and Artificial Photosynthesis , TOM MOORE, Arizona State University — This abstract not available.

9:12AM A39.00003 QM/MM and MD study on a light-harvesting molecular triad[1] , GUOXIONG SU, ARKADIUSZ CZADER, MARGARET CHEUNG, University of Houston — We investigated the hydrophobic interactions of an artificial photosynthetic molecular triad in nanoconfinement in various sizes using a combined approach of QM/MM method and all-atomistic molecular dynamics simulations with explicit water models. We use the Replica Exchange Method Dynamics (REMD) to investigate the effect of solvation and confinement on the distribution of the ensemble structures and the energy landscape of triad. The relationship of the charge distribution computed from QM/MM and the radial distribution function of water molecules at the proximity of triad will be discussed. The work presented here has profound implications for future studies of the photosynthetic function of triad that provides the opportunity for the insight into the molecular device of green energy.

[1]Department of Energy, Basic Energy Sciences (DE-FG02-10ER16175).

9:24AM A39.00004 Nanophotonics of Chloroplasts for Bio-Inspired Solar Energy Materials , PAUL L. GOURLEY, CHERYL R. GOURLEY, HighLight Research — In the search for new energy sources, lessons can be learned from chloroplast photonics. The nano-architecture of chloroplasts is remarkably well-adapted to mediate sunlight interactions for efficient energy conversion. We carried out experiments with chloroplasts isolated from spinach and leaf lettuce to elucidate the relationship between nano-architecture, biomolecular composition and photonic properties. We obtained high-resolution microscopic images of single chloroplasts to identify geometries of chloroplasts and interior grana. We performed micro-spectroscopy to identify strengths of absorption and fluorescence transitions and related them to broadband reflectance and transmittance spectra of whole leaf structures. Finally, the nonlinear optical properties were investigated with nanolaser spectroscopy by placing chloroplasts into micro-resonators and optically pumping. These spectra reveal chloroplast photonic modes and allow measurement of single chloroplast light scattering cross section, polarizability, and refractive index. The nanolaser spectra recorded at increasing pump powers enabled us to observe non-linear optics, photon dynamics, and stimulated emission from single chloroplasts. All of these experiments provide insight into plant photonics and inspiration of paradigms for synthetic biomaterials to harness sunlight in new ways.

9:36AM A39.00005 Direct Enzymatic Oxidation of Glucose with a Poly(Ionic Liquid) - Gold-Nanoparticle Composite , MILLICENT FIRESTONE, SUNGWON LEE, SOENKE SEIFERT, Argonne National Laboratory — In this work we describe the synthesis, fabrication and characterization of a gold nanoparticle - ionic liquid-derived polymer composite for conversion of biofuels into electricity. Glucose oxidase (GOx) electrostatically adsorbed on an ionic liquid-derived polymer containing internally organized columns of Au nanoparticles exhibits bioelectrocatalytic properties in the oxidation of glucose. The cationic poly(ionic liquid) provides an ideal substrate for the immobilization of GOx. The encapsulated Au nanoparticles serve two roles: promoting direct electron transfer with the recessed enzyme redox centers, and imparting electronic conduction to the composite, thereby allowing it to function as an electrode for electrochemical detection.

9:48AM A39.00006 Photosystem I assembly on chemically tailored SAM/ Au substrates for bio-hybrid device fabrication[1] , DIBYENDU MUKHERJEE, BAMIN KHOMAMI, Department of Chemical and Biomolecular Engineering, University of Tennessee — Photosystem I (PS I), a supra-molecular protein complex and a biological photodiode responsible for driving natural photosynthesis mechanism, charge separates upon exposure to light. Effective use of the photo-electrochemical activities of PS I for future bio-hybrid electronic devices requires controlled attachment of these proteins onto organic/ inorganic substrates. Our results indicate that various experimental parameters alter the surface topography of PS I deposited from colloidal aqueous buffer suspensions onto OH-terminated alkanethiolate SAM /Au substrates, thereby resulting in complex columnar structures that affect the electron capture pathway of PS I. Specifically, solution phase characterizations indicate that specific detergents used for PS I stabilization in buffer solutions drive the unique colloidal chemistry to tune protein-protein interactions and prevent aggregation, thereby allowing us to tailor the morphology of surface immobilized PS I. We present surface topographical, adsorption, and electrochemical characterizations of PSI /SAM/Au substrates to elucidate protein-surface attachment dynamics and its effect on the photo-activated electronic activities of surface immobilized PS I.

[1]Sustainable Energy Education and Research Center (SEERC)

Monday, March 21, 2011 8:00AM - 10:24AM –

Session A40 DPOLY: New Experimental, Theoretical, and Computational Methods in Polymer and Soft Matter Physics A122/123

8:00AM A40.00001 A First Principle Approach to Rescale the Dynamics of Simulated Coarse-Grained Macromolecular Liquids , IVAN LYUBIMOV, MARINA GUENZA, University of Oregon — A first-principle approach has been developed to rescale dynamical data from mesoscopic molecular dynamics simulations of polymer liquids. We derive rescaling factors from Generalized Langevin Equations (GLE) for the coarse-grained at the monomer level representation and coarse-grained at the mesoscopic level representation of the liquid, exploiting the Mori-Zwanzig projection operator formalism. The rescaling factors explicitly depend on coarse-grained model parameters and thermodynamic parameters. Two corrections need to be accounted to compensate the acceleration effect on dynamics caused by higher level of coarse-graining: change in entropy and change in friction. After applying our rescaling to data from mesoscopic simulations of unentangled and weakly entangled polyolefin melts we observe a good agreement with data of translational diffusion measured experimentally and from UA simulations. The method is used to predict self-diffusion coefficients for systems not yet investigated experimentally.

8:12AM A40.00002 Phase behavior of disk-coil molecules , YONGJOO KIM, ALFREDO ALEXANDER-KATZ, MIT — Using Monte Carlo simulations, we investigate the self-assembly of disk-coil molecules in the NPT ensemble. By changing the interaction parameters between the disk and the coil portion of the molecules, a full phase diagram of these four phases is constructed. Furthermore, we study the ordering of disks within the crystal phase and we find that the confinement imposed by the mesophase segregation induces stronger order compared to the pure disk case, which was also explicitly simulated. Our results show that by reducing the dimensionality of a system it is possible to induce higher order of the molecules and help orient the disks in the crystal phase. Furthermore, we simulated molecules with additional interaction and obtained interesting additional phases. Our results are relevant for organic photoactive (typically planar) molecules that are functionalized with tails to improve their processability and long-range order in the solid phase.

8:24AM A40.00003 A unified model Hamiltonian for polythiophene, polypyrrole, polyfuran, free base porphyrin, and polyaniline: Accuracy, transferability, and computational efficiency , ANDRE BOTELHO, XI LIN, Division of Materials Science and Engineering, Boston University, Boston MA — Two fully transferable physical parameters are incorporated into the historical Su-Schrieffer-Heeger Hamiltonian to model conducting polymers beyond polyacetylene, one parameter γ scales the electron-phonon coupling strength in aromatic rings and the other parameter ε specifies the heterogeneous core charges. This generic Hamiltonian predicts the fundamental band gaps of polythiophene, polypyrrole, polyfuran, free base porphyrin, polyaniline, and their oligomers of all lengths with an accuracy exceeding the time-dependent density functional theory. Additionally, its computational costs are four orders of magnitude or more lower than first-principles approaches.

8:36AM A40.00004 Fluctuating lattice-Boltzmann model for complex fluids , SANTTU OLLILA, Aalto University School of Science, COLIN DENNISTON, MIKKO KARTTUNEN, University of Western Ontario, TAPIO ALA-NISSILA, Aalto University School of Science — We develop, and test numerically, a lattice-Boltzmann (LB) model for non-ideal fluids that incorporates thermal fluctuations through a random component in the local stress tensor. The fluid model is a momentum-conserving thermostat, for which we demonstrate how the temperature can be made equal at all length scales present in the system by having noise both in the stress tensor of the fluid and by shaking the whole system in accord with the local temperature. The validity of the model is extended to a broad range of values of the sound velocity. Furthermore, our model features a consistent coupling scheme between the fluid and solid molecular dynamics objects, which allows us to use the LB fluid as a heat bath for solutes evolving in time $without$ external Langevin noise added to the solute. This property expands the applicability of LB models to dense, strongly correlated systems with thermal fluctuations and potentially non-ideal equations of state. We benchmark our model by performing tests on the fluid itself and on the static and dynamic properties of a coarse-grained polymer chain under strong hydrodynamic interactions. We find that our model produces results for single-chain diffusion that are in quantitative agreement with theory

8:48AM A40.00005 Polymer network stretching during electrospinning[1] , ISRAEL GREENFELD, ARKADII ARINSTEIN, Technion, KAMEL FEZZAA, Argonne National Laboratory, MIRIAM RAFAILOVICH, State University of New York, Stony Brook, EYAL ZUSSMAN, Technion — Fast X-ray phase contrast imaging is used to observe the flow of a semi-dilute polyethylene oxide solution during electrospinning. Micron-size glass particles mixed in the polymer solution allow viewing of the jet flow field, and reveal a high-gradient flow that has both longitudinal and radial components that grow rapidly along the jet. The resulting hydrodynamic forces cause substantial longitudinal stretching and transversal contraction of the polymer network within the jet, as confirmed by random walk simulation and theoretical modeling. The polymer network therefore concentrates towards the jet center, and its conformation may transform from a free state to a fully-stretched state within a short distance from the jet start.

[1]We acknowledge the financial support of the United States - Israel Bi-National Science Foundation (grant 2006061)

9:00AM A40.00006 Microscopic theory of topological entanglement constraints in fluids of rigid macromolecules , DANIEL SUSSMAN, KEN SCHWEIZER, University of Illinois at Urbana-Champaign — A theoretical description of the slow dynamics of an ideal gas of infinitely thin, non-rotating rods or three-dimensional crosses is presented. As objects with no excluded volume their equilibrium structure is trivial, and thus slow dynamics are determined solely by bond uncrossability and macromolecular connectivity. Our work builds on the dynamic mean-field theory of Szamel, which successfully predicted tube localization and reptation for non-rotating uncrossable rods. We derive an effective diffusion constant by exactly enforcing uncrossability at the two-molecule level in conjunction with a self-consistent renormalization to account for many-particle effects. For crosses and isotropically translating rods a topological localization transition is predicted at a critical density above which macromolecules are localized by a confinement potential with very strong anharmonicities. The spatial nature of the latter, including the density-dependent localization length, is analyzed and contrasted with recent experiments on entangled F-actin filaments. The stability of the localization transition to both an external force (yielding) and macromolecular collective density fluctuations is examined, and comparison with simulations on entangled crosses is performed.

9:12AM A40.00007 Tying Polymer Knots to Find the Entanglement Length , JIAN QIN, SCOTT MILNER, ChE at Penn State University — We propose two relations between the entanglement length and the probability distribution of topological states accessed by topologically equilibrated ring polymer melts. The first states that the rings are most likely entangled when the ring length exceeds the entanglement length. The second states that the topological entropy measuring the number of accessible topological states is about k_B per entanglement strand. To test these ideas, we simulated melts of ring polymers with hybrid MC/MD moves, and sampled their topological states by using various ring rebridging moves. Topological states are identified by mapping the molecular configurations to knots, and knots are distinguished by computing their invariant polynomials. We accumulated the state statistics, their ring length dependence, and extracted the entanglement length using these two approaches. The results are consistent with each other, and agree with those from the heuristic methods.

9:24AM A40.00008 Towards simulation of charges in the presence of varying dielectric response , VIKRAM JADHAO, Northwestern University, FRANCISCO SOLIS, Arizona State University, GUILLERMO GUERRERO-GARCIA, MONICA OLVERA DE LA CRUZ, Northwestern University — A variational formulation of electrostatics suitable for carrying out simulations of charges interacting in the presence of different dielectric media is developed. The variational principle employs the polarization charge density as the only variational field. A true energy functional is constructed to yield the correct electrostatic energy at its minimum and the correct force during the approach to the minimum. In the hope of applying the method to more realistic and complicated geometries, some numerical investigations of the variational procedure are also presented.

9:36AM A40.00009 Colloidal Particle Vibration Spectroscopy , TIM STILL, MPI for Polymer Research, Mainz, Germany, GEORGE FYTAS, MPI for Polymer Research, Mainz, Germany; Univ. of Crete and FORTH, Heraklion, Greece, MAURIZIO MATTARELLI, MAURIZIO MONTAGNA, Univ. Trento, italy — Brillouin light scattering (BLS) on dry colloidal particles resolves a large number of resonance vibrations (eigenmodes),[1] allowing determining the elastic properties at meso- and nanoscale and measure (polymer) physical properties not accessible by other methods.[2] So far, only the frequencies of the different eigenmodes, labeled by the "quantum numbers" (n,l) and calculated following Lamb's 19th century approach, were taken to identify the nature of the measured signals, however leading to some ambiguities. Herein, we present the first full theoretical representation of BLS eigenmode spectra, allowing an unprecedentedly precise access to the individual colloid's thermomechanical properties.[3] A longstanding discussion is resolved, showing that both even and odd l spheroidal modes are active. The theoretically predicted scattering angle dependence of the BLS intensity is verified.

[1]Cheng et al., *J. Chem. Phys.* **123**, 121104, 2005.
[2]Still et al., *Nano Lett.* **8**, 3194, 2008; *J. Coll. Int. Sci.* **340**, 42, 2009; *Macromolecules* **43**, 3422, 2010.
[3]Still et al., *J. Phys. Chem. Lett.* **1**, 2440, 2010.

9:48AM A40.00010 Physical properties of two-dimensional directed polymer systems obtained via bosonization and related techniques[1] , DAVID ZEB ROCKLIN, PAUL M. GOLDBART, University of Illinois at Urbana-Champaign — Classical directed polymers in 2 dimensions are well known to be equivalent to quantum particles in 1+1 dimensions, with polymer configurations corresponding to particle worldlines. This equivalence motivates the use of techniques designed for one-dimensional quantum systems for exploring many-polymer systems, as first exploited by de Gennes [1]. We discuss how thermodynamic quantities and certain correlation functions of a particular model polymer system can be calculated exactly from the Bethe ansatz solution for the Lieb-Liniger model of bosons with repulsive local interactions. We also discuss how the universal properties of more general polymer systems can be captured via Haldane's harmonic-fluid approach. Via this approach, we address various properties of strongly interacting many-polymer systems, focusing on aspects that display qualitative differences from those displayed by single polymers.

[1] P.-G. de Gennes, J. Chem Phys. 48, 2257-2259 (1968)

[1]D.Z. Rocklin acknowledges support from NDSEG.

10:00AM A40.00011 Adapted Su-Schrieffer-Heeger Hamiltonian for PPV, PPP, and polyacenes , YONGWOO SHIN, XI LIN, Boston university — This work presents a unified model Hamiltonian for poly-p-phenylenevinylene (PPV), poly-p-phenylene (PPP), and polyacenes based on the classical Su- Schrieffer-Heeger Hamiltonian for polyacetylene, with one single extra electron- phonon coupling parameter. Predicted band gaps of all these polymers and their oligomers of all lengths closely match to the available experimental results, with an accuracy exceeding the time-dependent density functional theory. Self-localized polaron states and their mobility are computed without any constraints.

10:12AM A40.00012 Rigid body constraints in HOOMD-Blue, a general purpose molecular dynamics code on graphics processing units , TRUNG D. NGUYEN, CAROLYN L. PHILLIPS, JOSHUA A. ANDERSON, SHARON C. GLOTZER, University of Michigan, Ann Arbor — Rigid body constraints are commonly used in a wide range of molecular modeling applications from the atomistic scale, modeling the bonds in molecules such as water, carbon dioxide, and benzene, to the colloidal scale, modeling macroscopic rods, plates and patchy nanoparticles. While the parallel implementations of rigid constraints for molecular dynamics simulations for distributed memory clusters have poor performance scaling, on shared memory systems, such as multi-core CPUs and many-core graphics processing units (GPUs), rigid body constraints can be parallelized so that significantly better performance is possible. We have designed a massively parallel rigid body constraint algorithm and implemented it in HOOMD-Blue, a GPU-accelerated, open-source, general purpose molecular dynamics simulation package. For typical simulations, the GPU implementation running on a single NVIDIA® GTX 480 card is twice as fast as LAMMPS running on 32 CPU cores. In the HOOMD-blue code package, rigid constraints can be used seamlessly with non-rigid parts of the system and with different integration methods, including NVE, NVT, NPT, and Brownian Dynamics. We have also incorporated the FIRE energy minimization algorithm, reformulated to be applicable to mixed systems of rigid bodies and non-rigid particles.

Monday, March 21, 2011 8:00AM - 11:00AM –
Session A41 DPOLY: Focus Session: Active Biopolymers and Biomaterials A115/117

8:00AM A41.00001 Connecting Atomic Structures with Continuum Mechanics in Cytoskeletal Polymers[1] , DAVID SEPT, University of Michigan — The mechanics of the cytoskeleton, namely actin filaments and microtubules, are key to many of their cellular functions. These polymers have been extensively studied using a wide range of biophysical techniques, and we have sought to connect the dynamics we observe in all-atom molecular dynamics simulations with continuum mechanics properties. We have developed coarse-graining techniques that allow us calculate mechanical properties of these polymers using a simple mesoscopic description. Our findings match very well with experimental measurements and allow us to probe how the atomic level effects of small molecules and/or point mutations manifest themselves at the level of the polymer.

[1]Supported by NSF Grant CMMI-0928540.

8:36AM A41.00002 The Interplay of Nonlinearity and Architecture and Nonequilibrium Dynamics in Cytoskeletal Mechanics , SHENSHEN WANG, Dept of Physics, UCSD, TONGYE SHEN, Dept of Biochemistry, Cellular and Molecular Biology, Univ. of Tennessee, PETER WOLYNES, Dept of Physics, Dept of Chemistry and Biochemistry, UCSD — The interplay between cytoskeletal architecture and the nonlinearity of the interactions due to bucklable filaments plays a key role in modulating the cell's mechanical stability and its structural rearrangements. We first study a model of cytoskeletal structure treating it as an amorphous network of hard centers rigidly cross-linked by nonlinear elastic strings, neglecting the effects of motorization. Using simulations along with a self-consistent phonon method, we show that this minimal model exhibits diverse thermodynamically stable mechanical phases that depend on excluded volume, crosslink concentration, filament length and stiffness. Within the framework set by the free energy functional formulation and making use of the random first order transition theory of structural glasses, we further estimate the characteristic densities for a kinetic glass transition to occur in this model system. Network connectivity strongly modulates the transition boundaries between various equilibrium phases, as well as the kinetic glass transition density. We further study the effects of motorization and polymerization upon the stability and dynamics of this model system.

8:48AM A41.00003 Buckling of Branched Cytoskeletal Filaments , D.A. QUINT, J.M. SCHWARZ, Syracuse University — *In vitro* experiments of growing dendritic actin networks demonstrate reversible stress-softening at high loads, above some critical load. The transition to the stress-softening regime has been attributed to the elastic buckling of individual actin filaments. To estimate the critical load above which softening should occur, we extend the elastic theory of buckling of individual filaments embedded in a network to include the buckling of branched filaments, a signature trait of growing dendritic actin networks. Under certain assumptions, there will be approximately a seven-fold increase in the classical critical bucking load, when compared to the unbranched filament, which is entirely due to the presence of a branch. Moreover, we go beyond the classical buckling regime to investigate the effect of entropic fluctuations. The result of compressing the filament in this case leads to an increase in these fluctuations and eventually the harmonic approximation breaks down signifying the onset of the buckling transition. We compute corrections to the classical critical buckling load near this breakdown.

9:00AM A41.00004 "Twist-state" transitions in parallel actin bundles induced by crosslinking proteins , HOMIN SHIN, GREGORY GRASON, University of Massachusetts Amherst — Parallel actin bundles are common structural motifs in many crucial cellular specializations, from filopodia to mechanosensory bundles of the inner ear. Here, we study a model of actin bundles, crosslinked by compact globular bundling proteins, known to modify the torsional state of filaments due to frustration between helical structure of the filaments and in-plane ordering of the bundle. Our coarse-grained model of parallel bundles maps the linker-induced "twist-state" transition of actin filament onto a *commensurate-incommensurate* phase transition, described by an effective Frenkel-Kontorowa model. We predict that the transition from the uncrosslinked, incommensurate helical symmetry to fully crosslinked, commensurate symmetry is highly sensitive to linker flexibility: flexible crosslinking smoothly distorts the twist state of bundled filaments, while rigidly crosslinked bundles undergo a phase transition, rapidly overtwisting filaments over a narrow range of free crosslinker concentrations. Additionally, we predict a rich spectrum of intermediate structures, composed of alternating domains of sparsely bound (untwisted) and strongly bound (overtwisted) filaments. This model reveals that subtle differences in crosslinking agents themselves modify not only the detailed structure of parallel actin bundles, but also the thermodynamic pathway by which they form.

9:12AM A41.00005 Elasticity of a cross-linked active bundle[1] , SILKE HENKES, Syracuse University, TANNIEMOLA B. LIVERPOOL, University of Bristol, M. CRISTINA MARCHETTI, A. ALAN MIDDLETON, JENNIFER M. SCHWARZ, Syracuse University — Understanding the effect of motor proteins, such as myosins, on the elasticity of crosslinked actin networks is essential to our understanding of cell mechanics. Both in vivo and in vitro, these active networks have radically different mechanical properties from their equilibrium counterparts, including contractile behavior and higher elastic moduli. Existing theoretical models do not address the relative role of passive and active crosslinkers in controlling the network contractility and stiffening. We construct a one dimensional lattice model with minimal ingredients, that is, rigid polar filaments, spring-like passive crosslinks and active crosslinks with on/off dynamics implemented through non-equilibrium Monte Carlo solution of the corresponding master equations. We find, consistent with experiments, that the network needs to be percolated through the passive crosslinks to be mechanically stable. Contractile behavior is observed for all concentrations of active crosslinks. We study the mechanical properties of the gel in the phase space of motor processivity, crosslink stiffness, and concentration of active crosslinks.

[1]This work is supported by the NSF through grants DMR-0806511, DMR-1004789, DMR-1006731 and DMR-0645373.

9:24AM A41.00006 Bursts of active transport in living cells , BO WANG, JAMES KUO, SUNG CHUL BAE, STEVE GRANICK, University of Illinois — This study of cargo motion in living cells, performed with nm resolution and an unprecedented large database, shows that the instantaneous speed of active transport deviates pervasively from the average speed yet with striking statistical regularity over several decades of time and space. The experimental approach involves single-particle tracking and special wavelet-based methods to discriminate active transport from passive diffusion, thus quantifying the instantaneous speed of endosomal and lysosomal active transport in living cells at times just longer than the motor stepping time. Pervasive bursts of acceleration stem from viscoelastic relaxation of the cytoplasm, the individual bursts displaying a time-averaged shape that we interpret to reflect stress buildup followed by rapid release. These statistical regularities did not change in response to changing the experimental conditions, specifically to changing the cell line and motor type, or to overexpressing microtubule binding proteins, thus indicating redundancy in regulation of cellular active transport. The power law of scaling is the same as seen in driven jammed colloids, powders, and magnetic systems, and is consistent with a simple heuristic argument. The implied regulation of active transport by environmental obstruction in the cytoplasm extends the classical notion of "molecular crowding."

9:36AM A41.00007 Mechanically Activated Motion of a Single Self-Propelled Polymeric Microcapsule , GERMAN KOLMAKOV, ALEXANDER SCHAEFER, Chemical Engineering Department, University of Pittsburgh, IGOR ARANSON, Materials Science Division, Argonne National Laboratory, ANNA BALAZS, Chemical Engineering Department, University of Pittsburgh — Using a hybrid computational approach, we demonstrate that a single nanoparticle-filled microcapsule on a rigid substrate can undergo self-sustained motion in response to initial mechanical deformation. Nanoparticles released from the capsule modify the underlying substrate and the adhesion gradients of the nanoparticle concentration formed at the surface sustain the motion of the capsule. The permeability of the microcapsule's shell increases with its deformation and therefore, more deformed microcapsules release nanoparticles at higher rates. An initial, non-uniform mechanical deformation of the capsule by an applied force causes an asymmetry in the nanoparticle distribution on the substrate that initiates the microcapsule motion. We also develop a two-dimensional model of the phenomenon within the phase-field approximation and compare the results of the two approaches.

9:48AM A41.00008 Coarse-grained models for biological simulations , ZHE WU, QIANG CUI, ARUN YETHIRAJ, UW Madison — The large timescales and length-scales of interest in biophysics preclude atomistic study of many systems and processes. One appealing approach is to use coarse-grained (CG) models where several atoms are grouped into a single CG site. In this work we describe a new CG force field for lipids, surfactants, and amino acids. The topology of CG sites is the same as in the MARTINI force field, but the new model is compatible with a recently developed CG electrostatic water (Big Multiple Water, BMW) model. The model not only gives correct structural, elastic properties and phase behavior for lipid and surfactants, but also reproduces electrostatic properties at water-membrane interface that agree with experiment and atomistic simulations, including the potential of mean force for charged amino acid residuals at membrane. Consequently, the model predicts stable attachment of cationic peptides (i.e., poly-Arg) on lipid bilayer surface, which is not shown in previous models with non-electrostatic water.

10:00AM A41.00009 Guided Transport of a Transmembrane Nanochannel , MEENAKSHI DUTT, OLGA KUKSENOK, ANNA BALAZS, University of Pittsburgh — Via the Dissipative Particle Dynamics approach, we design a system that allows transport of a nanochannel to a desired location by applying an external force. Each nanochannel encompasses an ABA architecture, with a hydrophobic shaft (B) with two hydrophilic ends (A). One of the hydrophilic ends of the nanochannel is functionalized with hydrophilic functional groups, or hairs. The hydrophilic hairs serve a dual role: (1) control transport across the membrane barrier when the channel diffuses freely in the membrane, and (2) enable the channel relocation to a specific membrane site. Our system comprises a transmembrane hairy nanochannel with the hairs extending into solution. In our earlier work, we demonstrated the spontaneous insertion of such a hairy nanochannel into a lipid bilayer (Nanoscale DOI: 10.1039/C0NR00578A). First, we hold a suitably functionalized pipette stationary above the membrane while the nanochannel freely diffuses within the membrane. For an optimal range of parameters, we demonstrate that the hairs find the pipette and spontaneously anchor onto it. We then show that by moving the pipette for a range of velocities, we can effectively transport the channel to any location within the membrane. This prototype system can provide guidelines for designing a number of biomimetic applications.

10:12AM A41.00010 Accidental Interactions and Purposeful Flaws in Polymer Brushes: Variations in Bioadhesive Mechanisms , MARIA SANTORE, University of Massachusetts — Water soluble brushes, such as polyethylene glycol and poly(hydroxyethyl methacrylate) are grafted, in many applications, to or from surfaces to prevent protein and cell adhesion. When brushes fail, as can be frequent in practice, protein adsorption becomes aggressive. Failure can occur if the brush architecture is simply too thin such that proteins can experience van der Waals and electrostatic attractions with the underlying substrate, or if the brush has flaws or holes, where the grafting procedure did not succeed. This talk compares the interactions of proteins and bacteria with nearly uniform brushes to the interactions of proteins and bacteria with patchy brushes. The latter are deliberately flawed by the inclusion of nanoscale adhesive elements (polymer coils and nanoparticles) at their base, which prevent local brush formation. The adhesive elements are smaller than the proteins themselves, but sufficient to perturb local brush structure. This talk demonstrates that large quantities of the appropriate types of random-coil (denatured) and globular (native) proteins can penetrate a brush and even displace it (if it is otherwise held in place by adsorbing anchor groups), while other proteins can be entirely repelled. The same is also true of the patchy brushes, but with patchy brushes, but the mechanism is different. With uniform brushes, small proteins and random coils sometimes penetrate sufficiently to experience electrostatic attractions once inside the brush. With patchy brushes, all proteins have the opportunity to interact electrostatically with the adhesive elements, but because large proteins can interact with greater numbers of adhesive elements, their capture is preferred. The result is different rankings of proteins which can ultimately adhere to thin uniform brushes or thicker patchy ones.

10:48AM A41.00011 Nanoparticle Self-Lighting Photodynamic Therapy For Cancer Treatment , WEI CHEN, University of Texas at Arlington — Photodynamic therapy has been designated as a "promising new modality in the treatment of cancer" since the early 1980s. Light must be delivered in order to activate photodynamic therapy. Most photosensitizers have strong absorption in the ultraviolet – blue range, therefore, UV -blue light is needed for their activation. Unfortunately, UV-blue light has minimal penetration into tissue and its application for *in vivo* activation is a problem. To solve the problem and to enhance the PDT treatment for deep cancers, we introduce a new PDT system in which the light is generated by afterglow nanoparticles with attached photosensitizers. When the nanoparticle-photosensitizer conjugates are targeted to tumor, the light from afterglow nanoparticles will activate the photosensitizers for photodynamic therapy. Therefore, no external light is required for treatment. More importantly, it can be used to treat deep tumor such as breast cancer because the light source is attached to the photosensitizers and are delivered to the tumor cells all together. This modality is referred as nanoparticle self-lighting photodynamic therapy.

Monday, March 21, 2011 8:00AM - 11:00AM –
Session A42 DPOLY: Focus Session: Directed Assembly of Hybrid Nanomaterials A302/303

8:00AM A42.00001 Magnetically Actuated Artificial Cilia with Controlled Length and Areal Density , JASON BENKOSKI, JENNIFER BREIDENICH, MICHAEL WEI, GUY CLATTERBAUGH, Johns Hopkins University APL, PEI-YUIN KENG, JEFFREY PYUN, University of Arizona — Artificial cilia have been explored for use in microrobotics, MEMS, and lab-on-a-chip devices for applications ranging from micromixers, microfluidic pumps, locomotion, acoustic detection, and heat transfer. We have previously demonstrated the ability to assemble dense brushes of magnetically actuated artificial cilia from the dipolar assembly of 24 nm ferromagnetic cobalt nanoparticles. Despite areal densities exceeding 1 cilim/μm^2, diameters below 25 nm, aspect ratios exceeding 400, and flexural rigidities below 3 x 10^{-28} Nm^2, these seemingly delicate structures resist collapse upon each other or the underlying substrate. The current study demonstrates the ability to rationally control their average length and areal density by changing the nanoparticle concentration and the dimensions of the rectangular capillary tube. We find that the length and areal density obey a simple conservation of mass relationship with concentration and capillary height such that the product of the former equals the product of the latter. Detailed statistical analysis supports a mechanism in which the role of the external field is to align pre-existing chains with the external field, assist stacking of chains along the axis of the field, and then draw them towards the ends of the permanent magnets, where the magnetic field gradient is steepest.

8:12AM A42.00002 Ordered ferrofluidic assemblies in polymer film formed by magnetically induced polymer-solvent phase separation , NATARAJ SANNA KOTRAPPANAVAR, MYUNGHWAN BYUN, PAUL ZAVAL-REVIERA, KEVIN CHONNON, Biological and Soft Sciences Sector, Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK, SHAHEEN S.A. AL-MUHTASEB, Department of Chemical Engineering, Qatar University, P.O. Box 2713, Doha, Qatar, EASAN SIVANIAH, Biological and Soft Sciences Sector, Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK, BIOLOGICAL AND SOFT SCIENCES SECTOR, CAVENDISH LABORATORY, UNIVERSITY OF CAMBRIDGE, CAMBRIDGE CB3 0H TEAM, DEPARTMENT OF CHEMICAL ENGINEERING, QATAR UNIVERSITY, P.O. BOX 2713, DOHA, QATAR COLLABORATION — Tri-block copolymer has been used as nonferrofluid to generate permanent magnetic structures with controlled dimension and architecture in a partially miscible ferrofluid-nonferrofluid mixture under the influence of a perpendicular magnetic field. The nature of the resultant assemblies was strongly dependent on the magnetic field and concentration of ferro/nonferrofluidic systems. These ordered cluster assemblies in a polymer film that can be used either directly, in applications such as membrane, or subsequently as a template for the formation of other nanostructured materials. The origin of the permanent structures, which have characteristic lateral dimensions ranging from 5 μm to submicron range, is the repartitioning of the ferrofluid carrier solvent into the nonferrofluid polymeric phase.

8:24AM A42.00003 Manipulating nanoparticles via polymer crystallization , CHRISTOPHER LI, BIN DONG, BING LI, XI CHEN, WENDA WANG, Department of Materials Science and Engineering, Drexel University, Philadelphia, PA 19104, USA — Directed nanoparticle (NP) assembly is of great interest in order to achieve desired NP structures for various application purposes. In this presentation, we will present our recent results on employing polymer single crystals (PSC) to direct NP assembly. First, tailor-made, free-standing NP frames and wires containing single or multiple types of NPs have been obtained by using an in-situ polymer crystallization method. End functionalized poly(ethylene oxide) single crystals were used as the templates. Gold and magnetite NPs were successfully patterned as evidenced by transmission electron microscopy experiments. Secondly, carbon nanotube induced PSCs were used to guide AuNPs to assemble into periodic pattern with controlled periodicity. Thirdly, polymer nanofibers decorated with block copolymer single crystals were used as templates to induce the formation of hydroxyapatite (HA) nanocrystals and the resultant nanofiber/HA hybrids mimic the structure of natural bones.

8:36AM A42.00004 Directed Assembly of Nano-Colloids: Toward Discrete and Defined Polymer-Inorganic Architectures , RICHARD VAIA, Air Force Research Laboratory — Analogies between controlled flocculation and the chemistry of macromolecular polymerization are informing new methods for bottom up fabrication of discrete polymer-inorganic architectures. Conceptually, hybrid nano-colloids with a narrow distribution of composition and structure ("monomers") are assembled via external control of the agglomeration kinetics ("polymerization"). The challenge however is to impart a level of predictability between nanoparticle design and resultant assembly, as embodied in monomer design and macromolecular architecture. Depending on the magnitude and directionality of the interparticle interactions, the controlled assembly of these hybrid nano-colloids can span from discrete, soluble proto-assemblies to single-component, bulk mediums with local order ranging from liquid-like to long-range translational coherence. Using nanoparticle shape, organic corona structure, and processing conditions (e.g. modulating the stability of the nano-colloid via solvent quality rather than number density), we demonstrate the fabrication of various discrete and defined metallic and metal oxide hybrid architectures, and discuss the unique properties of the assemblies, which reflect the uniformity of structure, nano-scale separation of the inorganic particles, and confinement of the polymer chains.

9:12AM A42.00005 Designing Functionalized Nanoparticles for Controlled Assembly in Polymer Matrix: Self consistent PRISM Theory and Monte Carlo simulation Study , ARTHI JAYARAMAN, NITISH NAIR, University of Colorado at Boulder — Significant interest has grown around the ability to create hybrid materials with controlled spatial arrangement of nanoparticles mediated by a polymer matrix. By functionalizing or grafting polymers on to nanoparticle surfaces and systematically tuning the composition, chemistry, molecular weight and grafting density of the grafted polymers one can tailor the inter-particle interactions and control the assembly/dispersion of the particles in the polymer matrix. In our recent work using self-consistent Polymer Reference Interaction Site Model (PRISM) theory- Monte Carlo simulations we have shown that tailoring the monomer sequences in the grafted copolymers provides a novel route to tuning the effective inter-particle interactions between the functionalized nanoparticles in a polymer matrix. In this talk I will present how monomer sequence and molecular weights (with and without polydispersity) of the grafted polymers, compatibility of the graft and matrix polymers, and nanoparticle size affect the chain conformations of the grafted polymers and the potential of mean force between the grafted nanoparticles in the matrix.

9:24AM A42.00006 High Fidelity Detection of Defects in Polymer Films using Surface-Modified Nanoparticles , ALAMGIR KARIM, MATTHEW BECKER, CHAITANYA PRATIWADA, Dept. of Polmyer Engg., University of Akron, Akron, OH, USA, UNIVERSITY OF AKRON TEAM — Surface defects are ubiquitous for most thin films, yet their systematic detection poses one of the most difficult challenges even to modern day technology. Polymer thin films are no exception to these problems. We address this issue by developing a novel, efficient method for the optical detection of surface topographical features using fluorescent nanoprobes, which are surface-modified CdSe quantum dots whose ability to detect surface features can be tuned via size and chemical properties. We have successfully applied this approach to detect numerous types of artificial and natural defects in polymer films including lines, pinholes, sharp edges, and chemically variant defect surfaces. This method can elucidate the surface structure of large areas in a minimal amount of time. It is estimated that this new method will decrease imaging time compared to traditional imaging methods like AFM and SEM by 50 fold. Our defect detection approach could be applicable for many problems where polymers are used as a component in hybrid nanomaterial films

9:36AM A42.00007 Directed Hierarchical Assemblies of Nanoparticles in Thin Films[1] , TING XU, UC, Berkeley — Controlling nanoparticle (NP) assemblies in thin films will enable one to capitalize on the unique properties of NPs so as to generate functional devices, such as hybrid photovoltaic, capacitors and optical devices. To this end, it is mandatory to control the macroscopic alignment of NP assemblies and inter-particle ordering with high precision to achieve a specific property. Recently, we described a new approach to assemble NPs over multiple length scales by combining small molecules with block copolymers (BCPs). Small molecules that favorably interact with NP ligands mediate polymer-NP interactions and solublize the NPs within the BCP microdomains. The small molecules also direct the spatial distribution of NPs within the BCP microdomains with exquisite precision. In the bulk, NPs were shown to readily assemble into ordered 1-D, 2-D and 3-D arrays. I will discuss our recent studies on directed hierarchical assemblies of NPs in thin films. Specifically I will focus on how to manipulate the macroscopic alignment and long-range ordering of NPs and generating NP superlattice within the BCP microdomains.

[1]Supported by NSF-DMR, ONR-YIP and DOE-BES

9:48AM A42.00008 Adsorption of particles at fluid interfaces: Jamming, structure control, and rheology , SACHIN VELANKAR, University of Pittsburgh — Various types of particles readily adsorb at the interface between two immiscible liquids or at the surface of a liquid. Such particles bear some similarity to conventional molecular surfactants. However, unlike surfactants, particles adsorb almost irreversibly at interfaces - a fact that can lead to interesting phenomena such as the stability of non-spherical jammed drops, spontaneous climbing of particle films, and particle-bridged emulsions. Similar phenomena - albeit with important differences - can be observed in polymeric systems and may lead to interesting new materials. This talk will review some of these phenomena, with a particular focus on the jamming of fluid interfaces due to particles, and discuss applications for controlling the structure of two-phase polymer systems such as polymer blends and foams.

10:24AM A42.00009 Additive-driven assembly of block copolymers , YING LIN, VIKRAM DAGA, ERIC ANDERSON, JAMES WATKINS, University of Massachusetts — One challenge to the formation of well ordered hybrid materials is the incorporation of nanoscale additives including metal, semiconductor and dielectric nanoparticles at high loadings while maintaining strong segregation. Here we describe the molecular and functional design of small molecule and nanoparticle additives that enhance phase segregation in their block copolymer host and enable high additive loadings. Our approach includes the use of hydrogen bond interactions between the functional groups on the additive or particle that serve as hydrogen bond donors and one segment of the block copolymer containing hydrogen bond acceptors. Further, the additives show strong selectively towards the targeted domains, leading to enhancements in contrast between properties of the phases. In addition to structural changes, we explore how large changes in the thermal and mechanical properties occur upon incorporation of the additives. Generalization of this additive-induced ordering strategy to various block copolymers will be discussed.

10:36AM A42.00010 Supramolecular Assembly of Gold Nanoparticles in PS-b-P2VP Diblock Copolymers via Hydrogen Bonding , SE GYU JANG, CRAIG J. HAWKER, EDWARD J. KRAMER, University of California Santa Barbara — We report a simple route to control the spatial distribution of Au nanoparticles (Au-NPs) in PS-*b*-P2VP diblock copolymers using hydrogen bonding between P2VP and the hydroxyl-containing (PI-OH) units in PS-*b*-PIOH thiol-terminated ligands on Au-NP. End-functional thiol ligands of poly(styrene-*b*-1,2&3,4-isoprene-SH) are synthesized by anionic polymerization. After synthesis of Au-NPs, the inner PI block is hydroxylated by hydroboration and the resulting micelle-like Au-NPs consist of a hydrophobic PS outer brush and a hydrophilic inner PI-OH block. The influence of the hydroxyl groups is significant with strong segregation being observed to the PS/P2VP interface and then to the P2VP domain of lamellar-forming PS-b-P2VP diblock copolymers as the length of the PI-OH block is increased. The strong hydrogen bonding between nanoparticle block copolymer ligands and the P2VP block allows the Au-NPs to be incorporated within the P2VP domain to high Au–NP volume fractions $\phi_p$without macrophase separation, driving transitions from lamellar to bicontinuous morphologies as ϕ_p increases.

10:48AM A42.00011 Role of defects on self-assembly of nanoparticles in block copolymer thin film , JENNY KIM, Universiy of Michigan, PETER GREEN, University of Michigan — The structure of A-b-B block copolymer (BCP) thin films is often exploited as scaffolds for directing nanoparticles into various, long-range ordered geometries. Depending on the affinity between nanoparticles and block chains, nanoparticles preferentially segregate to either A or B domains. We show that dislocations may play a dominant role in the assembly of large nanoparticles in BCP thin film that order at suboptimal thicknesses. Edge dislocations are ubiquitous in lamellar BCP thin films forming a partial surface layer, i.e. holes or island structures. When the ratio of the nanoparticle diameter, d, to the domain dimension, L, d/L < 0.15, the nanoparticles were distributed uniformly throughout the film. However for larger values of d/L, the nanoparticles reside primarily at the dislocation cores. In the case of films of initial film thicknesses between L $<$ h $<$ 3L the nanoparticles self-assemble into 2-dimensional planar shapes at the boundaries of holes or islands where edge dislocations are located.

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A43 DPOLY: Focus Session: Thin Film Block Copolymers I A306/307

8:00AM A43.00001 Study of Complex Morphology of ABC Triblock Copolymer with Resonant Soft X-ray Scattering , CHENG WANG, DONG HYUN LEE, LBNL, WEI ZHAO, THOMAS RUSSELL, UMASS, MYUNG IM KIM, TING XU, UCB, HIROKAZU HASEGAWA, UKyoto, ALEXANDER HEXEMER, LBNL — Combining the spectroscopy sensitivity with scattering, resonant soft x-ray scattering (RSoXS) is an ideal tool for characterizing morphology of multi-component soft materials thin films. Both elemental and chemical sensitivity can be achieved by changing incident photon energy close to the absorption edge of the constituent atoms. In this work, the morphologies in thin film and bulk of A-B-C triblock copolymer, Poly(1,4-isoprene)-block-polystyrene-block-poly(2-vinlypyridine), were investigated with RSoXS together with scanning force microscopy, small angle x-ray scattering and transmission electron microscopy. In thin film, hexagonal array of nanostructures were observed by all the techniques, however, RSoXS revealed the core-shell nanostructures. In bulk, hexagonally packed cylindrical microdomains was observed. By selectively staining different polymer block, TEM tomography results suggested spatial arrangement of two different cylindrical microdomains consisted of poly(1,4-isoprene) and poly(2-vinlypyridine) in polystyrene matrix. Using soft x-ray at selected photon energies to isolate the scattering contribution from two different polymer blocks, RSoXS unambiguously revealed the two different hexagonally packed lattice.

8:12AM A43.00002 STED Microscopy as a Characterization Tool for Three Dimensionally Nanostructured Block Copolymer Thin Films , CHAITANYA ULLAL, ROMAN SCHMIDT, ULRIKE BOEHM, Max Planck Institute for Biophysical Chemistry, SEBASTIAN PRIMPKE, PHILIPP VANA, Georg August Universitaet, Goettingen, STEFAN HELL, Max Planck Institute for Biophysical Chemistry — STED microscopy is an emerging method in the characterization of block copolymer film morphologies. We demonstrate a complete experimental platform that allows us to obtain in situ Three Dimensional images with microdomain specificity. IsoSTED, a variant of STED microscopy that coherently combines two opposing lenses, yields the necessary resolution, while the necessary fluorescence contrast is achieved by deterministically confining fluorophores to the targeted microdomain. These capabilities are combined to provide unambiguous images of various nano-structured block copolymer morphologies.

8:24AM A43.00003 Interfaces between Block Copolymer Domains , JAEUP KIM, UNIST, Korea, SEONG-JUN JEONG, University of California, Berkeley, SANG OUK KIM, KAIST, Korea — Block copolymers naturally form nanometer scale structures which repeat their geometry on a larger scale. Such a small scale periodic pattern can be used for various applications such as storage media, nano-circuits and optical filters. However, perfect alignment of block copolymer domains in the macroscopic scale is still a distant dream. The nanostructure formation usually occurs with spontaneously broken symmetry; hence it is easily infected by topological defects which sneak in due to entropic fluctuation and incomplete annealing. Careful annealing can gradually reduce the number of defects, but once kinetically trapped, it is extremely difficult to remove all the defects. One of the main reasons is that the defect finds a locally metastable morphology whose potential depth is large enough to prohibit further morphology evolution. In this work, the domain boundaries between differently oriented lamellar structures in thin film are studied. For the first time, it became possible to quantitatively study the block copolymer morphology in the transitional region, and it was shown that the twisted grain boundary is energetically favorable compared to the T-junction grain boundary. [Nano Letters, **9**, 2300 (2010)]. This theoretical method successfully explained the experimental results.

8:36AM A43.00004 Patterning of Multiple Block Copolymers per Layer with Orthogonal Processing , WEI MIN CHAN, Department of Electrical Engineering, Cornell University, EVAN L. SCHWARTZ, Department of Materials Science and Engineering, Cornell University, JIN-KYUN LEE, Department of Polymer Science and Engineering, Inha University, JOAN K. BOSWORTH, Hitachi Global Storage Technologies, JOHN DEFRANCO, Orthogonal Inc, SANDIP TIWARI, Department of Electrical Engineering, Cornell University, CHRISTOPHER K. OBER, Department of Materials Science and Engineering, Cornell University — In this work we demonstrate the concept of orthogonal processing of block copolymers. By using a semi-flourinated photoresist/solvent system, we are able to selectively pattern or lift-off and then recover the block copolymer film intact. This approach can enable removable templating of self- assembly and also multiple block copolymers, morphologies or domain sizes on the same layer which can open the door to self-assembly of a wider range of geometries than possible before. We highlight the interplay between the various parameters for a successful additive and subtractive patterning and directions for further theoretical investigation as well as the limitations of this technique.

8:48AM A43.00005 Highly specific placement of Au Nanoparticles on chemical brush patterns prepared by combination of top-down and block copolymer lithography , SERDAR ONSES, CHI-CHUN LIU, CHRISTOPHER THODE, SHENGXIANG JI, PAUL NEALEY, University of Wisconson-Madison — Metallic nanoparticles (NPs) with interesting optical, electronic and reactivity properties show great promise for a range of scientific fields and technological applications, such as plasmonics, catalysis, and nanowire growth. However taking advantage of these properties, particularly for device fabrication often requires immobilization of pre-synthesized particles with high specificity and precise control of density and spacing of NPs at sub 100 nm scale. Here we show that lithographic patterning of a cross-linkable polystyrene brush and subsequent filling with poly(2-vinyl pyridine) (P2VP) leads to high contrast chemical patterns leading to site-specific placement of pre-synthesized Au NPs (13 nm) with the precise control of number from single to tens of particles per spot. Moreover we show that this approach is extendible to large area patterning of NPs with costs and process times suitable for technological applications using block-copolymer (BCP) lithography.

9:00AM A43.00006 Synthesis and graphoepitaxial placement control of block copolymer mediated silver nanoparticles , DONG WOOK KIM, NOEL ARELLANO, CHARLES RETTNER, LESLIE KRUPP, TEYA TOPURIA, PHILIP RICE, GABRIELE RAINO, THILO STOFERLE, RAINER MAHRT, HO-CHEOL KIM, KRICT TEAM, IBM ZURICH RESEARCH CENTER TEAM — The strong interactions of plasmons in metal nanoparticle assemblies can render many possible applications ranging from sensors to imaging and information technology. To realize such applications, synthesis of well defined metal nanoparticles and precise control over assembly are critical. In this paper, we report a synthetic scheme of silver nanoparticles and their combination with dielectrics and/or gain media and their assembly on substrates. Silver nanoparticles are synthesized using a block copolymer of polystyrene and poly(4-vinyl pyridine) (PS-b-P4VP). Well defined nanoparticles were assembled on substrates using a graphoepitaxial approach with topographic patterns prepared by E-beam lithography. The effect of shapes and scales of topographic patterns on the nanoparticle assembly was investigated. Careful optical characterization and potential applications will be discussed.

9:12AM A43.00007 Functional Nanomaterials based on Nanoporous Block Copolymer Templates[1] , JIN KON KIM, Pohang University of Science and Technology — Nanoporous templates have been widely used for the development of new functional nanostructured materials suitable for electronics, optics, magnetism, and energy storage materials. We have prepared nanoporous templates by using thin films of mixtures of polystyrene-*block*-poly(methyl methacrylate) (PS-*b*-PMMA) and PMMA homopolymers. These nanoporous films were found to be very effective for the separation of human Rhinovirus type 14, major pathogen of a common cold in humans. We found that when the pore size was effectively controlled down to 6 nm, a long-term constant *in vitro* release of BSA and hGH was achieved without their denaturation up to 2 months. The long-term constant delivery based on this membrane for protein drugs within the therapeutic range can be highly appreciated for the patients with hormone-deficiency.

Work done in collaboration with Seung Yun Yang, Pohang University of Science and Technology.

[1]This work was supported by the National Creative Research Initiative Program supported by NRF.

9:48AM A43.00008 Effect of Boundary Conditions on the Directed Self-Assembly of Block Copolymer on Chemical Patterned Surfaces , GUOLIANG LIU, Chemical and Biological Engineering, University of Wisconsin-Madison, PAUL NEALEY, Department of Chemical and Biological Engineering, University of Wisconsin-Madison — Previously we determined the morphological phase behavior of lamellae-forming poly(styrene-block-methyl methacrylate) (PS-b-PMMA) density multiplication on chemically patterned surfaces in thin films. The stripe density of the chemical pattern was half of the block copolymer domain density. Parallel lamellae, vertical lamellae, mixed lamellae, PS-dots, and PMMA-dots were observed depending on the pattern stripe width and interaction strength between the polymer and the patterned surfaces. The density multiplied vertical lamellae exhibited three dimensional profiles, which was problematic in the subsequent pattern transfer process. Here we found that the block copolymer domain profiles could be improved by revising the boundary conditions. In the meanwhile, better line width and line edge roughness were obtained. The addition of homopolymers into the block copolymer and subsequent molecular transfer printing could offer a chemically patterned surface with improved boundary conditions for block copolymer directed assembly. The printed chemical patterns had a stripe density and a stripe width matching with block copolymer domains. The interfacial energies of the stripes were favorable to the block copolymer domains.

10:00AM A43.00009 Directed assembly of supramolecular copolymers in thin films , MARCUS MULLER, KOSTAS CH. DAOULAS, Institute for Theoretical Physics, Georg-August University, Goettingen, Germany, ANNA CAVALLO, Dept. of Physics, Salerno University, Fisciano, Italy, ROY SHENHAR, Institute of Chemistry, Hebrew University, Jerusalem, Israel — Using computer simulation of a coarse-grained model for supramolecular polymers we investigate the potential of quasi-block copolymers (QBCP) assembled on chemically patterned substrates for creating device-oriented nanostructures. QBCP are comprised of AB diblock copolymers and supramolecular B segments that can reversibly bond to any available B terminus, either on the copolymers or the B oligomers, creating a polydisperse blend of B homopolymers, AB and ABA copolymers. We focus on an AB incompatibility, χ, and strength of supramolecular bonds where a lamellar morphology, a bicontinous structure and a macrophase-separated state have comparable free energy in the bulk. We consider substrate patterns with perpendicularly crossing, A-preferential lines and demonstrate their defect-free replication by QBCP. The same QBCP replicates simultaneously patterns differing by up to 50% in their length scales, illustrating the high versatility of QBCP materials. We discuss the interplay between pattern geometry and distribution of molecular architectures and verify the key role of supramolecular associations for replicating patterns with different length scales.

10:12AM A43.00010 Self-Assembly of Block Copolymers on Well-modulated Sawtoothed Surface , DONG HYUN LEE, Lawrence Berkeley National Laboratory, TING XU, University of California, Berkeley, SUNG WOO HONG, University of Massachusetts, Amherst, ALEXANDER HEXEMER, HOWARD PADMORE, Lawrence Berkeley National Laboratory, THOMAS RUSSELL, University of Massachusetts, Amherst — The self-assembly of block copolymers on the faceted surfaces of sapphire and silicon substrates were investigated as a function of the amplitude and pitch of the sawtooth pattern. To generate these surfaces, sapphire substrates, cut along the M plane, were annealed at temperatures above 1000°C. The pitch and amplitude of the sawtooth pattern was controlled by varying the annealing temperature. In addition, surfaces with a sawtooth pattern in silicon were generated by an anisotropic etching of the silicon. Block copolymers were spin-coated onto the pattered surfaces. To induce ordering of the BCP, the thin films were solvent-annealed in organic solvent vapors. Long-range lateral ordering of the BCP microdomains persisted across the entire surface with both types of substrates without further treatment. The ordering of the BCP is very sensitive to the geometry of sawtooth pattern.

10:24AM A43.00011 Templating non-hexagonal monolayers of block copolymer spheres in confined geometries , ADETUNJI ONIKOYI, EDWARD KRAMER, GLENN FREDRICKSON, SU-MI HUR, UCSB — We investigate the ordering of poly(styrene-b-2vinylpyridine) [PS-PVP Mn = 56 kg/mol] sphere monolayers in wells of various shapes and sizes. Recent self-consistent field theory results on ordering of block copolymer (BCP) cylinders in square surroundings suggest that adding homopolymers of higher Mn can allow square arrays of BCP to form in small (4 to 5 cylinders across) square wells by relieving packing frustration. Experimentally, we adopt a similar strategy for ordering BCP spheres on silicon nitride membranes patterned by electron beam lithography to produce SiOx mesas, adding various volume fractions of PS homopolymer of different Mn. Scanning force microscopy, transmission electron microscopy and X-ray scattering has been used in a complementary manner to quantify the structures obtained after thermal annealing at 150 C. In the absence of PS additions, only defective hexagonal structures are observed even in wells containing 16 spheres. Adding 10% PS of Mn = 112 kg/mol to the BCP results in a square packing of spheres in square wells containing as many as 81 spheres.

10:36AM A43.00012 ABSTRACT WITHDRAWN –

10:48AM A43.00013 Dynamics of interacting edge defects in copolymer lamellae[1] , KARI DALNOKI-VERESS, JOSHUA D. MCGRAW, IAN D.W. ROWE, Department of Physics and Astronomy and the Brockhouse Institute for Materials Research, McMaster University — It is known that terraces at the interface of lamella forming diblock copolymers do not make discontinuous jumps in height. Rather, their profiles are smoothly varying. The width of the transition region between two lamellar heights is typically several hundreds of nanometres, resulting from a balance between surface tension, chain stretching penalties, and the enthalpy of mixing. What is less well known in these systems is what happens when two transition regions approach one another. In this study, we show that time dependent experimental data of interacting copolymer lamellar edges is consistent with a model that assumes a repulsion between adjacent edges. The range of the interaction between edge defects is consistent with the profile width of noninteracting diblock terraces.

[1]Financial support from NSERC of Canada is gratefully acknowledged.

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A44 DPOLY: Friction, Adhesion, and Fracture of Polymers A309

8:00AM A44.00001 Contact Adhesion of Wrinkled Surfaces , CHELSEA DAVIS, ALFRED CROSBY, University of Massachusetts Amherst — Inspired by examples in nature, recent research advances have demonstrated the ability to use topographic surface patterns rather than chemical modifications to control surface properties such as adhesion, wettability, and friction. Although most synthetic efforts have focused on the use of complicated lithographically-fabricated fibrillar structures, the use of spontaneously formed structures, such as surface wrinkles, have also proven advantageous. Wrinkles present many attributes, such as discretized length scales, which play an important role in adhesion control, yet the exact mechanisms for this control are not fully understood. We present a systematic study of the contact adhesion mechanics between a flat, rigid surface and a soft wrinkled surface. The wrinkles are fabricated using a technique that allows the effects of residual surface stresses and wrinkle topography to be decoupled in the context of adhesion control. We find that the maximum separation force for the wrinkled-flat interfaces increases with decreasing values of wrinkle wavelength and amplitude. These trends can be understood through the development of a simple scaling relationship, which links wrinkle geometry and materials properties to the maximum separation force.

8:12AM A44.00002 Structural Effects on the Friction of Tethered PDMS Networks[1] , CLAUDE COHEN, LUCAS LANDHERR, LYNDEN ARCHER, Cornell University — The interfacial properties of dry, surface-tethered end-linked polydimethylsiloxane (PDMS) films on silicon are examined. Thin network films (approximately 10 microns thick) were synthesized over a self-assembled monolayer supported on a silicon wafer. By systematically increasing the concentration of mono-functional PDMS chains in a mixture with telechelic precursor chains during cross-linking, structures ranging from near model elastic networks to very poorly cross-linked networks dominated by a preponderance of dangling/pendent chains were synthesized. Lateral force microscopy (LFM) employing a PE bead probe was used to quantify the effect of network structure and the role of viscoelasticity on the interfacial friction coefficient.

[1]Supported by DOE Grant DE-FG02-07ER46455 and NSF Grant DMR-0705565.

8:24AM A44.00003 Lithography-Free Microchannel Fabrication in PDMS[1] , JEYANTT S. SANKARAN, Department of Electrical Engineering, Nanotechnology Research and Teaching Facility, University of Texas at Arlington, WINTANA T. KAHSAI, UYEN H.T. PHAM, Department of Bioengineering, Nanotechnology Research and Teaching Facility, University of Texas at Arlington, SAMIR M. IQBAL, Department of Electrical Engineering, Nanotechnology Research and Teaching Facility, University of Texas at Arlington — We report a novel method for the fabrication of microchannels that could potentially be used for pervaporation experiments, cell adhesion and cell movement studies and detection of selective protein bio-markers. PDMS can sustain high temperatures, has a high young's modulus and it is biologically inert. Hydrophobic-hydrophilic interactions at gel point of PDMS form the basis of the presented technique. The repulsion of hydrophilic particles by the hydrophobic polymer matrix, stemming from the reduction of entropy and free energy variations during polymerization, provides an elegant lithography-independent approach for the fabrication of self-aligned microchannels.

[1]This work was supported by National Science Foundation CAREER Grant (ECCS 0845669).

8:36AM A44.00004 ABSTRACT WITHDRAWN –

8:48AM A44.00005 Polymer Brushes that Mimic Repulsive Properties of the Boundary Lubricant Glycoprotein Lubricin[1] , JAHN TORRES, Brown University/ Naval Undersea Warfare Center, GREGORY JAY, Brown University, QIAN NI, DAVID BELLO, GEOFFREY BOTHUN, University of Rhode Island, KYUNG-SUK KIM, Brown University — This is a report on the design of tailored functional groups which mimic the repulsive forces at work in the natural-joint boundary lubricant known as *lubricin*. *Lubricin*, an amphiphilic polyelectrolyte biomolecule, decreases friction and *cellular adhesion* by exhibiting surface force fields based on *steric hindrance*, *Debye electrostatic double layer repulsion* and *hydration repulsive forces*. We have identified a physically and chemically stable candidate polymers for anti-fouling coatings that will mimic lubricin's repulsive properties. Synthetic polymer brushes mimicking lubricin have been produced using these polymers grafted onto a glass surfaces. The average adhesive forces for the polymer brushes measured through atomic force microscopy are as low (56.796 $\pm$ 0.796 mN/m), similar to those exhibited by lubricin coated surfaces and on the same order of magnitude as superhydrophobic surfaces.

[1]This work was supported by the Coatings/Biofouling Program and the Maritime Sensing Program of the Office of Naval Research as well as the ILIR Program of the Naval Undersea Warfare Center DIVNPT.

9:00AM A44.00006 Activation-deactivation of self-healing in supramolecular rubbers , LAURENT CORTE, FLORINE MAES, DAMIEN MONTARNAL, SABINE CANTOURNET, FRANCOIS TOURNILHAC, LUDWIK LEIBLER, MINES-PARISTECH CNRS (UMR7633) TEAM, ESPCI-PARISTECH CNRS (UMR7167) TEAM — Self-healing materials have the ability to restore autonomously their structural integrity after damage. Such a remarkable property was obtained recently in supramolecular rubbers formed by a network of small molecules associated via hydrogen bonds [1]. Here we explore this self-healing through an original tack experiment where two parts of supramolecular rubber are brought into contact and then separated. These experiments reveal that a strong self-healing ability is activated by damage even though the surfaces of a molded part are weakly self-adhesive. In our testing conditions, a five minute contact between crack faces is sufficient to recover most mechanical properties of the bulk while days are required to obtain such adhesion levels with melt-pressed surfaces. We show that the deactivation of this self-healing ability seems unexpectedly slow as compared to the predicted dynamics of supramolecular networks. Fracture faces stored apart at room temperature still self-heal after days but are fully deactivated within hours by annealing. Combining these results with microstructural observations gives us a deeper insight into the mechanisms involved in this self-healing process. [1] P. Cordier, F. Tournilhac, C. Soulie-Ziakovic & L. Leibler, Nature, 451, 2008.

9:12AM A44.00007 Self-Healing of Polyethylene Oxide , DORINA MAGDALENA CHIPARA, MARITZA FLORES, NANCY PUENTE, KAREN LOZANO, The University of Texas Pan American — Autonomic self-healing is expected to enhance the lifetime of polymeric materials, resins, and composites subjected to long term mechanical stresses. The self-healing process is initiated by the rupture of some polyurea-formaldehyde microcapsules filled with monomer. The self-healing polymer is actually a compound containing microcapsules filled with monomer and catalyst particles. The monomer released from these broken microcapsules is diffusing within the polymer, reacting with the catalyst and starting a polymerization reaction. This new polymer, growing within the propagating crack, stops the mechanical failure. While the process is pretty slow (timescale of the order of 10 to 100 s), there are many important technological applications that would benefit from the availability of self-healing polymers. We report about the addition of self-healing capabilities to polyethylene oxide by using polyurea formaldehyde microcapsules filled with dicyclopentadiene and first generation Grubbs catalysts. Details regarding the physical and chemical steps used to add self-healing capabilities to polyethylene oxide will be presented. Self-healing efficiency was assessed by fatigues tests.

9:24AM A44.00008 Modeling the Nano-indentation of Self-healing Materials , SOLOMON F. DUKI, GERMAN V. KOLMAKOV, VICTOR V. YASHIN, Department of Chemical Engineering, University of Pittsburgh, TOMASZ KOWALEWSKI, KRZYSZTOF MATYJASZEWSKI, Department of Chemistry, Carnegie Mellon University, ANNA C. BALAZS, Department of Chemical Engineering, University of Pittsburgh — We use computational modeling to determine the mechanical response of crosslinked nanogels to an atomic force microscope (AFM) tip that is moved through the sample. We focus on two-dimensional systems where the nanogels are interconnected by both strong and labile bonds. We model each nanogel as a deformable particle using the modified lattice spring model that is applicable to a broad range of elastic materials.We utilize the Bell model to describe the bonds between these nanogel particles, and subsequently, simulate the rupturing of bonds due the force exerted by the moving indenter. The ruptured labile bonds can readily reform and thus, can effectively mend the cavities formed by the moving AFM tip. We determine how the fraction of labile bonds, the nanogel stiffness, and the size and velocity of the moving tip affect the self-healing behavior of the material. We find that samples containing just 10% of labile bonds can heal to approximately 90% of their original, undeformed morphology.

9:36AM A44.00009 Viscoelastic solid glue produced by orb-weaving spiders[1] , VASAV SAHNI, TODD BLACKLEDGE, ALI DHINOJWALA, The University of Akron — Modern orb-weaving spiders have evolved well-designed adhesives to capture preys. This adhesive is laid on a pair of soft and highly extensible axial silk fibers as micron-sized glue droplets that are composed of an aqueous coat of salts surrounding the nodules made of glycoproteins. Understanding the adhesion mechanism of these glue droplets has been challenging because both the glue droplets and the axial fibers contribute to the adhesive forces required to detach a thread from a surface. Here, we have decoupled these contributions by developing a novel experimental method to probe individual glue droplets and an energy model to separate the strain energy of the axial silk fibers from the adhesion energy required to peel the glue droplets. We observe that the glue droplets behave as a viscoelastic solid and are strongly affected by humidity and the rate of peeling. Knowledge of the adhesion and the mechanics of the glue will aid in developing bioinspired adhesives in the future.

[1]National Science Foundation

9:48AM A44.00010 Hydrophobic Interactions on a Protein-Polymer Functionalized Surface of Varying Hydrophilicity , KRISTEN KELLER, PINAR AKCORA, Stevens Institute of Technology — We have developed a novel heterogeneous surface consisting of streptavidin and poly(methyl methacrylate) (PMMA) grafted to silicon substrates. Such a system has been fabricated using the ever-growing click chemistry approach. Functionalities found at the surface of the substrates are characterized through FTIR while the hydrophobic effects arising from the interactions between the grafted components of differing hydrophilicities are investigated through AFM. Adhesive properties of such a heterogeneous surface are calculated using data acquired from force-distance measurements. Furthermore, changes in these properties resulting from variations in streptavidin surface coverage and PMMA chain length are similarly studied.

10:00AM A44.00011 Dissipative mechanisms of the lateral friction in contact-mode atomic force microscopy of flexible alkane molecule films , F.Y. HANSEN, Technical University Denmark, P. SOZA, Pontificia University Catolica Chile, H. TAUB, University of Missouri-Columbia, M. KIWI, U. VOLKMANN, Pontificia University Catolica Chile — Molecular dynamics simulations are used to investigate lateral friction in contact-mode Atomic Force Microscopy of tetracosane (n-$C_{24}H_{50}$) films. We find larger friction coefficients on the surface of monolayer and bilayer films in which the long axis of the molecules is parallel to the interface than on a surface of molecules with the long axis perpendicular to the surface, in agreement with experimental results. The simulations reveal that the strength of the attractive film-tip interaction is an important factor in energy dissipation and that molecular flexibility provides a major dissipative mechanism as manifested by torsional motion about the carbon-carbon bonds of the molecules.

10:12AM A44.00012 Stress-Induced Slip at Polymer-Polymer Boundaries , ANDREW GUSTAFSON, University of Minnesota — The phenomena of stress-induced tangential slip at polymer-polymer interfaces is studied by simulation and analytic theory. Simulations combine a slip-link model of entanglement with a self-consistent field description of the interface. We consider how the slip velocity depends upon shear stress, interfacial entanglement density, and polymer chain length. Our analysis assumes that the strongly non-linear shear thinning of the interface observed in experiment is a result of convective release of interfacial entanglements.

10:24AM A44.00013 Optical Properties of Isolated MEH-PPV polymers in Developing Crazes , MENG-KUAN WANG, Dept. of Photonics Engineering, Yuan Ze University, CHIAU-HENG TSAU, WEI-CHENG LI, ARNOLD CHANG-MOU YANG, Dept. of Materials Science, National Tsing Hua University, JUI-HUNG HSU, Dept. of Material Science and Opto-electronic Science, National Sun Yat-sen University, JONATHON D. WHITE, Dept. of Photonics Engineering, Yuan Ze University — Potential applications in light emitting devices and solar cells have led to extensive research into optimizing the optical properties of Luminescent Conjugated Polymers. Straining MEH- PPV/polystyrene thin films has been observed to result in craze formation and an enhancement of photoluminescence (PL). Using confocal microscopy, the optical properties of these crazes were investigated. Emission from developed crazes was found to be highly polarized while a variety of effects were found for developing crazes. The survival time of polymers in the crazed regions was increased by over 30% relative to the bulk. This suggests a stretch induced alignment of emitting segments in MEH-PPV as well as an increased resistance to photobleaching.

10:36AM A44.00014 Quantitative surface parameter maps using Intermodulation Atomic Force Microscopy , DANIEL FORCHHEIMER, DANIEL PLATZ, ERIK THOLÉN, CARSTEN HUTTER, DAVID HAVILAND, Royal Institute of Technology (KTH), Stockholm, Sweden — It is well known that the phase image in amplitude modulation atomic force microscopy (AM-AFM) is sensitive to material properties of the surface. However that information is not enough to fully quantify the tip-surface interaction. We have developed Intermodulation AFM, based on a spectral analysis of the cantilever's *nonlinear* dynamics, which increases the amount of information obtained without increasing scan time.[1] We show how it is possible to extract quantitative material properties of the surface from this additional information. The method works under the assumption of a tip-surface force model, such as the DMT model, fitting the model parameters to the measured spectral data. The parameters are obtained at each pixel of the AFM image and form surface property maps which can be displayed together with topography. We demonstrate this on different surfaces such as polymer blends, extracting stiffness and adhesive properties.

[1]D. Platz, E. A. Tholen, D. Pesen, and D. B. Haviland, Appl. Phys. Lett., 92, 153106 (2008)

10:48AM A44.00015 Direct Measurement of Acid-Base Interaction Energy at Polymer-Solid Interfaces[1] , ANISH KURIAN, SHISHIR PRASAD, ALI DHINOJWALA, The University of Akron — We have studied acid-base interactions at solid-liquid and solid- solid interfaces using interface-sensitive sum frequency generation (SFG) spectroscopy. The shift of the sapphire hydroxyl peak in contact with several polar and non-polar liquids and polymers was used to determine the interaction energy. The trend in the interaction energies cannot be explained by only measuring water contact angles. Molecular rearrangements at the sapphire interface, to maximize the interaction of the acid-base groups, play a dominant role and these effects are not accounted for in the current theoretical models. These results provide important insights in understanding adhesion, friction, and wetting on solid interfaces. In addition, we will present the consequences of the acid-base interactions on understanding surface segregation in polymer blends and copolymers.

[1]National Science Foundation

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A45 DAMOP: Focus Session: Exploring Quantum Phases in Cold Atom Systems A310

8:00AM A45.00001 Correlated phases of bosons in tilted, frustrated lattices , SUSANNE PIELAWA, TAKUYA KITAGAWA, EREZ BERG, SUBIR SACHDEV, Physics Department, Harvard University, Cambridge, MA 02138, USA — The search for correlated quantum phases of cold atoms in optical lattices has focused mainly on entangling the spin degrees of freedom on different lattice sites. We show that there are also rich possibilities for correlated phases in the density sector, and these are likely to be readily accessible by tilting Mott insulators into metastable states. It has been previously shown that a Mott insulator in a potential gradient undergoes an Ising quantum phase transition when the potential drop per lattice spacing is close to the repulsive interaction energy [1]. Here we theoretically study bosons in tilted, frustrated, two-dimensional lattices. The phases we find include phases with charge density order, a sliding Luttinger liquid phase, and a liquid-like ground state with no broken lattice symmetry.

[1] S. Sachdev, K. Sengupta, and S. M. Girvin, Phys. Rev. B 66, 075128 (2002).

8:12AM A45.00002 Pure Mott Phases in a Trapped 2D Hubbard Model[1] , DAVE CONE, Univ of California-Davis, VALY ROUSSEAU, Louisiana State University, SIMONE CHIESA, Univ of Tennessee-Knoxville, RICHARD SCALETTAR, Univ of California-Davis, GEORGE BATROUNI, Universite de Nice-Sophia Antipolis — In this talk, we report on Quantum Monte Carlo simulations of a Hubbard Hamiltonian which incorporates a proposed new method for confining ultracold atoms in an optical lattice. Termed "Off Diagonal Confinement (ODC)," this method employs an inhomogeneous array of hopping matrix elements which traps atoms by going to zero at the lattice edges. In contrast, the more conventional diagonal confinement(DC) trap uses a parabolic potential coupled to (diagonal) density operators. ODC has the advantage of producing systems which, while still being inhomogeneous, are entirely in the Mott phase. This makes the insulating behavior and associated antiferromagnetism more apparent, and also allows simulations which are free of the sign problem at low temperatures. We analyze the effects of using different ODC traps and compare results with those from DC traps, for density, spin, and pairing correlation functions, as well as entropy and temperature profiles. Finally, we will discuss the advantages and importance of this new confinement technique for modeling correlated systems, including the potential for reaching lower temperature scales by following constant entropy curves.

[1]Support from DOE, SCIDAC program, DOE-DE-FC0206ER25793.

8:24AM A45.00003 Exploring classical and quantum criticality in two-dimensional quantum gases , CHEN-LUNG HUNG, XIBO ZHANG, LICHUNG HA, SHIHKUANG TUNG, NATHAN GEMELKE[1], CHENG CHIN, The University of Chicago — Continuous phase transitions in two dimensions (2D) are expected to exhibit intriguing universal behaviors near the critical point. Prominent examples include the Berezinsky-Kosterlitz-Thouless (BKT) transition and the superfluid (SF) to Mott insulator (MI) transition described by the Bose-Hubbard model. Both transitions are investigated in our system based on ultracold Bose gases confined in a pancake-like optical trap with or without an optical lattice potential. In this talk, we will present a study of the universal behavior near the BKT transition by probing the density profiles and their fluctuations at various temperatures and atomic interaction strengths. We report the observation of global scale-invariance and universality in scaled thermodynamic observables. Our measurement agrees with the classical field theoretical prediction as well as the Monte Carlo calculations, and shows growing density-density correlations in the critical regime. Further extensions of this work, including exploration of quantum criticality near the SF-MI phase boundary, will be discussed.

[1]Current affiliation: Pennsylvania State University, University Park

8:36AM A45.00004 Fermions in Optical Lattices: Cooling Protocol to Observe Antiferromagnetism[1] , NANDINI TRIVEDI, The Ohio State University — Experiments on ultracold atoms in optical lattices have the potential of probing the complex phase diagrams arising from simple Hamiltonians. One of the most challenging problems for an optical lattice emulator is that of cooling fermions to observe interesting broken symmetry phases. In this talk I will discuss recent theoretical progress on this question for the simplest model of interacting fermions: the Hubbard model. We determine the equation of state, the density $\rho(\mu, T, U/t)$, and the entropy of the 3D repulsive Hubbard model using exact determinental Quantum Monte Carlo (QMC) simulations. Using the local density approximation (LDA), we calculate the spatial variation of density, entropy density, double-occupancy, local compressibility and local spin correlations for different trap curvatures and interaction strengths U/t. In contrast to a homogeneous system, we show that in a trap we can locally squeeze out the entropy from certain regions and observe antiferromagnetic order, even though the total entropy per particle in the cloud is quite high. We show that significant cooling due to entropy redistribution in the trap can be achieved by two mechanisms: (a) by increasing the lattice depth, and (b) by decompressing the cloud. Our calculations can be an important guide in the race to observe antiferromagnetic order in optical lattices.

[1]In collaboration with: Thereza Paiva (Rio de Janeiro, Brazil), Mohit Randeria (Ohio State), and Richard Scalettar (UC Davis). We acknowledge support from ARO W911NF-08-1-0338 and NSF-DMR 0706203 and the use of computational facilities at the Ohio Sup

9:12AM A45.00005 Criticality in Trapped Atomic Systems[1] , NIKOLAY PROKOFIEV, BORIS SVISTUNOV, Department of Physics, University of Massachusetts, Amherst, LODE POLLET, Theoretische Physik, ETH Zurich — We discuss generic limits posed by the trap in atomic systems on the accurate determination of critical parameters for second-order phase transitions, from which we deduce optimal protocols to extract them. We show that under current experimental conditions the in-situ density profiles are barely suitable for an accurate study of critical points in the strongly correlated regime. Contrary to recent claims, the proper analysis of time-of-fight images yields critical parameters accurately. L. POllet, N. Prokof'ev, and B. Svistunov, Phys. Rev. Lett. 104, 245705 (2010).

[1]Swiss National Science Foundation, the National Science Foundation under Grant PHY-0653183, and a grant from the Army Research Office with funding from the DARPA OLE program

9:24AM A45.00006 Inter-band coupling induced novel condensates in a double-well lattice[1] , QI ZHOU, Joint Quantum Institute and Condensed Matter Theory Center, University of Maryland, JAMES V. PORTO, Joint Quantum Institute, University of Maryland, SANKAR DAS SARMA, Joint Quantum Institute and Condensed Matter Theory Center, University of Maryland — We predict novel inter-band physics for bosons in a double-well lattice. An intrinsic coupling between the s and px band due to interaction gives rise to larger Mott regions on the phase diagram at even fillings than the ones at odd fillings. On the other hand, the ground state can form various types of condensates, including a mixture of single-particle condensates of both bands, a mixture of a single-particle condensate of one band and a pair-condensate of the other band, and a pair-condensate composed of one particle from one band and one hole from the other band. The predicted phenomena should be observable in current experiments on double-well optical lattices.

[1]Work supported by JQI-NSF-PFC, ARO-DARPA-OLE, and ARO-MURI.

9:36AM A45.00007 Unconventional Bose-Einstein condensation in high orbital bands , CONGJUN WU, The Department of Physics, University of Science and Technology of China, ZI CAI, The Department of Physics, University of California, San Diego, ANDREAS HEMMERICH, Institut für Laser-Physik, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — We perform the theoretical study on unconventional Bose-Einstein condensations (UBEC) in higher orbital bands of optical lattices observed by Hemmerich's group. These exotic states of bosons are non-zero condensation wavevectors, and thus beyond the "no-node" paradigm. We have studied various effects on UBECs including lattice asymmetry and interactions. The interplay between the kinetic and interaction energies gives rise to two different UBECs with the real and complex-valued condensation wavefunctions, respectively. The latter spontaneously breaks time-reversal symmetry, which is impossible in usual BEC systems.

9:48AM A45.00008 Topological semimetal: a probable new state of quantum optical lattice gases protected by D_4 symmetry[1] , KAI SUN, JQI and CMTC, University Of Maryland, W. VINCENT LIU, University of Pittsburgh and KITP UCSB, S. DAS SARMA, JQI and CMTC, University of Maryland — We demonstrate that a novel topological semimetal emerges as a parity-protected critical theory for fermionic atoms loaded in the p and d orbital bands of a two-dimensional optical lattice. The new quantum state is characterized by a parabolic band-degeneracy point with Berry flux 2π, in sharp contrast to the π flux of Dirac points as in graphene. We prove that this topological liquid is a universal property for all lattices of D_4 point group symmetry and the band degeneracy is protected by odd parity. Turning on interparticle repulsive interaction, the system undergoes a phase transition to a topological insulator, whose experimental signature includes chiral gapless domain-wall modes, reminiscent of quantum Hall edge states.

[1]KS and SDS acknowledge the support of JQI-NSF-PFC, AFOSR-MURI, ARO-DARPA-OLE and ARO-MURI. W.V.L. is supported by ARO and ARO-DARPA-OLE. We thank the KITP at UCSB for its hospitality where this research is supported in part by NSF Grant No. PHY05-51164.

10:00AM A45.00009 Unconventional superfluidity with non-collinear orbital order , HUBERT NGUYEN, ZI CAI, CONGJUN WU, UC San Diego — We propose an unconventional superfluid with spontaneous time-reversal symmetry breaking in p-orbital bands of cubic optical lattices. We find that in contrast to the square lattice which exhibits an antiferromagnetic orbital angular momentum (OAM), quantum fluctuations in the cubic lattice select an exotic superfluid state with non-collinear orderings of OAM moments. The collective excitations and phase transitions in this unconventional superfluid have also been discussed. This exotic superfluid state has no counterpart in solid state systems.

10:12AM A45.00010 Two distinct Mott-Insulator to Bose-glass transitions and breakdown of self averaging in the disordered Bose-Hubbard model , SEUNGMIN HONG, FRANK KRUGER[1], PHILIP PHILLIPS, University of Illinois, Urbana-Champaign — We show that two fixed points govern the Mott insulator to Bose glass transition in the disordered Bose-Hubbard model. At incommensurate fillings, the correlation length and the inverse compressibility diverge with exponents of $\nu = 1/D$ and $\gamma = 4/D - 1$, respectively, D the spatial dimension. We show that it is the breakdown of self-averaging (rare-region Griffiths physics) in the Bose glass that leads to a violation of the bound $\nu \geq 2/D$. At commensurate fillings, the transition is controlled by a different fixed point at which both the disorder and interaction vertices are relevant.

[1]Current affiliation: University of St Andrews

10:24AM A45.00011 Unbalanced fermion mixtures on an optical lattice , CHUNTAI SHI, University of California Riverside, TUN WANG, IQOQI-University of Innsbruck, Austria, SHAN-WEN TSAI, University of California Riverside — We study a two component fermion mixture on a square lattice. We describe such system by a Hubbard model wherein there is only on-site interaction between fermions of different species. Such a model can be realized by loading ultra cold fermions onto an optical lattice and by tuning the interaction strength via Feshbach resonance. We investigate the phase diagram of this system near half filling using the functional renormalization group approach for interacting fermions[1]. We focus on the interesting case where one species is at half filling so that their Fermi surface is nested while the other species is slightly doped so that their Fermi surface is not perfectly nested. We study both the cases with repulsive interaction and the cases with attractive interaction. For the attractive interaction, triplet pairing BCS instability among majority species compete with the singlet s-wave inter-species BCS pairing instability when the populations of two species are different. For the repulsive interaction, fermions with equal population are known to display d-wave singlet BCS pairing when both species are slightly doped away from half filling. When only one species of fermions is doped away from half filling, such d-wave instability is weakened while triplet pairing among majority species becomes possible.
[1]. R. Shankar, Rev. Mod. Phys. 66, 129 (1994).

10:36AM A45.00012 Bosonic models with Fermi-liquid kinematics: realizations and properties , PAUL GOLDBART, SARANG GOPALAKRISHNAN, Univ. of Illinois at Urbana-Champaign, AUSTEN LAMACRAFT, Univ. of Virginia — We consider models of interacting bosons in which the single-particle kinetic energy achieves its minimum on a surface in momentum space. The kinematics of such models resembles that resulting from Pauli blocking in Fermi liquids; therefore, Shankar's renormalization-group treatment of Fermi liquids [1] can be adapted to investigate phase transitions in these bosonic systems. We explore possible experimental realizations of such models in cold atomic gases: e.g., via spin-orbit coupling [2], multimode-cavity-mediated interactions [3], and Cooper pairing of Fermi gases in spin-dependent lattices. We address the phase structure and critical behavior of the resulting models within the framework of Ref. [1], focusing in particular on Bose-Einstein condensation and on quantum versions of the Brazovskii transition from a superfluid to a supersolid [3].

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10:48AM A45.00013 Pairing and crystallization of one-dimensional atomic mixtures with mass imbalance , TOMMASO ROSCILDE, Ecole Normale Superieure de Lyon - France, MARCELLO DALMONTE, CRISTIAN DEGLI ESPOSTI BOSCHI, Bologna University - Italy — We numerically investigate mass-imbalanced binary mixtures of hardcore bosons (or equivalently of fermions) loaded in one-dimensional optical lattices, with special focus on their instabilities towards the loss of first-order (one-body) coherence. We find a fundamental asymmetry between attractive and repulsive interactions. Attraction is found to always lead to pairing, and to pair crystallization for very strong mass imbalance and commensurate fillings. In the repulsive case away from half filling the two atomic components remain instead decoupled (and first-order coherent) over a large parameter range, and undergo crystallization or phase separation only for large mass-imbalance and/or strong interactions. This fundamental asymmetry is at odds with recent theoretical predictions, and can be tested directly via time-of-flight experiments on trapped cold atoms.

Monday, March 21, 2011 11:15AM - 2:15PM –
Session B1 DCMP: Quantum Devices Based on Semiconductor Nanowires Ballroom A1

11:15AM B1.00001 Cooper-pair splitter: towards an efficient source of spin-entangled EPR pairs , CHRISTIAN SCHONENBERGER, Department of Physics, University of Basel — In quantum mechanics the properties of two and more particles can be *entangled*. In basic science pairs of entangled particles, so called Einstein-Podolsky-Rosen (EPR) pairs, play a special role as toy objects for fundamental studies. They provide such things as "spooky interaction at distance," but they also enable secure encoding and teleportation and are thus important for applications in quantum information technology. Whereas EPR pairs of photons can be generated by parametric down conversion (PDC) in a crystal, a similar source for EPR pairs of electrons does not exists yet. In several theory papers, it has been suggested to use a superconductor for this purpose. The superconducting ground state is formed by a condensate of Cooper-pairs which are electron pairs in a spin-singlet state. Since there are many Cooper pairs in a metallic superconductor like Al, the main tasks are to extract Cooper pairs one by one and to split them into different arms. A controlled and efficient splitting is possible if one makes use of Coulomb interaction [1]. This has recently be demonstrated by two groups [2-4] using hybrid quantum-dot devices with both superconducting and normal metal contacts. In the present talk, I will discuss the Cooper-pair splitter results from the Basel-Budapest-Copenhagen team [3] and compare with the other experiments. As an outlook we discuss approaches that aim at entanglement detection. The Cooper pair splitter holds great promises because very large splitting efficiencies approaching 100% and large pair current rates appear feasible. This work has been done by L. Hofstetter, S. Csonka, A. Geresdi, M. Aagesen, J. Nygard and C. Schönenberger

[1] P. Recher, E. V. Sukhorukov, and D. and Loss, Phys. Rev. B **63**, 165314 (2001).
[2] C. Strunk, *Towards entangled electrons*, Nature Nanotechnology **5**, 11-12 (2009).
[3] L. Hofstetter, S. Csonka, J. Nygard, and C. Schönenberger, *Cooper pair splitter realized in a two-quantum-dot Y-junction*, Nature **460**, 906 (2009).
[4] L.G. Herrmann, F. Portier, P. Roche, A. Levy Yeyati, T. Kontos, and C. Strunk, *Carbon Nanotubes as Cooper Pair Beam Splitters*, Phys. Rev. Lett. **104**, 026801 (2010).

11:51AM B1.00002 Spin-orbit qubit in a semiconductor nanowire , SERGEY FROLOV, Kavli Institute of Nanoscience, Delft University of Technology — Spin-orbit interaction in InAs nanowires is so strong that spin and motion cannot be separated. The eigenstates of a single electron confined to a quantum dot become a spin-orbital doublet. We perform coherent manipulation of spin-orbit states of a single electron, thereby demonstrating a spin-orbit qubit. Fast and universal qubit control is achieved using gigahertz electric fields, which couple to the orbital part of the wavefunction. Qubits in adjacent quantum dots are addressed separately due to a gate-tunable difference in g-factors. Dephasing due to interaction with nuclear spins is studied in a Ramsey experiment. Coherence is extended using Hahn echo as well as Carr-Purcell-Meiboom-Gill dynamical decoupling pulse sequences. The next step is the demonstration of entanglement between neighbor qubits which can be achieved using exchange interaction.

12:27PM B1.00003 Prospecting for elusive Majorana particles in nanowires[1] , ROMAN LUTCHYN, Microsoft Station Q, UCSB — We propose and analyze theoretically an experimental setup for detecting the elusive Majorana particle in quasi-one dimensional semiconductor-superconductor heterostructures. The experimental system consists of a quasi one-dimensional semiconductor nanowire with strong spin-orbit Rashba interaction proximity coupled with an s-wave superconductor. Under appropriate conditions, such system can realize a non-trivial topological state supporting Majorana zero energy modes localized at the ends of the wire. These emerging Majorana quasiparticles, i.e. particles that are at the same time their own antiparticles, are effectively fractionalized objects (anyons) obeying non-Abelian statistics. We discuss several experiments for detecting Majorana fermions in nanowires.

[1]This work is supported by DARPA-QuEST and JQI-NSF- PFC.

1:03PM B1.00004 Spin States, Spin Correlations, Supercurrent, and Multiple Andreev Reflections in InSb Nanowire Quantum Devices , HONGQI XU, Lund University — Bulk InSb is one of the most promising materials for applications in spintronics and quantum information processing, due to the fact that it has the highest electron mobility μ_e = 77000 cm2/Vs, the smallest electron effective mass m_e* = 0.015 me, and the largest electron magnetic moment |g*| = 51 among all III-V semiconductors. Here, we report on realization and electrical measurements of InSb quantum dots and superconductor/InSb/superconductor hybrid quantum devices. The devices are made on a SiO2-capped Si substrate from InSb segments of InAs/InSb heterostructured nanowires grown by metal-organic vapor phase epitaxy. Spin states, effective g-factors, and spin-orbit interaction energy are measured for the fabricated InSb nanowire quantum dots [1]. We have also studied strong correlation phenomena and observed a new spin-correlation-induced phenomenon in the devices, namely the conductance blockade at the degeneracy of two orbital states with the same spin [2]. We attribute this conductance blockade to the effect of electron interference between two equivalent, strongly correlated, many-body states in the quantum dots. In superconductor/InSb nanowire/superconductor hybrid devices, we have observed supercurrent and multiple Andreev reflections, and have found that the fluctuations in the supercurrent are correlated to the conductance fluctuations of the corresponding InSb nanowires in the normal state. We have also observed multiple Andreev reflections and interplay between the Kondo correlation and proximity effect in the Coulomb blockade regime.

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[2] H. A. Nilsson et al., Phys. Rev. Lett. 104, 186804 (2010).

1:39PM B1.00005 Measurement of Spin Relaxation in SiGe nanowire quantum dots , CHARLES MARCUS, Department of Physics, Harvard University — This abstract not available.

Monday, March 21, 2011 11:15AM - 2:15PM –
Session B2 DCMP: Many-Body Effects for the Excited States of Graphene Ballroom A2

11:15AM B2.00001 Optical properties of single- and few-layer graphene: the role of interlayer and many-body interactions , JIE SHAN, Case Western Reserve University — Graphene, a single layer of carbon atoms, has attracted much attention in the past few years because of its unique 2D structure and linear dispersion relation near the K-point of the Brillouin zone. Optical spectroscopy provides a powerful tool for probing the electronic structure and interactions in graphene. In this talk we will discuss two types of interactions that affect the optical response – those arising from interlayer coupling of electrons and those arising from many-body effects. The possibility of altering the low-energy band structure of graphene through the interlayer interactions in few-layer graphene (FLG) was recognized theoretically several years ago and was demonstrated experimentally recently by infrared absorption spectroscopy. Two distinct classes of IR absorption spectra for crystalline samples of the same number of layers, but different stacking order, were also observed. These findings demonstrate the pronounced effect of interlayer interaction and stacking order on the electronic structure of FLG. Furthermore, significant many-body effects are revealed in the optical conductivity spectra. These were manifested as excitonic modifications to optical absorption near the saddle- point singularities. The strong electron-hole interactions produce an asymmetric resonance, significantly red-shifted from the value predicted by ab-initio GW calculations for the band- to-band transitions. Our experiment also showed a weak dependence of the excitonic resonance in FLG on layer thickness. This result reflects the effective cancellation of the increasingly screened repulsive electron-electron and attractive electron-hole interactions.

11:51AM B2.00002 Band structures of expitaxial graphene: the role of many-body interactions , ELI ROTENBERG, Lawrence Berkeley National Laboratory — This abstract not available.

12:27PM B2.00003 Ultrafast Carrier Dynamics in Graphene and Few Layer Graphite[1] , HENRY VAN DRIEL, University of Toronto — Graphene and its multilayer counterparts provide unique opportunities to study how the ultrafast carrier dynamics of layered systems evolve with layer number. We have carried out systematic investigations [1] of layered graphitic materials, from graphene to bulk graphite, exfoliated on to a Si/Silicon oxide substrate. The samples are excited using 150 fs, 800 nm pulses at room temperature and the time resolved reflectivity and transmission is probed using 150 fs, 1300 nm pulses. The response is governed by two times constants, one near 250 fs and the other near 3 ps, but both vary with the number of layers. The time constant are related to carrier cooling kinetics, interband transitions and hot phonon effects. The change in the first time constant with layer number is discussed in terms of alterations to the band structure with increasing number of layers over a few layers while the changes in the longer time constant over 10's of layers is related to substrate coupling effects. The results are compared with results from related experiments [2,3] using multilayer graphene, epitaxially grown on SiC, and also from results from experiments [4] using freestanding, thin graphite layers. *Work carried out with R.W. Newson and J.J. Dean.

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[2] D. Sun et al., Phys. Rev. Lett. 101, 157402 (2008).
[3] J.M. Dawlaty et al., Appl. Phys. Lett. 92, 043116 (2008).
[4] M. Breusing, C. Ropers and T. Elsaesser, Phys. Rev. Lett. 102, 086809 (2009).

[1]Research supported by NSERC.

1:03PM B2.00004 The Ordering and Electronic Structure of Multilayer Epitaxial Graphene on SiC[1] , EDWARD CONRAD, Georgia Institute of Technology — The structural definition of graphene as a single sheet of hexagonal carbon limits how we view this material. It is the electronic properties of a single isolated graphene sheet that actually defines and motivates current graphene research. Remarkably, the best example of the idealized band structure of graphene comes does not come from a single graphene layer but from multilayer films grown on SiC. Multilayer epitaxial graphene (MEG) not only shows all the 2D properties expected for an isolated graphene sheet, but it the scalability to large scale integrated carbon circuits. I will show that the reason for this remarkable property, i.e. that a multilayer graphene films behaving like a single graphene sheet, is due to MEG's unique stacking. MEG films have a quasi-ordered rotational stacking that breaks the Bernal stacking symmetry associated with graphite. Angle resolved photoemission spectroscopy (ARPES) data demonstrates that the bands are linear at the K-point of these films. We can also show that the rotated stacking is highly ordered and that less than 20% of the graphene sheets in the film are Bernal stacked. I will also show that ARPES measurements on MEG films demonstrate serious inadequacies with both tight binding and ab initio formalisms. In particular the data shows no reductions in the Fermi velocity or the formation of Van Hove singularity that have been consistently predicted for this material.

[1]I wish to acknowledge funding from the NSF under Grants No. DMR-0820382 and DMR-1005880.

1:39PM B2.00005 Raman spectroscopy of pristine, defected and strained graphene , ANDREA FERRARI, University of Cambridge — Raman spectroscopy is the most common and informative characterization technique in graphene science and technology. It is used to determine the number of layers, doping, strain, defects, functional groups, quality and type of edges [1-15]. I will discuss the historical development of the identification of the main Raman bands in graphene, focussing on the 2D" peak around 2450cm^{-1}, and its deep-UV Raman spectrum. I will then discuss the effects of defects, uniaxial and biaxial strain on the Raman spectrum. Combining strain and Raman measurements one can derive the constitutive relation for graphene, and gain insights in the resonant Raman process. The results on graphene are the basis to explain and unify analogous measurements on graphite, carbon fibres and carbon nanotubes reported over the past 30 years.

[1] A. C. Ferrari et al. Phys. Rev. Lett. 97, 187401 (2006).
[2] C. Casiraghi et al. Nano. Lett. 7, 2711 (2007).
[3] C. Casiraghi et al. Appl. Phys. Lett. 91, 233108 (2007).
[4] S. Pisana et al. Nat. Mater. 6, 198 (2007).
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[8] A. Das et al. Nature Nano. 3, 210 (2008).
[9] A. Das et al. Phys. Rev. B 79, 155417 (2009).
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[13] A. C Ferrari et al. Phys. Rev. B 61, 14095 (2000); 64, 075414 (2001).
[14] D. M. Basko et al. Phys Rev B 80, 165413 (2009).
[15] F. Schedin et al. ACS Nano 4, 5617 (2010)

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B3 FHP: The History of Superconductivity from its Discovery by Kammerlingh Onnes in 1911 Ballroom A3

11:15AM B3.00001 Heike Kamerlingh Onnes and the Road to Superconductivity , DIRK VAN DELFT, Director Museum Boerhaave — The discovery of superconductivity on 8 April 1911 came as a big surprise. It was stumbled upon in the Leiden cryogenic laboratory of Heike Kamerlingh Onnes in a moment of serendipity. Three years before, the liquefaction of helium on the other hand had been the culmination of a long battle with nature. It was a meticulously prepared operation, "big science" in its first appearance. Until recently, careless notebook entries by Kamerlingh Onnes and his terrible handwriting had hindered a complete view to the road to superconductivity. Even a date of the fascinating discovery was lacking. How did the discovery fit into the Leiden research program? What about the research effort Kamerlingh Onnes had to put in to be sure he had found superconductivity rather than a short-circuit? What about superfluidity? Once the right interpretation of the notebooks is clear, the real story can be told.

11:51AM B3.00002 From the Meissner Effect to the Isotope Effect: Precursors to the Microscopic Theory of Superconductivity , BRIAN SCHWARTZ, The Graduate Center of CUNY — After the discovery by Kamerlingh Onnes in 1911 of the low temperature disappearance of resistance in mercury to a state of perfect conductivity, there was a long period of more than two decades before there was a major experimental advance. In 1933, Meissner and Ochsenfeld discovered that a superconductor is not only a perfect conductor but in addition it is a perfect diamagnet. In 1935 F. and H. London presented a phenomenological understanding of the electromagnetic properties of the superconducting state, which included the London penetration depth for applied magnetic fields and later introduced the concept of a "stiffness" of the superconducting wave function. In 1950, Ginzburg and Landau developed a phenomenological theory for the superconducting state using general thermodynamic arguments.In the same year, Maxwell, and Serin et.al discovered the Isotope Effect which indicated that the electron-phonon interaction would play an important role in the theory of superconductivity.

12:27PM B3.00003 BCS: 50 Years , LEON COOPER, Brown University — The road to and from BCS: This talk was presented before an audience at Brown University on December 10th, 2010. The recording of the talk will be shown at the session in Dallas, as Professor Cooper will not be able to be present.

1:03PM B3.00004 Giaever, Nb3Sn, and Josephson , JOHN ROWELL, Arizona State University — The late 1950s and 1960s were times of remarkable progress in both the understanding and utilization of superconductivity. The majority of today's applications can be traced to key scientific advances made during a period of less than a decade, and the majority of those advances were made in the industrial research laboratories of the United States. As examples, in this talk I will mention the measurement of the specific heat and the critical current of Nb3Sn in high magnetic fields, the discovery by Giaever of tunneling between metal films and his direct observation of the superconducting energy gap, the understanding of strong coupling superconductors, leading to the development of tunneling spectroscopy of the electron-phonon pairing interaction, and the prediction by Josephson of pair tunneling.

1:39PM B3.00005 The arrival of high temperature superconductors[1] , PAUL C. W. CHU, Texas Center for Superconductivity, University of Houston and Lawrence Berkeley National Laboratory — The attainment of high temperature superconductivity has been considered a major advancement of modern science. It was the seminal discovery of the first cuprate high temperature superconductor, the Ba-doped La_2CuO_4, with a T_c of 35 K in 1986 by Alex Müller and George Bednorz of IBM Zurich Lab,[2] who were awarded the Nobel Prize in 1987, that ushered in the era of cuprate high temperature superconductivity. It was the first liquid nitrogen high temperature superconductor, $YBa_2Cu_3O_7$ with a T_c of 93 K discovered in 1987 by Paul C. W. Chu, Maw-Kuen Wu and colleagues in the respective groups at the University of Houston and the University of Alabama at Huntsville[3] that heralded the new era of high temperature superconductivity, drastically changing the psyche of superconductivity research and bringing superconductivity applications a giant step closer to reality. In the ensuing years, many high temperature superconductors have been found, leading to the current record T_c of 134 K which was observed by A. Schilling et al.[4] of ETH in 1993 in $HgBa_2Ca_2Cu_3O_{9-\delta}$ at ambient and later raised to 164 K under 30 GPa by L. Gao et al.[5] In the present talk, I shall briefly recall a few events leading to and during the arrival of high temperature superconductivity. The prospects for future superconductors with higher T_c will also be discussed.

[1]Supported in part by U.S. AFOSR, U.S. DoE through ORNL, U.S. AFRL CONTACT through Rice University, the T. L. L. Temple Foundation, the John J. and Rebecca Moores Endowment, and the State of Texas through TCSUH.

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Monday, March 21, 2011 11:15AM - 2:15PM –

Session B4 DPOLY: Hybrid Nanomaterials Assembly Ballroom A4

11:15AM B4.00001 "Hairy" Nanoparticles in Block Copolymers and Homopolymers: Modeling using Hybrid Self-Consistent Field Theory , VALERIY GINZBURG, The Dow Chemical Company — Today, dispersed nanoparticles play important role in various applications (toughened plastics, healthcare, personal care, etc.) Mesoscale simulations and theory are important in understanding what governs the morphology of nanoparticles under various conditions. In particular, for nanoparticle/block copolymer mixtures, two popular simulation methods are Self-Consistent Field/Density Functional Theory (SCF-DFT) (Thompson, Ginzburg, Matsen, and Balazs, Science 292, 2469 [2001]), and Hybrid Self-Consistent Field Theory (HSCFT) (Sides et al., Phys Rev Lett 96, 250601 [2006]). The two methods are shown to be very similar in their assumptions and end-results; the choice of the method to be used can depend on the specific problem. Here, we use modified HSCFT to explicitly account for the complicated role of short-chain ligands grafted onto nanoparticles to promote dispersion. In particular, we discuss the phase diagrams of such "hairy" nanoparticles in diblock copolymers as function of diblock composition, nanoparticle volume fraction, and ligand length. Depending on the particle size and ligand coverage, particles could segregate into favorable domain, stay close to the interface, or phase-separate from the block copolymer altogether. We also consider the dispersion of "hairy" nanoparticles in a homopolymer and analyze the morphologies of particle clusters as function of ligand length. The results could have interesting implications for the design of new nanocomposite materials.

11:51AM B4.00002 Direct hierarchical assemblies of nanoparticles in thin films , TING XU, Univ of California - Berkeley — This abstract not available.

12:27PM B4.00003 Aqueous foams stabilised solely by nanoparticles , DOMINIQUE LANGEVIN, CNRS — Particles are being increasingly used to stabilise foams and emulsions, the corresponding emulsions being known as "Pickering" emulsions. One of the peculiarities of these systems is the absence of Ostwald ripening: since the bubbles or drops do not grow (coalescence seems also suppressed) both foams and emulsions are stable over extremely long periods of time (months). These features make particles very interesting surface active agents as compared to standard surfactants or polymers/proteins. The origin of the suppression of ripening can be traced to the unusual behaviour of the interfacial layers made by these particles. The layers are solid-like and the usual characterisation methods (surface tension, surface rheology) are not straightforward to use. In this presentation, we will illustrate these difficulties with experiments made with partially hydrophobic silica nanoparticles. We will also discuss the relevance of foam characterisations methods such as multiple light scattering and X-ray tomography.

1:03PM B4.00004 Control of Nanoparticle Organization in Thin Homopolymer Films , PETER F. GREEN, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI 48109 — The morphological structure of mixtures of homopolymers with chain-grafted nanoparticles is determined by competing interactions between the nanoparticle cores, the free host chains and the grafted chains. In the bulk, when the nanoparticle grafting density is low, the phase behavior is largely determined by a competition between attractive nanoparticle core-nanoparticle core interactions, mediated by the chains grafted to the surface. At high grafting densities, the entropic brush layer/free host chain interactions are dominant, leading to miscibility or to microscopic/macroscopic phase separation. Thin film mixtures are thermodynamically less stable than their bulk analogs due to the preferential attraction of grafted nanoparticles to the external interfaces. The preferential attraction of the nanoparticles to the interfaces is driven by factors that include: entropic gains of the grafted nanoparticles and linear host chains; van der Waals interactions between the nanoparticles and the interfaces. If the grafted chains and host chains are of dissimilar chemical structure, then the nanoparticles exhibit a tendency to segregate to the free surface, provided its grafts possess a lower surface energy than the host chains. Consequences of these interactions on the overall nanoparticle organization in thin homopolymer films will be discussed.

1:39PM B4.00005 Nanoparticle Self-Assembly in a Polymer Matrix and Its Impact on Phase Separation , JACK DOUGLAS, Polymers Division, NIST — The ubiquitous clustering of nanoparticles (NPs) in solutions and polymer melts depends sensitively on the strength and directionality of the effective NP-NP interactions, as well as on the molecular geometry and interactions of the dispersing fluid. Surface functionalization apparently can also lead to emergent anisotropic interactions that can influence NP dispersion. Since NP clustering can strongly influence the properties of polymer nanocomposites and NP solutions, we investigate the reversible self-assembly of model NPs into clusters under equilibrium conditions through a combination of simulation and analytic methods. First, we performed molecular dynamics simulations of polyhedral NPs in a coarse-grained dense bead–spring polymer melt and find a transition from a dispersed to clustered NP state, consistent with the thermodynamic models of equilibrium particle association such as equilibrium polymerization. We also describe the competition between self-assembly and phase separation in an analytic lattice model of a mixture of polymers and NPs. We then focus on the particularly interesting situation where the associating "monomeric" NP species form high molecular mass dynamic polymeric clusters and where the assembly process then transforms the phase boundary from a form typical of a polymer solution to one that more resembles a polymer blend with increasing association near the critical point for phase separation. The model calculations elucidate basic physical principles governing the coupling of self-assembly and phase behavior in these complex mixtures.

Monday, March 21, 2011 11:15AM - 2:15PM –
Session B5 DCMP FEd: Mentoring Undergraduate Research Ballroom C1

11:15AM B5.00001 Using seminar-based instruction to convey contemporary research to undergraduates , ERIC MAZUR, Harvard University — This abstract not available.

11:51AM B5.00002 Flocking and self-defense: experiments and simulations of avian mobbing , SUZANNE AMADOR KANE, Physics Department, Haverford College, Haverford PA — We have performed motion capture studies in the field of avian mobbing, in which flocks of prey birds harass predatory birds. Our empirical studies cover both field observations of mobbing occurring in mid-air, where both predator and prey are in flight, and an experimental system using actual prey birds and simulated predator "perch and wait" strategies. To model our results and establish the effectiveness of mobbing flight paths at minimizing risk of capture while optimizing predator harassment, we have performed computer simulations using the actual measured trajectories of mobbing prey birds combined with model predator trajectories. To accurately simulate predator motion, we also measured raptor acceleration and flight dynamics, well as prey-pursuit strategies. These experiments and theoretical studies were all performed with undergraduate research assistants in a liberal arts college setting. This work illustrates how biological physics provides undergraduate research projects well-suited to the abilities of physics majors with interdisciplinary science interests and diverse backgrounds.

12:27PM B5.00003 Involving undergraduates in interdisciplinary research: The physics of biomineralization , PUPA GILBERT, University of Wisconsin-Madison — Biominerals include mollusk shells, the skeletons of sea urchins, corals, mammals, etc. Their formation mechanisms fascinate physicists, materials scientists, and chemists because they result in materials more robust than their components, with exquisitely intricate nano-structures, fill space more than synthetic nanoparticles, and directly control phase transitions. Because of the fundamental nature of research on the physical aspects of biominerals, their formation mechanisms, the potential for future bio-inspired materials synthesis, and the aesthetic beauty of biomineral structures, students of all ages are interested in biomineralization. While describing the involvement of undergraduates in this research, my talk will address two key questions: Q: How do biominerals achieve the beautiful morphologies we observe? A: By forming through amorphous precursor phases, with morphology and phase transitions directly under biological control [1, 2]. Q: How do organisms order their biominerals to be single-crystalline? A: By controlling crystal growth at the nanoscale, not atom by atom [3, 4].

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1:03PM B5.00004 Processing and Characterization of New Materials at Pomona College with External Collaborations , DAVID TANENBAUM, Pomona College — My research program focuses on the evolution of novel lithographic, growth, and characterization processes for use with thin films for microelectronics and photovoltaic technologies. We have established facilities at Pomona College for wet chemistry, spin coating, thermal evaporation, micro-contact printing, ultra violet ozone cleaning, oxygen plasma cleaning, Au/Pd sputter coating, critical point drying, optical microscopy, optical lithography, ellipsometry, spectral reflectance, electrical conductivity, current-voltage characterization, atomic force microscopy, scanning tunneling microscopy, electron microscopy, electron beam lithography, and energy dispersive x-ray spectroscopy. Active collaborations with researchers at Cornell University and at Risø National Laboratory for Sustainable Energy (in Denmark) keep the research program vibrant and relevant. Since 2001, I have been an active member of the Cornell Center for Nanoscale Systems. Recent research and publications have focused on carbon nanotubes, graphene sheets, and organic photovoltaics. Pomona College students have played significant roles in all these projects, as well as in the development of our facilities. Connections to a wide range of researchers are invaluable not only for scientific discussions, but provide many opportunities for summer REU internships for my research students. This provides valuable training, access to facilities, and seeds future collaborations. Collaborations at Cornell span 15 years including two sabbatical years and regular summer visits to work at sites such as the Cornell Nanofabrication Facility, the Cornell Center for Materials Research, and the Cornell Center for Nanoscale Systems.

1:39PM B5.00005 Mentoring undergraduates for experimental research in physic , JEREMY LEVY, Univ of Pittsburgh — This abstract not available.

Monday, March 21, 2011 11:15AM - 2:15PM –
Session B6 DAMOP: Few-body Aspects of Cold Atomic Gases Ballroom C2

11:15AM B6.00001 Interacting and Rotating Gases of a Few Trapped Atoms , NATHAN GEMELKE, Penn State University — I will discuss attempts to generate motionally entangled states in small clusters of repulsively interacting Bosonic atoms at nonzero angular momentum in two-dimensional harmonic traps.[1] By constructing an "array of rotating buckets" from an optical lattice of spinning and precisely controlled on-site potentials, small clusters of interacting atoms can be adiabatically transferred from uncorrelated states at zero angular momentum through a tabulated sequence of ground state level crossings with increasing atomic correlation and total angular momentum. Results will be shown probing these states with both time-of- flight techniques and by directly interrogating atomic correlation via photo-association to excited molecules. Comparison will be made to numeric models with no free parameters. I will discuss extension of these results to future experiments using Feshbach-resonant interactions, and the use of dynamically modulated lattice potentials to generate effective gauge fields.

[1] Gemelke, N., Sarajlic, E., Chu, S., arXiv:1007.2677

11:51AM B6.00002 Deterministic preparation and control of a tunable few-fermion system[1] , GERHARD ZUERN, Heidelberg University — Systems consisting of only few interacting fermions play a fundamental role in nature with atoms and atomic nuclei being the most prominent examples. In our experiments with ultracold atoms we have recently been able to prepare and control few-atom quantum states consisting of 1-10 fermions. We prepare such a system using ultracold ^{6}Lithium atoms in an optical dipole trap in which the interparticle interaction can be tuned over a wide range using a Feshbach resonance. By spilling all atoms occupying higher energy quantum states we can deterministically prepare samples from 1-10 particles in the ground state with fidelities exceeding 90%. In my talk I will present our first experiments controlling the interaction between particles in the ground state of the trap.

[1]Work done in collaboration with Selim Jochim, University of Heidelberg.

12:27PM B6.00003 Four-body Efimov effect , YVAN CASTIN, LKB - ENS — The few-body problem with resonant two-body s-wave interaction (that is with an infinite scattering length) can now be studied experimentally with ultracold atomic gases. In particular, the three-body Efimov phenomenon (Efimov, 1971), consisting in the existence of an infinite number of trimer states with an asymptotically geometric spectrum in the vicinity of a zero energy accumulation point, has now obtained experimental evidence. On the contrary, the four-body Efimov effect has remained elusive, both theoretically and experimentally. Strictly speaking, for same spin state bosons, as pointed out by Amado and Greenwood (1973), it is *a priori* excluded by the existence of the three-body Efimov effect: A tetramer state with an energy arbitrarily close to zero has eventually an energy larger than an Efimov trimer state and may decay into this trimer plus a free atom. We have found a system where a four-body Efimov effect takes place: It is made of three same spin state fermions of mass M interacting only with a lighter particle of mass m. The mass ratio $\alpha = M/m$ is used as a control knob: This system experiences a three-body Efimov effect if and only if $\alpha > \alpha_c(2;1) \simeq 13.607$ (Efimov, 1973; Petrov, 2003). Using a combination of symmetry arguments and a numerical solution of an integral equation,we show that Efimov tetramers exist over the interval of mass ratio $\alpha_c(3;1) < \alpha < \alpha_c(2;1)$, with $\alpha_c(3;1) \simeq 13.384$. The four-body Efimov exponent $|s|$ is also calculated as a function of α over that interval, and the experimental feasibility is discussed.

1:03PM B6.00004 Interferometry with ultra-cold few-atom states , EITE TIESINGA, Joint Quantum Institute — I will explain some of our recent modeling of experiments that loaded an atomic Bose-Einstein condensate into a three-dimensional optical lattice. In an optical lattice, a periodic trap for atoms, the condensate can be divided into millions of independent atomic coherent states. These states are superpositions of different atom number and the analogue of coherent states of light or photons. As in the case of coherent laser light these atomic states can be made to interfere. In fact, the time-evolution of the states leads to collapse and revivals in interference patterns observed in the atomic momentum distribution. I show that long-period revivals are associated to effective three-body interactions that are due to virtual excitations to higher vibrational states within a site of an optical lattice. This work has been published as P. R. Johnson, E. Tiesinga, J. V. Porto, and C. J. Williams, New Journal of Physics **11**, 093022 (2009).

1:39PM B6.00005 Virial Expansion for a Strongly Correlated Fermi Gas , HUI HU, Centre for Atom Optics and Ultrafast Spectroscopy, Swinburne University of Technology — Few-body physics can give considerable insight into the challenging many-body problem. A concrete example is the exact Tan relations [1] linking the "hard" (few-body) physics at short distance, large-momentum and high frequency to the "soft" physics of the equation of state via a contact parameter. This has been demonstrated clearly using the operator product expansion (OPE) method [2] which separates in a natural way few-body from many-body physics. In this talk, we present another example: the quantum virial expansion that bridges few-body and many-body physics. At large temperatures, the properties of a strongly correlated Fermi gas, either static or dynamic, can be expanded in terms of virial coefficients or expansion functions, calculable from the few-fermion solutions [3]. For the equation of state in the resonant unitarity limit [3], we obtain for the first time an accurate third order virial coefficient. This has been experimentally verified in a measurement at ENS (Paris) [4]. For the single-particle spectral function [5], we demonstrate that an expansion up to second order is able to explain the main features of momentum-resolved RF spectroscopy in a resonantly interacting Fermi gas, as recently reported by JILA [6]. We also obtain a virial expansion of the dynamic structure function, as measured at Swinburne University (Melbourne), and check that the second order expansion functions give the correct OPE coefficients in the limit of large momentum and frequency. The important feature of this expansion is the existence of a small parameter, the fugacity, even for strong interactions. In the future, we anticipate that higher-order virial expansions of dynamic properties such as the single-particle spectral function may provide useful insights into clarifying the debate on the pseudo-gap issue in resonantly interacting Fermi gases.

[1] S. Tan, *Ann. Phys.* **323**, 2952 (2008); **323**, 2971 (2008).
[2] E. Braaten, and L. Platter, *Phys. Rev. Lett.* **100**, 205301 (2008).
[3] X.-J. Liu, H. Hu, and P. D. Drummond, *Phys. Rev. Lett.* **102**, 160401 (2009).
[4] S. Nascimbène et al. *Nature* **463**, 1067 (2010).
[5] H. Hu, X.-J. Liu, and P. D. Drummond, *Phys. Rev. Lett.* **104**, 240407 (2010).
[6] J. T. Stewart, J. P. Gaebler, and D. S. Jin, *Nature* **454**, 744 (2008).

Monday, March 21, 2011 11:15AM - 2:15PM –
Session B7 DPB: Superconductivity in Accelerators Ballroom C3

11:15AM B7.00001 Superconducting Accelerator Structures: An Historical Overview[1] , PERRY WILSON, SLAC, Stanford — In 1961 I began doing active research on RF superconducting cavities at the High Energy Physics Laboratory (HEPL) at Stanford University. At that time there were already nascent research programs exploring superconducting cavities at four other laboratories around the world, including the one at the Stanford physics department. However, all attempts to produce a substantial accelerating field in a superconducting cavity had failed. Since a cavity that is capable of acceleration always has a surface electric field, I decided that my first research effort would be to build and test a cavity with only a magnetic field at the surface. The frequency would need to be 2856 MHz, that of the electron linac at HEPL, so that available instrumentation could be used. In order to have only a magnetic field at the surface, the cavity would have to operate in the so-called TE mode. But there was a problem: at 2856 MHz such a cavity would be considerably larger than the single-cell accelerating mode cavities previously built at the Stanford physics department. In collaboration with the low temperature physics group in the Stanford physics department, a larger electroplating facility was built that was capable of handling the cylindrical cavity body and two end plates. The initial measurements gave stunning results: a Q factor of about 10^8 at 4°K for a lead-plated cavity was obtained, and there was no degradation in Q up to a surface magnetic field of about 10 mT, (limited by the oscillator power). The results were published in 1963. Experimentation on superconducting accelerator cavities increased rapidly in the decade or so following this initial success. Successful niobium TM-mode (accelerating mode) cavities were built with Q's of about 10^{11}. Within a few years the multipactor problem in accelerating cavities was solved by changing the shape of the outer boundary. The initial impetus for superconducting accelerator research at Stanford was to design and build a long pulse superconducting linac with an energy of about one GeV. Such a linac has still not been realized, but in the years from 1970 to 1990 there have been successful applications of RF superconducting structures to storage rings, rf separators, drive linacs for FEL's, and heavy ion accelerators. The evolution superconducting structures and their applications, as outlined above, will be discussed in more detail in my talk

[1]Work supported by Department of Energy contract DE-AC03-76SF00515

11:51AM B7.00002 Superconductors for superconducting magnets , DAVID LARBALESTIER, National High Magnetic Field Laboratory — Even in 1913 Kamerlingh Onnes envisioned the use of superconductors to create powerful magnetic fields well beyond the capability provided by cooling normal metals with liquid helium. Only some "bad places" in his Hg and Pb wires seemed to impede his first attempts at this dream, one that he imagined would be resolved in a few weeks of effort. In fact, of course, resolution required another 50 years and development of both a true understanding of the difference between type I and type II superconductors and the discovery of compounds such as Nb_3Sn that could remain superconducting to fields as high as 30 T. And then indeed, starting in the 1960s, Onnes's dreams were comfortably surpassed. In the last 45 years virtually all superconducting magnets have been made from just two Nb-base materials, Nb-Ti and Nb_3Sn. Now it seems that a new generation of magnets based on cuprate high temperature superconductors with fields well above 30 T are possible using Bi-Sr-Ca-Cu-O and the RE-Ba-Cu-O compounds. We hope that a first demonstration of this possibility will be an all-superconducting 32 T magnet with RE-Ba-Cu-O insert that we are building for NHMFL users. The magnet application potential of this new generation of superconducting conductors will be discussed.

12:27PM B7.00003 State of the art superconducting magnet development , GIANLUCA SABBI, LBNL — This abstract not available.

1:03PM B7.00004 RF Superconductivity: the ultimate limit , HASAN PADAMSEE, Cornell University — This abstract not available.

1:39PM B7.00005 Cryogenic Systems: Recent Trends and New Directions , JOHN WEISEND, NSCL Michigan State University — The production of reliable cryogenic temperatures is vital for the use of superconductivity in accelerators. Cryogenics is found in the accelerating structures and magnets of the accelerator as well as in the magnets and calorimeters of the detectors in the experimental areas. In the century since the discovery of superconductivity, cryogenic systems have gone from small laboratory devices to very large industrial scale systems involving multiple refrigeration plants, containing over 100 tonnes of liquid helium. These systems, while specialized, represent a mature, well understood technology. This paper will survey the current status of cryogenic systems in accelerators and describe recent trends including: the large scale use of He II (superfluid helium) and the development of higher reliability and higher efficiency systems. It will also discuss future directions including the increased use of HiTc current leads, possible applications for small cryocoolers and the potential impact of the world helium supply on accelerator cryogenics.

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B8 FIP: Critical Materials for Global Science and Technology Ballroom C4

11:15AM B8.00001 Unobtainium? Critical Elements for New Energy Technologies , ROBERT JAFFE, MIT — I will report on a recently completed study jointly sponsored by the APS Panel on Public Affairs (POPA) and the Material Research Society (MRS). The twin pressures of increasing demand for energy and increasing concern about anthropogenic climate change have stimulated research into new sources of energy and novel ways to harvest, transmit, store, transform or conserve it. At the same time, advances in physics, chemistry, and material science have enabled researchers to identify chemical elements with properties that can be finely tuned to their specific needs and to employ them in new energy-related technologies. Elements like dysprosium, gallium, germanium, indium, lanthanum, neodymium, rhenium, or tellurium, which were once laboratory curiosities, now figure centrally when novel energy systems are discussed. Many of these elements are not at present mined, refined, or traded in large quantities. However new technologies can only impact our energy needs if they can be scaled from laboratory, to demonstration, to massive implementation. As a result, some previously unfamiliar elements will be needed in great quantities. We refer to these elements as energy-critical elements (ECEs). Although the technologies in which they are employed and their abundance in the Earth's crust vary greatly, ECEs have many features in common. The purpose of the POPA/MRS study was to evaluate constraints on availability of energy-critical elements and to make recommendations that can help avoid these obstructions.

11:51AM B8.00002 Using Earth Abundant Minerals for New Research Pathways in Solar PV and Battery Storage , CYRUS WADIA, Co-Director, Cleantech to Market - Directorate - Lawrence Berkeley National Laboratory — Dr. Wadia will provide an in-depth look at his research to discover and develop a new material system toward a more expansive solar photovoltaic future, covering topics of: materials selection based on abundance, new synthetic pathways for scaleable materials, and results of working solar cell devices he has fabricated with these principles in mind. He will also discuss the results of his latest paper exploring the resource constraints on electrochemical storage for both transportation and grid scale applications.

12:27PM B8.00003 Essentials for Successful and Widespread LED Lighting Adoption , NISA KHAN, LED Lighting Technologies — Solid-state lighting (SSL), with light-emitting diodes (LEDs) as the light source, is a growing and essential field, particularly in regard to the heightened need for global energy efficiency. In recent years, SSL has experienced remarkable advances in efficiency, light output magnitude and quality. Thus such diverse applications as signage, message centers, displays, and special lighting are now adopting LEDs, taking 2010's market to $9.1 billion - 68% growth from the previous year! While this is promising, future growth in both display and lighting applications will rely upon unveiling deeper understanding and key innovations in LED lighting science and technologies. In this presentation, some LED lighting fundamentals, engineering challenges and novel solutions will be discussed to address reduction in efficiency (a.k.a. droop) at high currents, and to obtain uniform light distribution for overcoming LEDs' directional nature. The droop phenomenon has been a subject of much controversy in the industry and despite several studies and claims, a widely-accepted explanation still lacks because of counter arguments and experiments. Recently several research studies have identified that the droop behavior in nitride-based LEDs beyond certain current density ranges can only be comprehensively explained if the current leaking beyond the LED active region is included. Although such studies have identified a few useful current leakage mechanisms outside the active region, no one has included current leakage, due to non-ideal, 3-D device structures that create undesirable current distribution inside and outside the active region. This talk will address achieving desirable current distributions from optimized 3-D device structures that should reduce current leakage and hence the droop behavior. In addition to novel LED design solutions for droop reduction and uniform light distribution, the talk will address cost and yield concerns as they pertain to core material scarcity. Such solutions are expected to make LED lights more energy efficient, pleasant in appearance, longer-lasting, affordable, and thus suitable for green living.

1:03PM B8.00004 Niobium and its Impact on Superconducting Radiofrequency Technology , ANDREW HUTTON, Thomas Jefferson National Accelerator Facility — The Continuous Electron Beam Accelerator Facility at Jefferson Lab in Newport News, Virginia, was the first large-scale deployment of superconducting radiofrequency (RF) technology, and was optimized for nuclear/high energy physics research. The success of this technology led to the creation of a Free Electron Laser (FEL) facility at Jefferson Lab that has achieved world-record power, and is leading the way towards the next generation of FELs based on superconducting energy-recovery linacs. Superconducting RF technology has been adopted for other large accelerators (LEP, SNS) and is proposed for many of the future large accelerator facilities (ESS, FRIB, ILC, Project X, etc.). All these applications rely on the superconducting properties of niobium. While the performance of niobium accelerating cavities has been excellent, there are still improvements being developed, in particular, the new ingot niobium technology. This talk will provide a review of superconducting RF technology and the impact it has had, and will continue to have, on the accelerator field.

1:39PM B8.00005 Isotopes for Research - Can We Continue to Depend on Them? , ROBERT ATCHER, Los Alamos National Laboratory — The use of isotopes as tracers has been critical to many scientific endeavors. The discovery of radioactivity was quickly followed by experiments in which radioisotopes were being used to trace the behavior of those elements in biologic systems including humans. More recently, the ability to separate and enrich stable isotopes has facilitated their use as probes in a variety of applications using magnetic resonance, mass spectrometry and post facto neutron activation to determine their distribution, concentration and chemical form. Recently, shortages of both stable enriched and radioisotopes have had an impact on endeavors on which they play an important role.

Monday, March 21, 2011 11:15AM - 1:51PM –
Session B9 DFD: Nanofluidics D220

11:15AM B9.00001 Message in a bottle: the statistical behavior of nanoparticles in optical confinement[1] , H. DANIEL OU-YANG, JOSEPH JUNIO, LIANGCHENG ZHOU, Lehigh University — In an aqueous medium, container surfaces can significantly alter the behavior of suspended nanoparticles. We propose a method to investigate nanoparticle behavior in a boundary-free environment by transiently trapping them with a focused laser beam. While optical confined, as in an optical bottle, these particles are affected by both particle-light and particle-particle interactions. Time-averaged fluorescence imaging produces results in 3D mapping of the nanoparticle concentration in the bottle. We report how we analyze the messages in the bottle, i.e. the statistical behavior of these particles, by using the 3D distributions obtained under both controlled optical and interparticle forces.

[1]This project is supported in part by NSF DMR 0923299, Pennsylvania Department of Commerce and Economic Development through the Center for Optical Technologies at Lehigh University and the Pennsylvania Department of Health CURE Formula Funds.

11:27AM B9.00002 Low-frequency dielectric response of a single particle in aqueous suspensions , JINGYU WANG, Physics, Lehigh University, Bethlehem, PA, USA 18015, H. DANIEL OU-YANG, Physics and Bioengineering, Lehigh University, Bethlehem, PA, USA 18015 — $\alpha-$relaxation, the counterion diffusion in the electric double layer, has been used to described the anomalous low frequency dielectric dispersion of aqueous suspensions of colloidal particles. A microscopic theory describing this relaxation process proposed by Schwarz, however, has not been investigated systematically. We propose to use a single particle dielectrophoresis (DEP) force spectroscopy to study the relaxation mechanism as a function of particles size, temperature and solvent viscosity. Specifically, we measure the dependence of the DEP crossover frequency force and compare results with predictions by Schwarz.

11:39AM B9.00003 Investigation of MEMS force sensors for nano-scale water measurements[1] , SOYOUNG KWON, WONHO JHE, COREY STAMBAUGH, Seoul National University — Nanoscale water formed by capillary condensation has typically been studied by means of an atomic force microscope (AFM). While this approach can provide details about the dynamic visco-elastic properties, it is limited in the type of information that can be measured. Here we propose replacing the fixed sample surface generally used in AFM systems with movable micro-mechanical force sensors (MEMS) fabricated specifically for tapping mode or shear mode. By incorporating a MEMS device we can directly measure the adhesion force, pull-in distance and capillary force of nano confined water while the AFM collects information pertaining to the dynamic visco-elastic properties. In this talk, we will characterize the force measurement in the system and discuss the behavior of the device in the presence of nano-scale water.

[1]Work supported NRF of Korea and NSF grant OISE #0853104.

11:51AM B9.00004 Investigation of the Static and Dynamic Mechanical Properties of Nano-scale Water[1] , COREY STAMBAUGH, SOYOUNG KWON, WONHO JHE, Seoul National University — The behavior of liquids on the nano-scale has become an area of interest as new fabrication techniques have allowed for increasingly smaller structures to be made. While much work has been done on the interactions forces at liquid and solid interfaces, questions still remain regarding the behavior of nano-scale liquids. By incorporating a micro-electromechanical force sensor (MEMS) into the quartz tuning fork based atomic force microscope (QTF-AFM) probe setup we are able to both manipulate and measure nano-scale water, which in turn provides information beyond the standard AFM approach. Here we look at both the static and dynamic mechanical properties of water formed between the tip of a (QTF-AFM) probe and the polysilicon surface of a MEMS device.

[1]Work supported by NSF grant OISE #0853104.

12:03PM B9.00005 Thermophoretic stretching of DNA in polymer nanochannels , JONAS PEDERSEN, LASSE THAMDRUP, HENRIK FLYVBJERG, ANDERS KRISTENSEN, Technical University of Denmark — We demonstrate that thermophoretic forces generated by light-induced local heating can enhance the extension of genomic-length DNA confined in a polymer nanochannel. By temperature control on the micron-scale, bacteriophage T4 DNA is locally stretched to 80% of its contour length, although the cross-section of the nanochannel is as large as 250x250nm^2. A coarse-grained model of the forces at play captures the DNA-molecule's response to thermophoretic forces with accuracy and precision, and allows for fitting the density profile of the stretched DNA with only a single fit-parameter. The forces involved are relatively strong, because they add up along the molecule. They are measured by using the molecule as an entropic spring balance. Pending a calculation of these forces, this experiment might discriminate between the competing theories for thermophoretic forces.

12:15PM B9.00006 Poisson or not Poisson: Probability distribution of colloidal nanoparticles in an optical trap , YI HU, XUANHONG CHENG, H. DANIEL OU-YANG — In a colloidal suspension of nanoparticles, the presence of an optical trap can exponentially enhance the probability of finding the particles in the vicinity of the trap. Intriguing questions arise regarding whether the probably distribution of particle number in the trap follows Poisson approximation, and if so, what is the upper limit of the trapping energy at which Poisson is followed. To answer these questions, we conduct experiments to determine directly the variance and the mean particle number in the trap at different trapping energies and compare with the predictions of the probability theory.

12:27PM B9.00007 Charging Dynamics of Sub-nanometer Pores , YING LIU, Clemson University, GUANG FENG, JINGSONG HUANG, BOBBY SUMPTER, Oak Ridge National Laboratory, VINCENT MEUNIER, Rensselaer Polytechnic Institute, RUI QIAO, Clemson University — Electrodes featuring sub-nanometer pores can potentially improve the energy density of supercapacitors significantly. However, ions entering such narrow pores often need to pay an energy penalty because part of their salvation shell must be removed. This can potentially limit the charging kinetics of such nanopores. In this work, we investigate the charging dynamics of sub-nanometer pores connected with an electrolyte bath. We quantify the energy barrier for ions to enter 0.82-nm wide slit pores and determine the time constant for charging of the pores using Molecular Dynamics simulations. Strong concentration polarization is found during the charging process and the charging kinetics is much slower than that predicted using the classical equivalent circuit model. The results are rationalized using a modified Poisson-Nernst-Planck model.

12:39PM B9.00008 Statics and Dynamics of Stretched Single DNA Molecules Tug-of-War at Micro-Nanofluidic Interfaces , JIAWEI YEH, Institude of Physics, National Taiwan University, ALESSANDRO TALONI, Tel Aviv University, YENG-LONG CHEN, CHIA-FU CHOU[1], Institute of Physics, Academia Sinica — Understanding single molecule dynamics at micro-nanoscale interfaces has implications to polymer transport in biological processes, device design for single molecule analysis and biotechnological applications. We report our study on single DNA molecules straddling across a nanoslit, bridging two micro-nanofluidic interfaces, for both its tug-of-war behavior and confinement-induced entropic recoiling at varying length and height (h: 30∼100 nm) of a nanoslit. From a modified worm-like chain model in the tug-of-war scenario and the scaling analysis in the entropic recoiling process, we demonstrate the entropic recoiling force is essentially constant, given the degree of confinement, irrespective of the DNA length inside the nanoslit and the slit length. The scaling exponents for the entropic force will also be discussed.

[1]corresponding author

12:51PM B9.00009 Long time dynamics of single linear and circular ds-DNA confined in sub-100nm nanoslits , PO-KENG LIN, JEN-FANG CHANG, I. STACHIV, CHIA-FU CHOU, Y.- L. CHEN, Institute of Physics, Academia Sinica, Taipei Taiwan — We investigate the role of topological constraints on DNA dynamics in very strong confinement to study the dynamics of nuclear chromosome and DNA viral packaging. Experiments and simulations were carried out to investigate the equilibrium shape and dynamics of the single linear and circular λ-DNA confined in a silicon/glass nanoslit. We measured the chain extension r, shape asphericity A, extensional ($\tau_{||}$) and rotational relaxation time τ_r, and examined the dependence on chain topology as functions of the slit height h(20 $\sim$ 780 nm) and the solvent ionic strength I (0.8 $\sim$250 mM). We observed that the shape asphericity increases as h and$I$ decrease as the chain shape becomes anisotropic. Moreover, in sub-Kuhn length confinement, the DNA relaxation time increases with decreasing h in a smooth and broad transition.

1:03PM B9.00010 Heat-Driven Release of a Drug Molecule From Carbon Nanotubes , VITALY CHABAN, OLEG PREZHDO, University of Rochester — Hydrophobicity and ability to absorb light that penetrates through living tissues make carbon nanotubes (CNTs) promising intracellular drug delivery agents. Following insertion of a drug molecule into a CNT, the latter is delivered into a tissue, is heated by near infrared radiation, and releases the drug. In order to assess the feasibility of this scheme, we investigate the rates of energy transfer between CNT, water and the drug molecule, and study the temperature and concentration dependence of the diffusion coefficient of the drug molecule inside CNTs. We use ciprofloxacin (CIP) as a sample drug: direct penetration of CIP through cell membranes is problematic due to its high polarity. The simulations show that a heated CNT rapidly deposits its energy to CIP and water. All estimated timescales for the vibrational energy exchange between CNT, CIP and water are less than 10 ps at 298 K. As the system temperature grows from 278 K to 363 K, the diffusion coefficient of the confined CIP increases 5-7 times, depending on CIP concentration. The diffusion coefficient slightly drops with increasing CIP concentration. This effect is more pronounced at higher temperatures. The simulations support the idea that optical heating of CNTs can assist in releasing encapsulated drugs.

1:15PM B9.00011 Characterization of Nanostructured Silicon Membranes for Control of Molecular Transport , BERNADETA SRIJANTO, SCOTT RETTERER, JASON FOWLKES , MITCHEL DOKTYCZ, Oak Ridge National Laboratory — Fabrication of nanoporous membranes for selective transport of molecular species requires precise engineering at the nanoscale. The membrane permeability can be tuned by controlling the physical structure and the surface chemistry of the pores. We use a combination of electron-beam and optical lithography, along with cryogenic deep reactive ion etching, to fabricate silicon membranes that are physically robust and have uniform pore sizes. Pore sizes are further reduced using plasma enhanced chemical vapor deposition and atomic layer deposition of silicon dioxide onto the membrane surfaces. Integrating nanoporous membranes within a microfluidic network provides a platform for tailoring molecular exchange between microchannels, independent of hydrodynamic effects. In enzymatic reactions, for example, tuning the pores size will allow smaller enzymatic substrates to traverse the membrane at controlled rates while larger enzymes remain spatially separated. Our results from membrane cross-sectioning using focused ion beam milling show that pore sizes can be controlled at dimensions below 10nm. Functional characterization was performed by quantitative fluorescence microscopy to observe the selective transport of molecular species of different sizes.

1:27PM B9.00012 Thermal resistance of thin water films during phase-change , NITIN SHUKLA, NENAD MILJKOVIC, RYAN ENRIGHT, EVELYN N. WANG, Device Research Laboratory, Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139 — The thermal resistance of a thin water film during phase-change processes is of interest for fundamental studies and of importance for various engineering systems. In particular, as the thickness of the water film approaches the nanoscale, the thermal resistance across the liquid-vapor interface can contribute significantly to the overall heat transport. In this work, we experimentally investigate the thermal resistance of thin water films during phase change on metallic substrates using transient thermoreflectance (TTR) spectroscopy. This technique offers a novel method to examine heat transport in evaporating liquid films less than a 100 nm in thickness. The understanding gained from this work will aid in the design of high performance phase-change based micro/nanoscale devices.

1:39PM B9.00013 Effect of hydrogen bond cooperativity on the behavior of water , KEVIN STOKELY, Boston University — Four scenarios have been proposed for the low–temperature phase behavior of liquid water, each predicting different thermodynamics. The physical mechanism which leads to each is debated. Moreover, it is still unclear which of the scenarios best describes water, as there is no definitive experimental test. Here we address both open issues within the framework of a microscopic cell model by performing a study combining mean field calculations and Monte Carlo simulations. We show that a common physical mechanism underlies each of the four scenarios, and that two key physical quantities determine which of the four scenarios describes water: (i) the strength of the directional component of the hydrogen bond and (ii) the strength of the cooperative component of the hydrogen bond. The four scenarios may be mapped in the space of these two quantities. We argue that our conclusions are model-independent. Using estimates from experimental data for H bond properties the model predicts that the low-temperature phase diagram of water exhibits a liquid–liquid critical point at positive pressure.

Monday, March 21, 2011 11:15AM - 2:15PM –
Session B10 SPS: SPS Undergraduate Research I D221

11:15AM B10.00001 Which String Breaks? Revisited[1] , CHRISTOPHER FRYE, University of Central Florida — Many have seen the common introductory physics demonstration in which a heavy ball hangs from a string, with another identical string hanging freely from the ball. When the instructor pulls the bottom string slowly, the top string breaks. However, when the instructor pulls the bottom string very rapidly, the bottom string breaks. This simple experiment is used to demonstrate inertia and Newton's laws. In The Physics Teacher of November 1996, there is an article in which the authors create a model of this problem in an attempt to explain the outcomes quantitatively. However, their analysis gave strange results. Using an improved model, I will show that the results of this demonstration can be obtained using only simple calculations.

[1]This work was funded by a RAMP grant from the University of Central Florida.

11:27AM B10.00002 Synchronization effects in chaotic oscillators with spatially dependent frequency mismatch[1] , PHILIP JAVERNICK, TRINANJAN DATTA, Augusta State University — We investigate the phenomena of synchronization for two coupled chaotic oscillators with a frequency mismatch which is explicitly spatially dependent. We compute the frequency synchronization plot in the parameter space of coupling strength and frequency mismatch of the chaotic system. We find regimes where the system is frequency locked corresponding to a synchronous state and regimes of non-synchronous state. In the non-synchronous state the frequencies are either zero individually (quenched oscillations) or the difference between them is non-zero. We also find that the region with oscillation quenching is reduced compared to the case when the frequency mismatch is a constant.

[1]Automated Data Processing (ADP) research funds

11:39AM B10.00003 Rolling vs. Sliding: The inclusion of non-conservative work in the classic comparison , BENJAMIN LEE, JUSTIN MUELLER, California Baptist University, TERRY BUEHLER, U.C. Berkeley, ALEX CHEDIAK, California Baptist University — If a rolling and sliding object, each of the same material, were to race down the same incline plane, which would win? Last year, we presented a theoretical model with confirming experimental data which showed that the winning object depends on the angle, the effective coefficient of friction, C, and kinetic coefficients of friction: If C $<$ μ_{k_block}, the rolling object is faster, but if C $>$ μ_{k_block}, the sliding object is faster. Though the materials were the same, we previously reported that the $\mu_{s_sphere}$was apparently not equal to μ_{s_block}. This year, we are directly determining the coefficients of friction using a force sensor, seeking to resolve this apparent discrepancy. We plan to report more accurate values of $\mu_{s_sphere}$and μ_{s_block} and, if they are found to be different, explain why. Steps will be taken to improve track uniformity. We will more precisely determine the transition angle, where the block becomes faster than the sphere, by taking data at smaller angular increments. In addition, we will incorporate results for rolling *with* slipping, as it is expected that as slipping increases, so will linear velocity, as less energy is lost to rotational kinetic energy. Beyond this, we hope to extend the model to different geometries (with different moments of inertia).

11:51AM B10.00004 Is Ball Milling An Innovative Technique For the Production of Zn From ZnO?[1] , JEFF MCLEOD, ALI BAKHSHAI, Goucher College — The process of mechanical alloying using ball milling transfers mechanical energy to reactants in powder form, causing the particle size of the reactant powders to be reduced until defects in the lattice structure of the reactants are created. For reactions of sufficient exothermicity, this facilitates a complete mechanochemical reaction through self-heat propagating synthesis (SHS). The oxide reduction reaction of ZnO with Al, which yields pure Zn as a product, cannot be induced using ball milling alone because of its low exothermicity. This study used a systematic combination of ball milling and annealing in order to induce the reaction. Parameters tested were milling time, annealing time, and annealing temperature with the purpose of establishing the importance of each of these variables in inducing a complete reaction in the sample. The completeness of the reaction was determined using XRD analysis and inspection with an optical microscope. Results confirmed that neither ball milling nor heat treatment could induce the reaction individually; only ball milling followed by annealing could cause the reaction to take place. This study suggests that using ball milling in conjunction with heat treatment can produce Zn from ZnO in a less costly, more efficient, and less wasteful manner than traditional methods.

[1]This work is supported by Goucher College summer research award.

12:03PM B10.00005 Women in Physics: an Analysis of the Gender Gap , LILLIE GHOBRIAL, MICHAEL EVANS, GREGORY MASLAK, MARK STEWART, ANNA BONTORNO, BRITTANY BARRETT, NICOLE SCOTT, CAROLINA ILIE, Dept. of Physics, SUNY Oswego — It is not a surprise that the number of women in physics is not impressive, and the reasons are diverse and well-known [1]. We conducted several surveys at SUNY Oswego regarding the gender gap. We examined the source of the problem and we developed possible solutions. We propose herein various strategies for short-term and long-term improvement of female representation in Physics. This insight will hopefully benefit other physics departments in which women are underrepresented.

[1] Rachel Ivie and Katie Stowe. June 2000. Women in Physics, 2000, AIP Publication Number R-430.

12:15PM B10.00006 STAIRSTEP – a research-oriented program for undergraduate students at Lamar University , CRISTIAN BAHRIM, Department of Physics, Lamar University — The relative low number of undergraduate STEM students in many science disciplines, and in particular in physics, represents a major concern for our faculty and the administration at Lamar University. Therefore, a collaborative effort between several science programs, including computer science, chemistry, geology, mathematics and physics was set up with the goal of increasing the number of science majors and to minimize the retention rate. Lamar's Student Advancing through Involvement in Research Student Talent Expansion Program (STAIRSTEP) is a NSF-DUE sponsored program designed to motivate STEM students to graduate with a science degree from one of these five disciplines by involving them in state-of-the-art research projects and various outreach activities organized on-campus or in road shows at the secondary and high schools [1]. The physics program offers hands-on experience in optics, such as computer-based experiments for studying the diffraction and interference of light incident on nettings or electronic wave packets incident on crystals, with applications in optical imaging, electron microscopy, and crystallography. The impact of the various activities done in STAIRSTEP on our Physics Program will be discussed. [1] Doerschuk P, Bahrim C, Daniel J, Kruger J, Mann J, and Martin Ch, *39th ASEE/IEEE Frontiers in Education Conference,* San Antonio 2009, M3F-1-2.

12:27PM B10.00007 Modeling Surface Acoustic Waves on Liquid Loaded Surfaces , MICHAEL MITCHELL, MATTHEW KWAN, MADELEINE MSALL, Bowdoin College — Ultrasound excitation of crystals creates acoustic waves that propagate on the surface. The wave velocities vary with directions based on the properties of the crystal. Experiments typically use ultrasound transducers submerged in water. The water loading on the surface creates a perpendicular stress. This alters the boundary conditions of the surface waves, changing their propagation. We model the phase and group velocities of Rayleigh surface waves on water loaded Si (100) and $CaWO_4$. The addition of water loaded boundary conditions improves the match between model and experimental data.

12:39PM B10.00008 Characterization of a MEMS Actuator through Simulation[1] , ERIK GARCELL, MIGUEL GONZALEZ, BYOUNG HEE MOON, PRADEEP BHUPATHI, PAN ZHENG, GEORGE LING, YOONSEOK LEE, Department of Physics, University of Florida, Gainesville, FL 32611, HO BUN CHAN, Department of Physics, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong — Simulations of a laterally shifting micro-electro-mechanical-system (MEMS) were performed to characterize the device for use in liquid ^{3}He experimentation. Using the multiphysics software COMSOL, we were able to identify the relevant electrostatic and mechanical properties of our device, as well as its various vibrational modes. When actuated with a DC voltage, simulations demonstrated comparatively large out-of-plane displacements, which are in agreement with optical measurements taken from the actual device. New simulations were performed to test the effectiveness of possible efforts to dampen this displacement. Using the data collected from these simulations, future generations of the MEMS will be designed and improved for use in liquid ^{3}He experiments.

[1]This work is supported by NSF DMR-0851707 (REU Program) and DMR-0803516 (YL).

12:51PM B10.00009 Scanning Tunneling Microscopy of Manganites[1] , ICON MAZZACCARI, HYOUNGJEEN JEEN, AMLAN BISWAS, Department of Physics, University of Florida, Gainesville, FL 32611 — We have built a scanning tunneling microscope (STM) which employs a mechanical coarse approach mechanism. We have tested the mechanical and electronic components of the system and calibrated the piezoelectric scanning mechanism by imaging highly ordered pyrolytic graphite (HOPG) at room temperature. Atomic resolution HOPG images were obtained when the STM was placed inside a vibration isolated liquid helium dewar. We have also scanned single crystals and thin-films of hole-doped manganese oxides (manganites) and obtained images on the scale of about 100 nm to about 10 nm. After obtaining satisfactory images at room temperature, we will cool the apparatus first down to liquid nitrogen temperature (77 K) and then down to liquid helium temperature (4.2 K) to investigate micrometer and nanometer scale phase separation in manganites.

[1]NSF DMR-0804452

1:03PM B10.00010 Magnetic field dependence on neutrino-induced electron-positron creation rates[1] , HANNAH MCWILLIAMS, Hendrix College — The study of neutrino processes in magnetic fields are immensely important for astrophysical phenomena where neutrino interactions are the dominant mode of energy loss and large fields exist. In this talk I will present a phenomenological relationship for the production rate of one such process, the creation of electron-positron pairs $\nu \rightarrow \nu\ e\ \bar{e}$, as a function of the magnetic field. I will show that above the critical magnetic field strength and at large neutrino energies there exists a power law dependence on the magnetic field.

[1]This work is supported by the Hendrix Odyssey Program and the Arkansas Space Grant Consortium

1:15PM B10.00011 Emergent magnetic monopoles and their dynamics in artificial spin ice[1] , YICHEN SHEN, OLGA PETROVA, PAULA MELLADO, OLEG TCHERNYSHYOV — Electrically charged particles such as electrons are common in our world. In contrast, no elementary particles with a net *magnetic* charge have ever been observed. After a recent discovery that magnetic monopoles can emerge in a system of magnetic dipoles [1], much attention has been paid to the behavior of magnetic monopoles in artificial spin ice, arrays of nano-scale magnetic islands or wires that mimic the behavior of geometrically frustrated materials [2]. We have developed a theoretical model of magnetization dynamics in artificial spin ice under the action of an external magnetic field [3]. Magnetization reversal is mediated by the creation, propagation and absorption of domain walls carrying two units of magnetic. Domain walls are emitted from lattice junctions when the local field becomes large enough to overcome the Coulomb attraction between the magnetic charges of the domain wall and the junction. This interaction is also responsible for a positive feedback that triggers magnetic avalanches observed experimentally in artificial spin ice.

[1] C. Castelnovo, R. Moessner, and S. L. Sondhi, Nature **451**, 42 (2008).
[2] O. Tchernyshyov, Nat. Phys. **6**, 323 (2010).
[3] P. Mellado, O. Petrova, Y. Shen, and O. Tchernyshyov, Phys. Rev. Lett. **105**, 187206 (2010).

[1]This work was supported in part by the NSF Grant DMR-0520491.

1:27PM B10.00012 Antihydrogen Production in a Paul Trap[1] , GUY GEYER, REINHOLD BLUMEL, Wesleyan University — We investigate the dynamics of anti-hydrogen production within a Paul trap through computational means with the intent to develop a strategy for confining the anti-atom for further experimentation. We obtained first preliminary results on the transient production of anti-hydrogen. We present these results, discuss the experimental implementation of our system, and suggest ways to lengthen the lifetime of anti-hydrogen in the trap.

[1]This research was funded in part by the APS.

1:39PM B10.00013 Effects of interactions on interference pattern formed after release and expansion of two identical Bose-Einstein condensates[1] , CATHERINE LEE, COURTNEY LANNERT, Wellesley College — We numerically simulate the expansion and interference of two adjacent, identical Bose-Einstein condensates initially trapped by harmonic potentials. We use explicit finite-difference methods to solve the Gross-Pitaevskii equation and time-evolve the condensates. We repeat the simulation, varying the interaction strength of the condensates, and analyze how the interactions affect the time-evolution of the interference pattern.

[1]This work was supported by the NSF under grant DMR-0605871.

1:51PM B10.00014 Search for an Entanglement Measure for N-Qubit States via Phase Symmetry[1] , JOSHUA GELLER, University of Rochester — While quantitative measures of entanglement exist for two-qubit systems, there are no equivalent measures for larger systems. Phase patterns within multi-qubit density matrices could yield clues to constructing quantitative measures for these larger systems. One such pattern within the N-qubit density matrix is observed by reordering the matrix according to the types of coherence terms in the first row and first column so the number of phases in each element increases from left to right in the first row, and from top to bottom in the first column. The resultant matrix contains blocks on its diagonal with elements having only bipartite entanglement. All remaining diagonal elements are part of GHZ-type states in this configuration. A benefit to this matrix structuring is the ability to apply concurrence, a measure of two-qubit entanglement, to the sub-matrix blocks formed on the diagonal. Exploring the meaning of these concurrences with regard to the entanglement of the whole system of N-qubits represented by the full density matrix is a possible next step toward finding a measure of N-qubit entanglement.

[1]This project was supported in part by NSF Grant PHY-0851243.

2:03PM B10.00015 Plasmon Enhancement of Organic Solar Cells using Embossed Gratings , DAVID SHOPE, Department of Chemistry and Physics, Trinity University, JENNIFER STEELE, Department of Physics and Astronomy, Trinity University — Organic photovoltaic cells (OPV) are attractive because of their low cost and easy fabrication. However, because the diffusion length of excitons in most organic photovoltaic material is about 100 nm, the overall thickness and therefore the optical absorbance of the device is limited, reducing the overall efficiency. Surface plasmon excitations have been studied as a possible mechanism to increase the absorption of light in solar cell active layers because of their ability to manipulate and enhance local electromagnetic fields. This work focuses on using metal gratings as one electrode. Gratings support a broad range of surface plasmons that can be tuned by changing the incident angle of light, making them ideal to isolate the contribution of surface plasmons to increases in the quantum efficiency of solar cells. OPV cells are made using a conjugated polymer and fullerene-based active layer with either an aluminum or silver bottom electrode patterned with a grating through microcontact printing. By measuring the efficiency of the solar cells as a function of both incident angle and wavelength, we can match increases in efficiency with specific surface plasmon modes.

Monday, March 21, 2011 11:15AM - 2:15PM –
Session B11 FIAP: Compound and Oxide Semiconductors D222

11:15AM B11.00001 Terahertz radiation mechanism of native n-Type InN with different carrier concentrations , KUANG-I LIN, JUNG-TSE TSAI, JENN-SHYONG HWANG, Department of Physics, National Cheng Kung University, HON-WAY LIN, SHANGJR GWO, Department of Physics, National Tsing Hua University, MENG-CHU CHEN, Institute of Nuclear Energy Research — InN has received considerable attention due to its lower effective mass, higher mobility, and higher velocity saturation compared with GaN or AlN. The fundamental band gap of InN has recently been reevaluated to be around 0.6–0.7 eV, being therefore a promising candidate for terahertz (THz) applications. In this study, the polarity and mechanism of THz radiation from native n-type InN excited by femtosecond optical pulses are investigated. The optical properties, electron concentrations, and crystalline quality are characterized by photoluminescence and Raman scattering spectra. The electron concentrations are estimated to be between 0.35×10^{19} and 3.87×10^{19} cm^{-3}. The intensity ratio of the A_1(LO) to E_2(high) mode increases with increasing electron concentration. The polarity of THz radiation field from the samples with higher electron concentrations is opposite to that from p-InAs, indicating that the dominant radiation mechanism is the drift current. However, the samples with lower electron concentrations show the same polarity as p-InAs. Under this condition, the radiation mechanism is dominated by the photo-Dember effect.

11:27AM B11.00002 Self-confined GaN hetero-phased quantum wells , YU-CHI HSU, IKAI LO, CHIA-HO HSIEH, WEN-YUAN PANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan, MITCH M.C. CHOU, Department of Materials and Optoelectronic Science, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan, YEN-LIANG CHEN, CHENG-HUNG SHIH, YING-CHIEH WANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan — Wurtzite/zinc-blende/wurtzite GaN hetero-phased quantum wells (QWs) were grown by plasma-assisted molecular beam epitaxy. A self-assembling mechanism was used to simulate the hetero-phased QW, in which a wurtzite/zinc-blende phase transition was created by rotating the threefold symmetric N-Ga vertical bond of wurtzite 60°. From the cathodoluminescence measurement, we observed an additional peak (energy ∼3.2eV) associated with GaN zinc-blende phase. From the transmission electron microscopy images and selective area electron diffraction patterns, we confirmed the formation of hetero-phased quantum wells with a transition of wurtzite/zinc-blende GaN [1].

[1] I. Lo, Y.-C. Hsu, C.-H. Hsieh, W.-Y. Pang, M. M.C. Chou, Y.-L. Chen, C.-H. Shih, and Y.-C. Wang, Appl. Phys. Lett. **96**, 222105 (2010).

11:39AM B11.00003 Growths of InGaN Quantum Wells on GaN Micropyramids , RENBO SONG, LE ZHAO, GUANGYU LIU, JING ZHANG, NELSON TANSU, Lehigh University — Selective area epitaxy (SAE) of InGaN quantum wells on GaN micropyramids were grown by using metalorganic chemical vapor deposition (MOCVD). The pattern prepared for the SAE was fabricated by the deposition of 300 nm SiO_2 film on n-type GaN substrate by using plasma enhanced chemical vapor deposition (PECVD) and followed by photolithography. The grown micropyramid structures were characterized by scanning electron microscope (SEM) and photoluminescence (PL). Uniformly-distributed defect-free GaN micropyramids were observed by SEM. The growths of InGaN quantum wells were performed on the GaN micropyramids, and broadband luminescence were observed from the PL measurements applicable for white light-emitting diodes applications.

11:51AM B11.00004 Charge Carriers in Boron Nitride Nanotubes Appear to confirm Quantum Capillary Action , RICHARD KRISKE, University of Minnesota — A recent article in Physics Today confirmed a previous Theory put forward by this author in that electrons and perhaps other fundamental particles should find the easiest transmission path to be in the center of nanotubes not on the walls. Of course this is somewhat astonishing in that the center of the tube has nothing in it. This author had previously suggested that this might ultimately give a quantum mechanical explaination for capillary action. In any case a model could now be confirmed that this author previously put forward to show that in many cases the flow of particles should occur in the centers of nanotubes not on the walls and this would allow the exploration of the use of nanotubes as reaction devices, and transport devices with a general theory to show how molecules as well as elementary particles could be transported down the centers of these tubes and reacted in the tubes or in chambers attached to the tubes. This would also explain some vexing biological problems involving tubes and capillary action.

12:03PM B11.00005 Transport Electron Scattering by Structural Defects in InSb Quantum Wells , T.D. MISHIMA, M.B. SANTOS, University of Oklahoma — Among all the binary III-V semiconductors, InSb has the highest electron mobility and the narrowest band-gap. Field effect transistors and magnetic-field sensors are examples of devices based on InSb quantum wells (QWs) that exploit these material properties. In this study, we have investigated electron scattering due to two dominant structural defects, micro-twins (MTs) and threading dislocations (TDs), in InSb QWs grown on GaAs (001) substrates via AlInSb buffer layers. A linear regression analysis shows that the room-temperature electron mobility in InSb QWs has a strong correlation with the densities of both MTs and TDs, with an R^2 value of 0.9791. The MT-originated energy barrier and reflection coefficient for electron conduction in InSb QWs are estimated to be 0.09 eV and 0.33, respectively. The TD-limited electron mobility in InSb QWs is explained by electric charge with a density of 1.3 $\times10^{-10}$ C/m along a TD line. In addition to further discussion of the data, we will show the derivations of some key equations used for the mathematical analyses. This work was supported by the NSF under Grants Nos. DMR-0520550 and DMR- 0808086.

12:15PM B11.00006 Strain, Confinement and Density Dependence of the Effective Mass of Holes in InSb Quantum Wells , CHOMANI GASPE, M. EDIRISOORIYA, T.D. MISHIMA, R.E. DOEZEMA, M.B. SANTOS, University of Oklahoma, L.C. TUNG, Y.J. WANG, NHMFL, Florida State University — The valence band structure in a III-V quantum well (QW) is complicated by the presence of two highly non-parabolic bands. The lower (higher) energy band has a hole mass that is lighter (heavier) for motion in the plane of the QW. The energy separation between the two bands increases with increasing biaxial compressive strain and decreasing well width. An expected anticrossing between the two bands can add significantly to their non-parabolicity. We report an experimental study of the effective mass of 2D holes in a series of remotely doped InSb QWs under biaxial compressive strain. Only the lower energy band is occupied at low tempearture. Cyclotron resonance measurements at 4.2K show that the hole effective mass increases with increasing hole density from 0.045m$_e$ at 2.1×10^{11} cm^{-2} to 0.083m$_e$ at 5.1×0^{11} cm^{-2}. The smallest effective mass of 0.017m$_e$ was observed in the QW with the largest compressive strain (1.06%) and narrowest well width (7nm). This work was supported by the NSF Grants Nos. DMR-0520550 and DMR-088086.

12:27PM B11.00007 Carrier and Spin Dynamics in Narrow Gap Parabolic Quantum Well Structures[1] , M. BHOWMICK, T. MERRITT, G.A. KHODAPARAST, Virginia Tech, T.D. MISHIMA, M.B. SANTOS, University of Oklahoma, D. SAHA, G.D. SANDERS, C.J. STANTON, University of Florida — Heterostructures with parabolic confinement potentials are important systems to study for many reasons. In a perfect Parabolic Quantum Well (PQW), the subbands are equally spaced and electron-electron interactions are virtually non-existent, allowing coupling of long-wavelength radiation only to the center-of-mass coordinate of the electron system. Narrow band PQW systems are well suited for THz devices because by careful design, one can tune the transition frequency, temperature stability, and narrow-band emission. In our studies, the parabolic confinement was created by an effective parabolic Al compositional gradient inside each well. We studied carrier/spin dynamics in an InSb/$Al_xIn_{1-x}Sb$ multiple-PQW structure using several time resolved differential transmission schemes in the mid-infrared. Our results demonstrate the unique and complex dynamics in InSb heterostructures that can be important for electronic and optoelectronic devices.

[1]Supported by: NSF-DMR-0507866, DMR-0520550, DMR-0706313, and NSF-Career Award DMR-0846834.

12:39PM B11.00008 Electrical characterization of GeSn grown on Si using ultra high vacuum chemical vapor deposition method , MO AHOUJJA, S. ELHAMRI, University of Dayton, J. KOUVETAKIS, J. TOLLE, Department of Chemistry and Biochemistry, Arizona State University, Arizona, MEE YI RYU, Y.K. YEO, Department of Engineering Physics, Air Force Institute of Technology, Wright-Patterson AFB, Ohio — Recently, there has been considerable interest in growing $Ge_{1-x}Sn_x$ alloys on Si with x< 0.2 for the purpose of developing optoelectronic devices that can be integrated with Si-based electronic technology. Here we report Hall coefficient and resistivity measurements as a function of temperature from thin epitaxial layers of GeSn grown on Si substrates using ultra high vacuum chemical vapor deposition. The Hall measurements show that GeSn samples with Sn concentrations of 1.5 and 2 % are of high quality. The hole concentration for the boron doped $Ge_{0.98}Sn_{0.02}$ sample at room temperature is 7.1x10^{18} cm^{-3} while that of the as-grown undoped sample is 9.8x10^{16} cm^{-3}. The measured hole mobility for $Ge_{0.98}Sn_{0.02}$ alloys with carrier concentrations greater than 10^{18} cm^{-3} are found to be comparable to those found in Ge samples with similar doping concentrations.

12:51PM B11.00009 An extensive study to observe the effects of thermal annealing and ion fluences in the ion beam synthesis of β-SiC , P.R. POUDEL, B. ROUT, D.R. DIERCKS, F.D. MCDANIEL, University of North Texas, J.A. PARAMO, Y.M. STRZHEMECHNY, Texas Christian University — A systematic study of the formation of β-SiC structures by low energy carbon ion (C^-) implantation into Si followed by high temperature thermal annealing will be presented. The effects of thermal annealing in the formation of β-SiC structures has been studied. It is observed that the thermal annealing of 1100 $^\circ$C for 1 hr is required to observe the formation of β-SiC. The quantitative analysis in the formation of β-SiC nanostructures has been performed by the implantation of various carbon ion fluences in the range of 1×10^{17} - 8×10^{17} atoms /cm^2 at an ion energy of 65 keV into Si. It is observed that the average size of β-SiC crystals decreases whereas the amount of β-SiC increases monotonically with ion fluence up to a fluence of 5 $\times$ 10^{17} atoms/cm^2 and appears to saturate for a higher fluence of 8 $\times$ 10^{17} atoms/cm^2 when the samples were annealed at 1100 $^\circ$C for 1 hr. The stability of graphitic C-C bonds at 1100 $^\circ$C limits the growth of SiC precipitates in the sample implanted at a fluence of 8×10^{17} atoms /cm^2 which results in the saturation behavior of SiC formation in the present study as predicted by various characterization techniques such as FTIR, Raman, XRD, XPS and Transmission electron microscopy.

1:03PM B11.00010 Complimentary Ferromagnetic Mechanisms in Mn doped ZnO Thin films deposited using Pulsed Laser Ablation[1] , DEVAJYOTI MUKHERJEE, TARA DHAKAL, HARIHARAN SRIKANTH, PRITISH MUKHERJEE, SARATH WITANACHCHI, University of South Florida — We show evidence through experiments and analysis that the ferromagnetism (FM) in 2% Mn doped ZnO (ZMO) thin films is a combination of two complementary mechanisms - the bound magnetic polaron (BMP) percolation at low temperatures and the Ruderman-Kittel-Kasuya-Yosida (RKKY) exchange interaction at higher temperatures. Pulsed laser deposition was used to grow ZMO thin films on c-cut sapphire substrates. Films were deposited at various temperatures and background oxygen pressures to study the effect of growth parameters on the FM. While no impurity-phase contributions were detected, a strong correlation between effective carrier densities and FM was established. FM in amorphous films with high defect densities were described by the BMP model whereas that in highly conducting films was consistent with the RKKY mechanism. Detailed characterization of the structural, electrical and magnetic properties of the as-deposited ZMO films will be presented.

[1]This work was supported by NSF (Grant Nos. DMI-0217939 and DMI-0078917) and DOD (Grant No. W81XWH-07-1-0708).

1:15PM B11.00011 Excitation of atomic zinc during excimer laser ablation of zinc oxide at 193 nm , ENAMUL KHAN, STEPHEN LANGFORD, THOMAS DICKINSON, Washington State University — Atomic excitations during UV laser ablation usually involve collisions with energetic electrons. When zinc oxide is ablated with a 193 nm excimer laser, we observe light emission at pulse energies —well below the threshold for normal electron heating processes. At pulse energies near the threshold for visible light emission, the source is localized and moves away from the surface at a nearly constant velocity. Time-resolved quadrupole mass spectrometry confirms the presence of zinc atoms with velocities consistent with this motion. We propose that these excited zinc atoms are generated by two-photon excitation into the autoionizing $3d^{10}4p$ ($^2P^\circ_{3/2}$) 5s $^2[3/2]^\circ$ state of atomic zinc at 103 001 cm^{-1}. The broad "window resonance" associated with this state in single-photon absorption is associated with a *drop* in absorption, because the main decay channel (ionization) is hindered by destructive interference effects. We propose that radiative decay, which is otherwise a minor decay channel, produces bound excited states that subsequently decay to yield the observed light.

1:27PM B11.00012 Role of ligands on the photoluminescence of colloidal CdSe quantum dots and enhancement of photoconductivity of ZnO nanowires by quantum dots , SYAMANTA KUMAR GOSWAMI, TAE SOO KIM, BYOUNG WOO LEE, EUNSOON OH[1], CH. KIRAN KUMAR, EUI TAE KIM, Chungnam National University, DEPARTMENT OF PHYSICS TEAM, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING TEAM — Colloidal core-shell CdSe/ZnS quantum dots (QDs) encapsulated by trioctylphosphine oxide ligand were synthesized via pyrolysis. Then the TOPO ligands by 3-mercaptopropionic acid ligands were replaced under Ar environment. ZnO nanowires were fabricated by sonochemical method on pre-patterned alumina electrodes. With increasing temperature above 220 K, the PL lifetime was found to be increased in case of the TOPO capped QDs, whereas for the MPA capped QDs, the lifetime was short and almost independent of temperature. The conductivity of ZnO nanorods was increased after the deposition of the QDs, which was further enhanced by the exposure of light. This increase in the conductivity with and without light can be explained by the photo-carrier transport and surface modification effect, respectively. The photo-generated electrons in the CdSe QDs will tend to move toward the ZnO nanowires, resulting in the enhancement of photo-conductivity in the ZnO nanowires.

[1]corresponding author

1:39PM B11.00013 Preparation and characterization of nanostructured ZIO thin films , VIPIN KUMAR JAIN, Thin film & Membrane Science Laboratory, University of Rajasthan, Jaipur -302004, India, PRAVEEN KUMAR, Surface Physics and Nanostructures Group, National Physical Laboratory, New Delhi -110012, India, Y.K. VIJAY, Thin film & Membrane Science Laboratory, University of Rajasthan, Jaipur -302004, India, VIPIN KUMAR JAIN TEAM, PRAVEEN KUMAR COLLABORATION — ZnO–In2O3 system has attracted much attention because of chemical and thermal stability in addition to properties comparable to those of ITO. In the present work Zinc indium oxide (ZIO) thin films were deposited on glass substrate with varying concentration (ZnO: In2O3 - 100:0, 90:10, 70:30 and 50:50 wt %) at room temperature by flash evaporation technique. These deposited ZIO films were annealed in vacuum to study the thermal stability and to see the effects on the structural, chemical and electrical properties. Each film has been characterized ex-situ by XRD, XPS, XRF, AFM, SEM, optical band gap and Hall measurements. Results show the properties of the ZIO films strongly depend on the In2O3 concentration and also influenced by the post annealing of these films. XPS core level spectra of Zn(2p), O(1s) and In(3d) have been deconvoluted into their Gaussian components, while valence band spectra shows the change in electronic structures of the films.

1:51PM B11.00014 M-plane ZnO grown on m-plane sapphire by radio-frequency magnetron sputtering , BI-HSUAN LIN, WEI-REIN LIU, SHAO-TING HSU, CHIN-CHIA KUO, SONG YANG, CHIA-HUNG HSU, WEN-FENG HSIEH, DEPARTMENT OF PHOTONICS AND INSTITUTE OF ELECTRO-OPTICAL ENGINEERING, NATIONAL CHIAO TUNG UNIVERSITY TEAM, DIVISION OF SCIENTIFIC RESEARCH, NATIONAL SYNCHROTRON RADIATION RESEARCH CENTER TEAM, DEPT OF PHOTONICS & INST. OF ELECTRO-OPTICAL SCIENCE AND ENGINEERING, NATL. CHENG KUNG UNIVERSITY TEAM — High quality m-plane orientated ZnO films with in-plane epitaxial relationship of $(0002)_{ZnO}||(11\text{-}20)_{sapphire}$ and $(11\text{-}20)_{ZnO}||(0006)_{sapphire}$ have been successfully grown on m-plane sapphire by using radio-frequency magnetron sputtering. The introduction of a nanometer thick low temperature grown ZnO buffer layer effectively eliminated other undesirable orientations. The significant anisotropy of the strain field breaks the hexagonal symmetry and leads to the different physical properties from that of c-plane oriented ZnO films. The structural properties, including crystalline quality, strain state, and defect structures, of the m-plane ZnO layers are thoroughly examined by synchrotron x-ray scattering, transmission electron microscopy and atomic force microscopy. The optical properties are investigated by temperature, polarization as well as power dependent photoluminescence, and polarization dependent Raman spectroscopy. The correlation between the structural and optical properties will be discussed.

2:03PM B11.00015 Phase diagram, structure, and electronic properties of $(Ga_{1-x}Zn_x)(N_{1-x}O_x)$ solid solution[1] , LI LI, PHILIP B. ALLEN, Stony Brook University — We studied $(Ga_{1-x}Zn_x)(N_{1-x}O_x)$ solid solution by Density Functional Theory (DFT). To conduct thermodynamic simulations, we built a database of structures and constructed a Cluster Expansion(CE). The subsequent Monte Carlo simulation gives a calculated phase diagram with a wide miscibility gap and an ordered x=0.5 compound. The disordered phase displays strong short range ordering (SRO) at experimental temperatures. We then used snapshots from MC to investigate structural and electronic properties by DFT on large supercells. Consistent with previous theoretical and experimental findings, lattice parameters appear to deviate from Vegard's law with small upward bowing. Bond lengths depend strongly on local environment, with a variation much larger than the difference of bond length between ZnO and GaN. The downward band gap bowing deviates from parabolic by having more rapid onset of bowing at low and high concentrations. Our results show that SRO influences both the structural and electronic properties.

[1]This work is supported by DOE Grant DE-FG02-08ER46550

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B12 DMP: Focus Session: Dopants and Defects in Semiconductors: Compound Semiconductors I D223/224

11:15AM B12.00001 ABSTRACT WITHDRAWN –

11:27AM B12.00002 Optimized basis sets for coarse-grained electronic structure calculations of point defects , BJÖRN LANGE, CHRISTOPH FREYSOLDT, JÖRG NEUGEBAUER, MPIE Düsseldorf — Density-functional theory is a powerful tool to study the properties of point defects in the supercell approach. Yet, the size limitations make a description of the extended tails of defect states, especially for shallow defects, cumbersome. Atomic orbital basis sets are the method of choice to coarse-grain electronic structure calculations, but are in general not flexible enough for describing the unusual bonding situations, which occur in point defects. We employ a newly developed method that, based on a variational principle, allows to generate small atomic basis sets which optimally mimic the Kohn-Sham wavefunctions with a plane-wave basis set. We show that these basis sets accurately reproduce the underlying plane-wave calculation. We analyze how the atomic orbitals close to the defect are modified in comparison to their bulk counterparts. We are able to extend basis sets generated from small supercells and to reproduce the bandstructure of larger cells. Using this approach we construct and solve a reliable sparse model Hamiltonian for a shallow defect test system containing $10^3..10^4$ atoms.

11:39AM B12.00003 Strain-Enhanced Doping in Semiconductors: Effects of Dopant Size and Charge State[1] , JUNYI ZHU, 1 National Renewable Energy Lab 2 University of Utah, FENG LIU, GERALD STRINGFELLOW, University of Utah, SU-HUAI WEI, National Renewable Energy Lab — When a semiconductor host is doped by a foreign element, it is inevitable that a volume change will occur in the doped system. This volume change depends on both the size and charge state difference between the dopant and the host element. Unlike the "common expectation" that if the host is deformed to the same size as the dopant, then the formation energy of the dopant would reach a minimum, our first-principles calculations discovered that when an external hydrostatic strain is applied, the change of the impurity formation energy is monotonic: it decreases if the external hydrostatic strain is applied in the same direction as the volume change. This effect also exists when a biaxial strain is applied. A simple strain model is proposed to explain this unusual behavior, and we suggest that strain could be used to significantly improve the doping solubility in semiconductor systems.

[1]The work at NREL was supported by the DOE/OS/BES under Grant No. DE-AC36-08GO28308. The work at University of Utah was supported by DOE/OS/BES under Grant No. DE-FG0204ER46148.

11:51AM B12.00004 Defects and Carrier Compensation in CdTe[1] , MAO-HUA DU, Materials Science and Technology Division and Center for Radiation Detection Materials and Systems, Oak Ridge National Laboratory — CdTe is a very useful semiconductor material for its radiation detection and thin-film solar cell applications. Good carrier mobility and lifetime are needed for CdTe since efficient carrier collection is essential for the success of both applications. On the other hand, high resistivity is required for radiation detection for suppressing dark current and device noise. This is in contrast to CdTe-based solar cells, in which low resistivity is desired. In this talk, I will discuss the properties of native defects and impurities in CdTe with emphasis on carrier compensation and its implications in radiation detection and solar cell applications.

[1]This work was supported by the U.S. DOE Office of Nonproliferation Research and Development NA22 and DOE ORNL LDRD program.

12:27PM B12.00005 n-type doping in Cu_2O by halogen impurities: a first-principles study[1] , QIONG BAI, MENG TAO, QIMING ZHANG, University of Texas at Arlington — The present work focuses on first-principles calculations on n- type doping by F, Cl, and Br impurities in Cu_2O under solution-grown environments. From the formation energy point of view, the substitution of oxygen in Cu_2O is favored over the interstitial sites. The electronic structures after doping are carefully studied.

[1]supported by the U.S. DOE, Office of BES, under No. DE-SC0002062.

12:39PM B12.00006 Diffusion of ion implanted indium in ZnO crystals , FAISAL YAQOOB, MENGBING HUANG, University at Albany-SUNY, DAVID LOOK, Wright State University and Air Force Research Laboratory — We report on diffusion behaviors for ion implanted indium atoms in ZnO crystals. A c-plane ZnO crystal was implanted with In ions for four different energies (40, 100, 200, and 350 keV, respectively) and doses (8.0×10^{13}, 1.2×10^{14}, 1.6×10^{14} and 6.5×10^{14} /cm^2, respectively), resulting in a uniform concentration profile of In from surface to the depth $\sim$ 150 nm. The samples were annealed for 30 minutes at temperatures between 700-1000 $^\circ$C with an argon or oxygen gas flow. The distributions of In atoms, either aligned or nonaligned along the crystalline directions, were measured by Rutherford backscattering combined with ion channeling. The diffusivities for nonaligned (interstitial) and aligned In atoms varied with annealing temperature via the Arrhenius relationship. The diffusion activation energies (E_a) for aligned In atoms were lower than those for interstitial In atoms, e.g., for annealing in an Ar gas, $E_a \sim 0.61$ eV for <1010> aligned In atoms and $E_a \sim 1.1$ eV for interstitial In atoms between <1010> atomic rows. Furthermore, the diffusion activation energies were affected by the gas species used during annealing, e.g., for annealing in an O_2 gas, $E_a \sim 0.39$ eV for <1010> In atoms and $E_a \sim 0.79$ eV for interstitial In atoms between <1010> atomic rows. These experimental results will be compared with first-principle calculations for In diffusion in ZnO crystals.

12:51PM B12.00007 Surface effects in Co-doped ZnO nanocrystals[1] , ALINE L. SCHOENHALZ, GUSTAVO M. DALPIAN, Universidade Federal do ABC — Semiconducting nanostructures have received high attention by scientific community due to their unusual properties and wide rage of possible applications. In this scale, the understanding of the surface effects of the material is fundamental to explain its properties. By using the Density Functional Theory within the Local Density Approximation, we report on the effects of the surface on the magnetic properties of Co-doped ZnO nanocrystals. For bulk ZnO, it is well known that the most stable magnetic interaction between Co impurities is antiferromagnetic. This is also the case for saturated nanostructures, where surface effects are not taken into account. However, when surface effects are considered, the interaction between transition metal impurities becomes ferromagnetic. We will discuss the interaction between surface and impurity states, comparing our results to experimental findings.

[1]Brazilian agencies CAPES, FAPESP and CNPq support this work.

1:03PM B12.00008 Vacancy-assisted migration of group-III impurities in ZnO[1] , DANIEL STEIAUF, JOHN L. LYONS, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106 — Zinc oxide is a wide-band-gap material used as transparent conductor. As grown it often shows n-type conductivity, probably due to impurity contamination. High electron concentrations can be achieved by intentional doping with group-III elements, a process that usually involves annealing. It is thus important to understand the diffusion properties of the dopants. We perform first-principles calculations for the vacancy-assisted migration process of Al, Ga and In in ZnO, using both standard density functionals and hybrid functionals to correct the underestimated band gap. Indium induces the largest distortions in the lattice and has the highest formation energy. Its migration barrier to a neighboring Zn vacancy is the lowest. Al shows the highest barrier and thus has the best thermal stability. From the calculated migration barriers and formation energies, we determine diffusion activation energies and estimate annealing temperatures. The results are compared with recent experiments.

[1]This work was supported by Saint Gobain Research and by the NSF MRSEC Program.

1:15PM B12.00009 Improved LDA+U model for band gap corrected ZnO defect calculations , ADISAK BOONCHUN, WALTER LAMBRECHT, Case Western Reserve University — The local density approximation (LDA) is known to fail dramatically for point defects in ZnO. In the case of the oxygen vacancy, the one electron level of the 1+ charge state lies above the conduction band and leads to improper filling of the levels. Different points of view on how to implement a-posterior gap corrections still leave large uncertainty on the position of the defect levels. For the Zn-vacancy, LDA leads incorrectly to a delocalized wave function of the hole on all four neighbors. Our approach is to apply LDA+U corrections to various orbitals, O-sp and Zn-spd. The U-parameters which lead to orbital shifts $V_i = U_i(1/2 - n_i)$ are adjusted to quasiparticle self-consistent GW (QSGW) calculations of the band structure, including the shifts of the band structure relative to the LDA one on an absolute scale. With this improved LDA+U model, good agreement is obtained for the minimum gap, the conduction band mass and the valence and conduction band shifts separately. The structural properties of ZnO also remain intact. When applied to the oxygen vacancy, we find the 2+/0 transition level in good agreement with recent hybrid functional calculations. Applications of the same LDA+U model to the Zn-vacancy are in progress and show that localization of the wave function on two oxygen neighbors is obtained.

1:27PM B12.00010 Hybrid density functional study of gallium in ZnO , DENIS DEMCHENKO, Virginia Commonwealth University — The properties of interstitial and substitutional gallium impurities as well as their complexes in wurtzite ZnO are modeled using hybrid density functional theory. This approach reproduces experimental band gap and avoids any artificial gap corrections necessary when using LDA/GGA/LDA+U methods. We find that the lattice relaxations at the LDA/GGA level can also introduce large errors to the defect formation energies (up to 1.5 eV). The error is particularly large in cases where shallow occupied defect levels are formed and LDA can produce incorrect charges. The correct defect structure therefore should be obtained by relaxation using hybrid DFT method. We find both interstitial and substitutional Ga forming donor-like defect states, with substitutional Ga being energetically favorable. Acceptor-like Zn vacancy has high formation energy in the isolated state but exhibits strong preference to form defect complexes with both substitutional and interstitial gallium. (Ga_i-V_{Zn}) complex acts as a shallow donor, while ($Ga_{Zn} - V_{Zn}$) is a deep acceptor. The low formation energies of both complexes suggests an appreciable degree of self-compensation.

1:39PM B12.00011 Study of defects in TlBr, InI as potential semiconductor radiation detectors[1] , KOUSHIK BISWAS, MAO-HUA DU, Materials Science and Technology Division and Center for Radiation Detection Materials and Systems, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — Group III-halides such as TlBr and InI are receiving considerable attention for application in room temperature radiation detector devices. It is however, essential that these detector materials have favorable defect properties which enable good carrier transport when operating under an external bias voltage. We have studied the properties of native defects of InI and Tlbr and several important results emerge: (1) Schottky defects are the dominant low-energy defects in both materials that can potentially pin the Fermi level close to midgap, leading to high resistivity; (2) native defects in TlBr are benign in terms of electron trapping. However, anion-vacancy in InI induces a deep electron trap similar to the F-centers in alkali halides. This can reduce electron mobility-lifetime product in InI; (3) low diffusion barriers of vacancies and ionic conductivity could be responsible for the observed polarization phenomenon in both materials at room temperature.

[1]U.S. DOE Office of Nonproliferation Research and Development NA22.

1:51PM B12.00012 Information-based screens for deep traps in semiconducting materials[1] , KIM FERRIS, KUNAL SHAH, Pacific Northwest National Laboratory, DUMONT JONES, Proximate Technologies, LLC. — The key to a successful materials search is the ability to suggest promising materials and a priori eliminate unfruitful inquiry. For semiconducting radiation detection materials, performance is characterized by several key properties; band gap, density, electron mobility, and carrier lifetime. The material's proclivity to form defects is critical, as even simple antisite and vacancy defects can be sufficiently deep to affect effective carrier lifetime and mobility. We have developed a new model for defect formation proclivity, leveraging prior defect models (van Vechten and Feichter) and our information-based work. Our approach is based upon classification of materials chemistry and properties consistent with high concentrations of particular defects (e.g. antisites and vacancies). One issue is that nearly any charged local defect can potentially form a deep trap, so the screen must cover different defect types. Second, the screening model for new materials cannot rely on generally unknown factors such as 3D crystal geometry. The resulting model is intended to provide design guidance on expected defect behavior for candidate detection materials for which there is little or no prior information.

[1]The authors gratefully acknowledge financial support from U.S. Department of Homeland Security under Contract No. HSHQDC-08-X-00872.

2:03PM B12.00013 Ab-Initio analysis of TlBr: limiting the ionic current without degrading the electronic one , CEDRIC ROCHA LEAO, VINCENZO LORDI, Lawrence Livermore National Lab — Although TlBr in principle presents all the theoretical requirements for making high resolution room temperature radiation detectors, practical applications of TlBr have proven to be nonviable due to the polarization that is observed in the crystal after relatively short periods of operation. This polarization, that is believed to be caused by accumulation of oppositely charged ionic species at the ends of the crystal, results in an electric field that opposes that of the applied bias, counter-acting its effect. In this work, we use state of the art quantum modeling to benchmark the theoretical limits for the performance of TlBr as a radiation detector, showing that the best experimental reports demonstrate near-ideal electronic characteristics. We then propose a model to inhibit the detrimental ionic current in the material without impacting the excellent properties of the electronic current. Prepared by LLNL under Contract DE-AC52-07NA27344.

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B13 DFD: Focus Session: Polymer Colloids: Structure, Function, and Dynamics II

D225/226

11:15AM B13.00001 Predicting long-time Brownian dynamics of ultrasoft colloid suspensions from thermodynamics , MARK POND, The University of Texas at Austin, JEFFREY ERRINGTON, State University of New York at Buffalo, THOMAS TRUSKETT, The University of Texas at Austin — Suspensions of ultrasoft colloids, such as Gaussian-core particles and Hertzian spheres, have received significant research interest due to their reentrant melting behavior and dynamic anomalies. Many of the previous dynamic studies of these systems have focused on molecular dynamics simulations, which by their nature ignores the solvent medium. We have conducted Brownian dynamics simulations of these ultrasoft colloid suspensions to show their long-time dynamic behavior near the reentrant melting transition. In addition, we have developed a novel method for quantitatively and qualitatively predicting the long-time Brownian dynamics of ultrasoft colloidal suspensions from their thermodynamic properties.

11:27AM B13.00002 Development of surfaces repelling negatively buoyant solid particles , CARINA SEMMLER, ALEXANDER ALEXEEV, Georgia Institute of Technology — Using a hybrid computational method that integrates the lattice Boltzmann model for fluid dynamics and the lattice spring model for solids, we examine the motion of negatively buoyant solid microparticles in shear flow near a solid wall decorated with regularly distributed rigid posts. The posts are arranged in a square pattern and tilted relative to the flow direction. We show that when rigid posts are tilted against flow, secondary flows emerge that prevent the deposition of suspended particles on the solid surface. We probe the effect of post geometry on the development of secondary flows and identify the optimal post architecture in terms of the mass of levitated solid particles. Our results are useful for designing anti-fouling surfaces that repel colloidal particles carried by fluid.

11:39AM B13.00003 Microscopic structure of confined colloidal suspensions under shear , XIN-LIANG XU, STUART RICE, AARON DINNER, James Franck Institute, University of Chicago, XIANG CHENG, ITAI COHEN, Department of Physics, Cornell University — We report a study of driven colloidal suspensions by Stokesian dynamics simulation. The suspension is confined by two parallel plates, and is being driven far away from equilibrium by shearing induced by translation of the parallel plates. The separation of the plates is varied so the suspensions form either a single layer or two layers. Both the structure of the non-equilibrium steady state and the dynamics of the relaxation of the non-equilibrium state back to the equilibrium are examined, at a wide range of shearing strengths (the non-dimensional ratio quantifying the driven motion relative to the Brownian motion of the colloidal particles, the Peclet number is tuned from 0.1 to 100) and packing fractions. We observe string-like structures at low packing fractions and shear-induced crystallization at high fractions. A mechanism is proposed for how hydrodynamic interactions give rise to these structures.

11:51AM B13.00004 Evaporation of Lennard-Jones Fluids , SHENGFENG CHENG, JEREMY LECHMAN, STEVEN PLIMPTON, GARY GREST, Sandia National Laboratories — Solvent evaporation is a process frequently used to disperse particles in a bulk material or at a substrate. The local order and packing of particles can be controlled by controlling the evaporation rate. The first step to fully understand this complicated process is to understand the evaporation process of pure liquid at the microscopic scale. We have carried out large scale molecular dynamics simulations to study the evaporation of Lennard-Jones (LJ) fluids composed of monomers, dimers, or trimers. For LJ monomers in contact with a vacuum, the evaporation rate is found to be very high with significant evaporative cooling and an accompanying density gradient in the liquid domain near the liquid/vapor interface. Increasing the chain length to just dimers significantly reduces the evaporation rate. The velocity distributions of evaporated monomers are measured and compared to a kinetic theory and their dependence on the evaporation conditions is discussed. For nanoparticle suspensions, the nanoparticles order at the surface, which causes the evaporation to significantly slow down.

12:03PM B13.00005 Rotational and Translational Diffusion of PMMA Colloidal Clusters , HYUN JOO PARK, MARK T. ELSESSER, New York University, KAZEM V. EDMOND, Emory University, DAVID J. PINE, New York University, NEW YORK UNIVERSITY COLLABORATION, EMORY UNIVERSITY COLLABORATION — Colloidal clusters, 3-7 μm in size, are a good model system for various 2D and 3D structures depending on the aggregation number, N. We measure the translational and rotational diffusion of individual dyed PMMA clusters of dimers and trimers using high speed confocal scanning microscopy and particle tracking. We report measurements of the rotational and translational diffusion coefficients (and their ratios) as a function of volume fraction.

12:15PM B13.00006 A diversity of binary colloidal crystals using DNA-directed interactions , JOHN CROCKER, MARIE UNG, W. BEN ROGERS, RAYNALDO SCARLETT, TALID SINNO, University of Pennsylvania — DNA is the premier tool for directing the controlled self-assembly of nanoscopic and microscopic objects. The interactions between microspheres due to the hybridization of DNA strands grafted to their surface have been measured and can be modeled in detail, using well-known polymer physics and DNA thermodynamics. Knowledge of the potential, in turn, enables the exploration of the complex phase diagram and self-assembly kinetics in simulation. In experiment, at high densities of long grafted DNA strands, and temperatures where the binding is reversible, these system readily form colloidal crystals having a diverse range of symmetries. For interactions that favor alloying between two same-sized colloidal species, our experimental observations compare favorably to a simulation framework that predicts the equilibrium phase behavior, crystal growth kinetics and solid-solid transitions. We will discuss the crystallography of the novel alloy structures formed and address how particle size and heterogeneity affect nucleation and growth rates.

12:27PM B13.00007 Correlating Structural and Spectral Fluctuations in a Lasing Colloidal Suspension , JASON W. MERRILL, Yale University, Department of Physics, HUI CAO, Yale University, Departments of Physics and Applied Physics, ERIC R. DUFRESNE, Yale University, Departments of Mechanical Engineering, Physics, Chemical Engineering, and Cell Biology — When multiply scattering media with optical gain are optically pumped above a critical threshold, they emit coherent radiation in many spectral lines. This phenomenon is known as random lasing. The wavelengths of these spectral lines depend sensitively on the spatial distribution of scatterers, but this relationship has only just begun to be explored. We study the time and frequency domain statistics of random laser spectra emitted from dense colloidal suspensions doped with laser dye with an eye toward using this information as a probe of the underlying colloid dynamics.

12:39PM B13.00008 Smart colloidosomes with tunable permeability and a dissolution trigger , ADRIANA SAN MIGUEL, JAN SCRIMGEOUR, JENNIFER CURTIS, SVEN BEHRENS, Georgia Tech — Self-assembly of colloidal particles in the liquid interface of double emulsion droplets can be used to fabricate "colloidosome" microcapsules, which have great potential as vehicles for the controlled delivery of drugs or other cargoes. Here we present a novel class of aqueous core colloidosomes that combine the benefit of low capsule permeability (good cargo retention) with the option of a stimulus-triggered fast release in a target environment. Complete or partial dissolution of the capsule walls in response to a mild pH change is achieved in each case through the use of responsive particles made from polymers with pH-switchable solubility. We demonstrate three methods of controlling the capsule permeability prior to release while maintaining the intended response to the release trigger.

12:51PM B13.00009 A theoretical study of colloidal forces near an amphiphilic polymer brush , JIANZHONG WU, University of California, Riverside — Polymer-based "non-stick" coatings are promising as the next generation of effective, environmentally-friendly marine antifouling systems that minimize nonspecific adsorption of extracellular polymeric substances (EPS). However, design and development of such systems are impeded by the poor knowledge of polymer-mediated interactions of biomacromolecules with the protected substrate. In this work, a polymer density functional theory (DFT) is used to predict the potential of mean force between spherical biomacromolecules and amphiphilic copolymer brushes within a coarse-grained model that captures essential nonspecific interactions such as the molecular excluded volume effects and the hydrophobic energies. The relevance of theoretical results for practical control of the EPS adsorption is discussed in terms of the efficiency of different brush configurations to prevent biofouling. It is shown that the most effective antifouling surface may be accomplished by using amphiphilic brushes with a long hydrophilic backbone and a hydrophobic end at moderate grafting density.

1:03PM B13.00010 Phase transition of colloidal particles on curved surfaces , GUANGNAN MENG, JAYSON PAULOSE, DAVID NELSON, Department of Physics, Harvard University, VINOTHAN MANOHARAN, Department of Physics and School of Engineering and Applied Sciences, Harvard University — Defects and disclinations have to appear in crystalline domains on a curved surface with non-zero Gaussian curvature. These geometrical frustrations can qualitatively change the physics of phase transition. We encapsulate micron sized polystyrene (PS) colloidal particles within emulsion droplets and use nanometer sized polyNIPAM hydrogel particles to introduce depletion attraction between PS particle and interface, as well as between PS particles. We use this experimental model system and confocal microscopy to study phase transitions on curved surfaces. We will present both experimental phenomena and theoretical analysis.

1:15PM B13.00011 Dielectric effects in self-assembly of binary colloid mixtures , ERIK LUIJTEN, KIPTON BARROS[1], Northwestern University — Colloidal self-assembly is often controlled by electrostatic interactions. The solvent and colloids typically have different dielectric constants, thereby inducing polarization charge at the colloid surfaces. A shortcoming of previous simulations of charged colloids with implicit solvent is the neglect of the effective many-body interactions resulting from such dielectric effects. We study colloidal self-assembly using a method that properly accounts for polarization charge. In simulations of weakly charged colloids with large size asymmetry, we find that dielectric effects modify the pair correlation function in a nontrivial way and at low temperatures alter the observed crystal phase.

[1]Currently at Los Alamos National Laboratory.

1:27PM B13.00012 Formation of three-dimensional colloidal nanoparticle supercrystals and probing the formation kinetics , IRVING HERMAN, Columbia Univeristy, CHENGUANG LU, AUSTIN AKEY, Columbia University — A multiple solvent system consisting of colloidal nanoparticles in several solvents of gradually decreasing vapor pressures was investigated in the self assembly of hundred-layer thick colloidal nanoparticle superlattices in lithographically defined capillaries. Such a solvent system allows a very slow and tunable drying rate of solvents, which, together with the microfluidic flow into the capillaries, leads to the controllable formation of large, single crystalline 3D nanoparticle supercrystals. The underlying mechanism of superlattice formation was investigated via the drying rates for nanoparticle assembly for solvent systems of specific compositions. This technique generates single-crystalline 3D supercrystals of $\sim$micrometer size at spatially controlled locations, and large chunks (up to 40 μm by 40 μm by 5 μm) of single crystalline supercrystals on a flat Si substrate. The ordered nature of the structures formed was probed by high-resolution SEM and small angle x-ray scattering. In-situ x-ray scattering reveals the formation kinetics of the transition of nanoparticle assemblies from amorphous to ordered. This technique is versatile and has been applied to various types and sizes of colloidal nanocrystals, including those composed of CdSe, Au, PbS and Fe_3O_4.

1:39PM B13.00013 Nanoparticle-induced self-assembly of functionalized tetrapods , DANIEL W. SINKOVITS, University of Illinois at Urbana-Champaign, ERIK LUIJTEN, Northwestern University — Recent advances in synthesis have made it possible to create monodisperse particles with well-defined shapes. In particular, tetrapods have been fabricated in a wide range of well-controlled dimensions and have been functionalized in several different ways. We present Monte Carlo simulations of the self-assembly of functionalized tetrapods. We consider how the addition of charged spherical nanoparticles provides another means to control the self-assembled structure. In addition, we report the results of simulations of planar tripods confined to two dimensions and demonstrate that highly regular structures can be achieved without functionalization, through nanoparticle-mediated depletion interactions.

1:51PM B13.00014 A "diffusing diffusivity" model of "anomalous yet Brownian" diffusion of colloidal particles , MYKYTA V. CHUBYNSKY, GARY W. SLATER, Department of Physics, University of Ottawa, Canada — "Anomalous yet Brownian" diffusion of colloidal beads, with a mean-square displacement (MSD) exactly linear in time (as in simple Fickian diffusion) but an exponential (rather than Gaussian) displacement distribution (DD) at short times for large displacements, has been reported recently by Granick's group [1] in several systems. We argue that a strictly linear MSD with a non-Gaussian DD is a universal feature of systems with "diffusivity memory" (a particle diffusing faster is likely to keep diffusing faster for some time), but without "direction memory" (a jump in a particular direction does not change the probability of subsequent jumps in that direction). We consider a series of toy models reproducing this behavior in which a particle undergoes regular diffusion, but its diffusivity itself performs a (perhaps biased) random walk. The DD is strictly exponential at short times when the diffusivity distribution itself is exponential, but an exponential remains a good fit for a variety of diffusivity distributions.

[1] Wang et al., PNAS 106 (2009) 15160.

2:03PM B13.00015 Reentrant and Isostructural Transitions in the Cluster-Crystal Forming GEM-4 , KAI ZHANG, PATRICK CHARBONNEAU, Duke University, BIANCA MLADEK, University of Cambridge — Systems governed by soft, bounded, purely repulsive interactions show two possible equilibrium behaviors under compression: reentrant melting, as in the Gaussian core model (GCM), or clustering, as in the penetrable sphere model (PSM). The generalized exponential model of power 4 (GEM-4), which is the intermedia of the GCM and PSM with a simple isotropic pair interaction $u(r) \sim e^{-r^4}$, is thought to belong to the second family and was indeed found to form clusters at sufficiently high densities at high temperatures. Here, we present the low-temperature behavior of GEM-4 through Monte Carlo simulations using a specially developed free energy integration scheme. We find the phase behavior to be hybrid between the GCM and the PSM limits, showing a surprisingly rich phase behavior in spite of the simplicity of the interaction form. For instance, S- shaped doubly reentrant phase sequences and evidence of a cascade of critical isostructural transitions between crystals of different average lattice site occupancy are observed. The possible annihilation of lattice sites and accompanying clustering moreover leads to an unusual softening upon compression, which suggest that these materials may have interesting mechanical properties. We discuss possible experimental realizations and challenges of this class of materials.

Monday, March 21, 2011 11:15AM - 2:03PM –

Session B14 GSNP: Applications of Statistical and Nonlinear Physics to Social Systems and GSNP Student Speaker Award Talks D227

11:15AM B14.00001 Characterization of stock market regimes by data compression[1] , EUGENIO E. VOGEL, GONZALO SARAVIA, Universidad de La Frontera, Temuco, Chile — It has been shown that data compression can characterize magnetic phases (Physica A 388 (2009) 4075). In the introduction of this presentation we briefly review this result. We then go onto introducing a new data compressor (wlzip) developed by us to optimize recognition of meaningful patterns in the compressing procedure, yielding sharp transition curves at the magnetic critical temperatures. The advantages of the new compressor, such as better definition and tuning capabilities are presented. The rest of the talk consists of applying wlzip to the Chilean stock market along several months during 2010. The accumulated daily data allow to recognizing days with different types of activity. Moreover, the data recorded every minute allow to analyzing the "present" status of the stock market by applying wlzip to the data of the last hour or couple of hours. Possible extensions of the application of this technique to other fields are discussed.

[1]Partial support from Fondecyt 1100156, ICM and CEDENNA is acknowledged.

11:27AM B14.00002 Relativistic statistical arbitrage , ALEXANDER WISSNER-GROSS, Massachusetts Institute of Technology, CAMERON FREER, University of Hawaii — Recent advances in high-frequency financial trading have made light propagation delays between geographically separated exchanges relevant. Here we show that there exist optimal locations from which to coordinate the statistical arbitrage of pairs of spacelike separated securities, and calculate a representative map of such locations on Earth. Furthermore, trading local securities along chains of such intermediate locations results in a novel econophysical effect, in which the relativistic propagation of tradable information is effectively slowed or stopped by arbitrage.

11:39AM B14.00003 The Impact of Competing Time Delays in Stochastic Coordination Problems[1] , G. KORNISS, D. HUNT, B.K. SZYMANSKI, RPI — Coordinating, distributing, and balancing resources in coupled systems is a complex task as these operations are very sensitive to time delays. Delays are present in most real communication and information systems, including info-social and neuro-biological networks, and can be attributed to both non-zero transmission times between different units of the system and to non-zero times it takes to process the information and execute the desired action at the individual units. Here, we investigate the importance and impact of these two types of delays in a simple coordination (synchronization) problem in a noisy environment. We establish the scaling theory for the phase boundary of synchronization and for the steady-state fluctuations in the synchronizable regime[2]. Further, we provide the asymptotic behavior near the boundary of the synchronizable regime. Our results also imply the potential for optimization and trade-offs in stochastic synchronization and coordination problems with time delays.

[1]Supported in part by DTRA, ARL, and ONR.

[2]D. Hunt, G. Korniss, B.K. Szymanski, e-print arXiv:1011.2957 (2010).

11:51AM B14.00004 Statistical regularities in the rank-citation profile of individual scientists , ALEXANDER PETERSEN, H. EUGENE STANLEY, Boston University, SAURO SUCCI, Istituto Applicazioni Calcolo C.N.R. — Citation counts and paper tallies are ubiquitous in the achievement ratings of individual scientists. As a result, there have been many recent studies which propose measures for scientific impact (e.g. the h-index) and the distribution of impact measures among scientists. However, being just a single number, the h-index cannot account for the full impact information contained in an author's set of publications. Alternative "single-number" indices are also frequently proposed, but they too suffer from the shortfalls of not being comprehensive. In this talk I will discuss an alternative approach, which is to analyze the fundamental properties of the *entire* rank-citation profile (from which all single-value indices are derived). Using the complete publication careers of 200 highly-cited physicists and 100 Assistant professors, I will demonstrate remarkable statistical regularity in the functional form of the rank-citation profile $c_i(r)$ for each physicist $i = 1...300$. We find that $c_i(r)$ can be approximated by a discrete generalized beta distribution over the entire range of ranks r, which allows for the characterization and comparison of $c_i(r)$ using a common framework. Since two scientists can have equivalent h_i values while having different $c_i(r)$, our results demonstrate the utility of a scaling parameter, β_i, in conjunction with h_i, to quantify a scientist's publication impact.

12:03PM B14.00005 Modeling the decline of religion[1] , RICHARD WIENER, Research Corporation for Science Advancement and Department of Physics, University of Arizona, HALEY YAPLE, DANIEL ABRAMS, Department of Engineering Sciences and Applied Mathematics, Northwestern University — People claiming no religious affiliation constitute the fastest growing "religious" minority in many countries throughout the world.[2] Here we use a minimal model of competition between social groups[3] to explain historical data on the growth of religious non-affiliation in 85 regions around the world. We also describe numerical experiments that support the validity of the model. According to the model, for societies in which the perceived utility of not adhering is greater than the utility of adhering, religion will be driven toward extinction.

[1]This work was funded by Northwestern University and The James S. McDonnell Foundation.

[2]Zuckerman, P. "Atheism: Contemporary rates and patterns," in Cambridge Companion to Atheism, University of Cambridge Press, 2007.

[3]Abrams, D. M. and Strogatz, S.H. Modelling the dynamics of language death. Nature 424(6951), 900 (2003).

12:15PM B14.00006 Spontaneous Time Symmetry Breaking in System with Mixed Strategy Nash Equilibrium: Evidences in Experimental Economics Data , ZHIJIAN WANG, BIN XU, Experimental social science laboratory, Zhejiang University, ZHEJIANG UNIVERSITY COLLABORATION — In social science, laboratory experiment with human subjects' interaction is a standard test-bed for studying social processes in micro level. Usually, as in physics, the processes near equilibrium are suggested as stochastic processes with time-reversal symmetry (TRS). To the best of our knowledge, near equilibrium, the breaking time symmetry, as well as the existence of robust time anti-symmetry processes, has not been reported clearly in experimental economics till now. By employing Markov transition method to analysis the data from human subject 2x2 Games with wide parameters and mixed Nash equilibrium, we study the time symmetry of the social interaction process near Nash equilibrium. We find that, the time symmetry is broken, and there exists a robust time anti-symmetry processes. We also report the weight of the time anti-symmetry processes in the total processes of each the games. Evidences in laboratory marketing experiments, at the same time, are provided as one-dimension cases. In these cases, time anti-symmetry cycles can also be captured. The proposition of time anti-symmetry processes is small, but the cycles are distinguishable.

12:27PM B14.00007 The Sign Effect in Emerging Markets: the Inherent Instability of Bad News , JOEL TENENBAUM, Boston University Department of Physics, BORIS PODOBNIK, Faculty of Civil En- gineering, University of Rijeka, 51000 Rijeka, Croatia, DAVOR HORVATIC, Faculty of Natural Sciences, University of Zagreb, 10000 Zagreb, Croatia, SLAVICA BAJIC, Electrical Engineering Department, Polytechnic of Zagreb, 10000 Zagreb, Croatia, BECO PEHLIVANOVIC, Faculty of Educational Sciences, University of Bihac, Bihac, Bosnia and Hercegovina, H. EUGENE STANLEY, Boston University Department of Physics — In developed economy market indices, the sign of a term in a series influences the volatility in an asymmetric fashion — bad news results in larger subsequent fluctuations while good news results in smaller fluctuations. We study this phenomenon of volatility asymmetry using a stochastic process, exploring whether this asymmetry manifests in emerging markets, and if so, how such asymmetry changes over time as economies develop, mature, and react to crises such as the present one. We find that while both developed and emerging markets show distinctive behavior with respect to volatility asymmetry during times of economic tumult, they do so in ways that could be viewed either as universal or qualitatively different, posing interesting questions for further research. B. Podobnik et al., Phys. Rev. E **80**, 015101(R) (2009). J. Tenenbaum et al., Phys. Rev. E **82**, 046104 (2010).

12:39PM B14.00008 Quantized expected returns in terms of dividend yield at the money , LAMINE DIENG, City University of New York — We use the Bachelier (additive model) and the Black-Scholes (multiplicative model) as our models for the stock price movement for an investor who has entered into an America call option contract. We assume the investor to pay certain dividend yield on the expected rate of returns from buying stocks. In this work, we also assume the stock price to be initially in the out of the money state and eventually will move up through at the money state to the deep in the money state where the expected future payoffs and returns are positive for the stock holder. We call a singularity point at the money because the expected payoff vanishes at this point. Then, using martingale, supermartingale and Markov theories we obtain the Bachelier-type of the Black-Scholes and the Black-Scholes equations which we hedge in the limit where the change of the expected payoff of the call option is extremely small. Hence, by comparison we obtain the time-independent Schroedinger equation in Quantum Mechanics. We solve completely the time independent Schroedinger equation for both models to obtain the expected rate of returns and the expected payoffs for the stock holder at the money. We find the expected rate of returns to be quantized in terms of the dividend yield.

12:51PM B14.00009 Competition in social systems: three and a half models , DANIEL ABRAMS, HALEY YAPLE, Northwestern University, Department of Engineering Sciences and Applied Mathematics, RICHARD WIENER, Research Corporation for Science Advancement and Department of Physics, University of Arizona — When groups compete for members, the resulting dynamics of human social activity may be understandable with simple mathematical models. Here, we use techniques from dynamical systems and perturbation theory to analyze a theoretical framework for the growth and decline of competing social groups in three limits. We apply our analysis to an international data set tracking the growth of religious nonaffiliation, and find that data suggest a particular case of our general growth law, leading to clear predictions about possible future trends in society.

1:03PM B14.00010 Extraordinary Elasticity of the Distorted Kagome Lattice , ANTON SOUSLOV, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104, KAI SUN, Joint Quantum Institute and Condensed Matter Theory Center, University of Maryland, College Park, MD 20742, XIAOMING MAO, TOM LUBENSKY, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104 — J. C. Maxwell discovered that a system of particles in d-dimensions will be marginally rigid, or *isostatic*, if each particle interacts on average with $2d$ of its neighbors. Isostatic models have been used to describe such diverse soft phenomena as the jamming transition and the elasticity in networks of semi-flexible polymer gels. We develop models based on the isostatic kagome lattice, which has a subextensive number of floppy phonon modes. We show that these can be extended into soft deformations by changing the particle configurations while keeping the bond lengths fixed. Thus, we create families of novel isostatic lattices, which exhibit highly tunable elastic properties as a consequence of isotropic linear elasticity with a zero bulk modulus. They have a negative Poisson ratio, or auxetic (anti-rubber) behavior. Further, we find no bulk soft phonons at large length scales due to conformal symmetry. We discuss the intimate relationship between various symmetries and soft response in these models as well as the relation of these models to other marginally rigid systems.

1:15PM B14.00011 Theory of cooperation in a micro-organismal snow-drift game[1] , ZHENYU WANG, NIGEL GOLDENFELD, Department of Physics, Center for the Physics of Living Cells and Institute for Genomic Biology, University of Illinois at Urbana-Champaign — We present a mean field model for the phase diagram of a community of micro-organisms, interacting through their metabolism so that they are, in effect, engaging in a cooperative social game. We show that as a function of the concentration of the nutrients glucose and histidine, the community undergoes a phase transition separating a state in which one strain is dominant to a state which is characterized by coexisting populations. Our results are in good agreement with recent experimental results, correctly predicting quantitative trends and the phase diagram.

[1]We thank Jeff Gore for sharing with us his experimental data. This work was supported in part by the National Science Foundation through grant number NSF-EF-0526747.

1:27PM B14.00012 Intrinsic noise in stochastic models of gene expression with molecular memory and bursting , TAO JIA, RAHUL V. KULKARNI, Department of Physics, Virginia Polytechnic Institute and State University — Regulation of intrinsic noise in gene expression is essential for many cellular functions. Correspondingly, there is considerable interest in understanding how different molecular mechanisms of gene expression impact variations in protein levels across a population of cells. In this work, we analyze a stochastic model of bursty gene expression which considers general waiting-time distributions governing arrival and decay of proteins. By mapping the system to models analyzed in queueing theory, we derive analytical expressions for the noise in steady-state protein distributions. The derived results extend previous work by including the effects of arbitrary probability distributions representing the effects of molecular memory and bursting. The analytical expressions obtained provide insight into the role of transcriptional, post-transcriptional and post-translational mechanisms in controlling the noise in gene expression.

1:39PM B14.00013 Search for Euler Singularity using Vortex Filaments , SAHAND HORMOZ, MICHAEL BRENNER, Harvard University — A promising mechanism for generating a finite-time singularity in the incompressible Euler equations is stretching of vortex filaments. An exhaustive search of all possible initial conditions involving filaments, however, is not practically feasible. In this talk, I will show that two interacting vortex filaments can not generate a singularity for any initial conditions, by analyzing the asymptotic self-similar limit of their collapse. Essentially, our approach entails a separation of the dynamics of the filament shape, from the shrinking of its core. We solve for the dynamics using a self-similar ansatz and show that the core does not shrink fast enough for a self-consistent collapse. The similarity solution allows for many different collapse geometries, consistent with the tireless effort in the past of investigating new initial conditions. Potential for a singularity at higher number of filaments is also discussed.

1:51PM B14.00014 Vibrofluidized melting of geometrically cohesive granular media , NICK GRAVISH, GEOFFREY RUSSELL, Georgia Tech, SCOTT V. FRANKLIN, Rochester Institute of Technology, DAVID HU, DANIEL I. GOLDMAN, Georgia Tech — Dry granular media composed of particles of special shapes (e.g. long rods or c-shaped particles) can display cohesive effects through particle geometry alone. We study the solid to gas transition in piles of c-shaped particles under vertical vibration as we vary acceleration and frequency. A cylindrical solid of particles is formed with wall angles near 90° and is placed on a solid surface. For fixed frequency as acceleration increases, the pile undergoes two transitions. The first is from the solid-like state to a liquid-like state in which the wall angles relax but the mobile particles remain spatially localized. The second is from the liquid-like state to the gaseous state in which particles become separated (not entangled). Using video and accelerometer measurements, we record the temporal evolution of the spatial density and pile-plate collisional impulse. A critical energy scale, set by the particle geometry and gravitational potential energy, governs the liquid-gas transition.

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B15 DMP GMAG FIAP: Focus Session: Spins in Semiconductors - Spin Currents I

D171

11:15AM B15.00001 Optical effects of spin currents in semiconductors[1] , JING WANG, Department of Physics, Tsinghua University — BANG-FEN ZHU, Department of Physics and Institute of Advanced Study, Tsinghua University, REN-BAO LIU, Department of Physics, The Chinese University of Hong Kong – We predict the linear and second-order nonlinear optical effects of spin currents in semiconductors, based on systematic symmetry analysis and microscopic calculations with realistic models [1, 2]. By an analogue to the Ampere effect and Oersted effect, we conceived and verified that a spin current can be coupled to a "photon spin curren" carried by a polarized light beam, which causes sizeable Faraday rotation without involving net magnetization. Furthermore, a spin current can have a strong second-order nonlinear optical effect with unique polarization-dependence due to the special symmetry properties of the spin current. In particular, for a longitudinal spin current, in which the spins point parallel or anti-parallel to the current direction is a chiral quantity, a chiral sum-frequency effect will be induced. The second-order optical effects of spin currents have been experimentally verified immediately after the theoretical prediction [3]. These discoveries represent new phenomena in magneto-optics, with potential spin-photonic applications. They bring new opportunities to research of spintronics and may also facilitate research of topological insulators where the edge states form pure spin currents. References:

[1] J. Wang, B. F. Zhu, and R. B. Liu, *Phys. Rev. Lett.* 100, 086603 (2008); see also Erratum, *ibid* 101, 069902 (2008)
[2] J. Wang, B. F. Zhu, and R. B. Liu, *Phys. Rev. Lett.* 104, 256601 (2008).
[3] L. K. Werake and H. Zhao, *Nature Physics* 6, 875 (2010).

[1]This work was supported by the NSFC Grant Nos.10574076, 10774086, and the Basic Research Program of China Grant 2006CB921500, Hong Kong RGC HKU 10/CRF/08 and Hong Kong GRF CUHK 402207.

11:51AM B15.00002 Magnetoelectric Photocurrent Generated by Direct Interband Transitions in InGaAs/InAlAs Two-Dimensional Electron Gas , JUNFENG DAI, HAI-ZHOU LU, The University of Hong Kong, CHUNLEI YANG, Sun Yat-Sen University, SHUN-QING SHEN, FU-CHUN ZHANG, XIAODONG CUI, The University of Hong Kong, NANOSTRUCTURE CHARACTERIZATION GROUP TEAM, CENTRE OF THEORETICAL AND COMPUTATIONAL PHYSICS COLLABORATION, DEPARTMENT OF PHYSICS IN SUN YAT-SEN UNIVERITY COLLABORATION — We report the observation of magnetoelectric photocurrent generated via direct interband transitions in an InGaAs/InAlAs two-dimensional electron gas by a linearly polarized incident light. The electric current is proportional to the in-plane magnetic field, which unbalances the velocities of the photoexcited carriers with opposite spins and consequently generates the electric current from a hidden spin photocurrent. The spin photocurrent can be evaluated from the measured electric current, and the conversion coefficient of spin photocurrent to electric current is self-consistently estimated to be 10^{-3}–10^{-2} per Tesla. The observed light-polarization dependence of the electric current is well explained by a theoretical model which reveals the wave vector angle dependence of the photoexcited carrier density.

12:03PM B15.00003 Anisotropic conductivity caused by spin-orbit interactions , DAVID H. BERMAN, MICHAEL E. FLATTÉ, University of Iowa — Free propagation in a two-dimensional electron gas with both Rashba and Dresselhaus spin-orbit coupling shows strong anisotropy depending on the ratio of the coupling strength to the Fermi energy and on the ratio of the strengths of the Rashba and Dresselhaus interactions [1]. This spin-orbit induced anisotropy appears also in the local density of states near impurities. In addition the non-local conductivity, $\sigma_{i,j}(\mathbf{r},\mathbf{r}')$, computed in the absence of impurities is anisotropic. This is in contrast to the macroscopic conductivity in the presence of impurities which shows no anisotropy when only ladder diagrams are considered [2]. In all these instances, the degree of anisotropy can be controlled by application of electric fields perpendicular to the 2DEG.

[1] D. H. Berman and M. E. Flatté, PRL **105**, 157202 (2010).
[2] O. Chalaev and D.Loss, Phys. Rev. B **71**, 245318 (2005).

12:15PM B15.00004 Drift and diffusion of spin and charge density waves in a two-dimensional electron gas , LUYI YANG, J.D. KORALEK, J. ORENSTEIN, Lawrence Berkeley National Laboratory and University of California Berkeley, D.R. TIBBETTS, J.L. RENO, M.P. LILLY, Sandia National Laboratories — We use transient grating spectroscopy (TGS) to study the persistent spin helix (PSH) state and electron-hole density wave (EHDW) in a 2D electron gas in the presence of an in-plane electric field parallel to the wavevector of the PSH or EHDW. By directly measuring the phase, we can measure the PSH and EHDW displacement with 10 nm spatial and sub-picosecond time resolution. We obtain both the spin diffusion and mobility and ambipolar diffusion and mobility from the TGS measurements of PSH and EHDW, respectively. The spin transresistivity extracted from the spin diffusion is in excellent agreement with the RPA theory of spin Coulomb drag (SCD). The spin mobility data indicate that SCD may also play a role in the spin wave drifting process. From the ambipolar diffusion and mobility, we obtain the transresistivity of electrons and holes in the same layer, which is much stronger than is typically seen in the conventional Coulomb drag experiments on coupled quantum wells.

12:27PM B15.00005 Radial spin helix in two-dimensional electron systems with Rashba spin-orbit coupling , VALERIY SLIPKO, Department of Physics and Technology, V. N. Karazin Kharkov National University, 4 Svobody Sq., Kharkov 61077, Ukraine, YURIY PERSHIN, Department of Physics and Astronomy and USC Nanocenter, University of South Carolina, 712 Main Street, Columbia, SC 29208, USA — We suggest a new long-lived spin-polarization structure, a radial spin helix [1], and study its relaxation dynamics. For this purpose, starting with a system of equations for spin-polarization density, we find its general solution in the axially symmetric case. It is demonstrated that the radial spin helix of a certain period relaxes slower than homogeneous spin polarization and plain spin helix [2]. Importantly, the spin polarization at the center of the radial spin helix stays almost unchanged at short times. At longer times, when the initial nonexponential relaxation region ends, the relaxation of the radial spin helix occurs with the same time constant as that describing the relaxation of the plain spin helix. Experimentally, such a structure can be created using spin injection or extraction in a system with cylindrical electrodes or, possibly, by a modified spin gratings technique.

[1] Y. V. Pershin and V. A. Slipko, Phys. Rev. B 82, 125325 (2010).
[2] Y. V. Pershin, Phys. Rev. B 71, 155317 (2005).

12:39PM B15.00006 Anholonomic spin manipulation in drift transport in semiconductors , BEN J. MOEHLMANN, MICHAEL E. FLATTÉ, Optical Science and Technology Center and Department of Physics and Astronomy, University of Iowa — We find that the electronic spin rotation induced by drift transport around a closed path in a wide variety of nonmagnetic semiconductors at zero magnetic field depends solely on the physical path taken. Physical paths that produce any possible spin rotation due to transport around a closed path are constructed for electrons experiencing strain or electric fields in (001), (110), or (111)-grown zincblende semiconductor quantum wells. Spin decoherence due to travel along the path is negligible compared to the background spin decoherence rate. The small size of the designed paths (< 100 nm scale in GaAs) may lead to applications in nanoscale spintronic circuits. This work was supported by an ONR MURI.[1]

[1]B. J. Moehlmann and M. E. Flatté, arXiv:1007.0909

12:51PM B15.00007 Mapping Spin-Orbit Splitting in Strained (In,Ga)As Epilayers , B.M. NORMAN, C.J. TROWBRIDGE, V. SIH, Department of Physics, University of Michigan, Ann Arbor, MI 48109, J. STEPHENS, A.C. GOSSARD, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — Time-resolved and spatially resolved Faraday rotation spectroscopy is used to measure the magnitude and direction of the momentum-dependent spin splitting in strained InGaAs epilayers. The epilayers are lattice-matched to the GaAs substrate and designed to reduce inhomogeneous effects related to strain relaxation. Measurements of momentum-dependent spin splitting as a function of electron spin drift velocity along [100], [010], [110] and $[1\bar{1}0]$ directions enable separation of isotropic and anisotropic effective magnetic fields that arise from uniaxial and biaxial strain along $\langle 110 \rangle$. Such electrically induced effective magnetic fields can be used for spin generation and manipulation in spintronics devices. We find that anisotropic and isotropic strain-induced effective magnetic fields are comparable in magnitude. [1]

[1]B. M. Norman, C. J. Trowbridge, J. Stevens, A. C. Gossard, D. D. Awschalom, and V. Sih, Phys. Rev. B. **82**, 081304(R) (2010).

1:03PM B15.00008 Spin-orbit interaction from low-symmetry localized defects in semiconductors[1] , OLEG CHALAEV, G. VIGNALE, University of Missouri, MICHAEL FLATTÉ, University of Iowa — The presence of low-symmetry impurities or defect complexes in the zinc-blende direct-gap semiconductors (e.g. interstitials, Jahn-Teller distortions) results in a novel spin-orbit term in the effective Hamiltonian for the conduction band. The new spin-orbit interaction is proportional to the matrix element of the defect potential between the conduction and the valence bands. Because this interaction arises already in the first order of the expansion of the effective Hamiltonian in powers of $\Delta/E_g \ll 1$ (where Δ is the valence band spin-orbit splitting, and E_g is the band gap), its contribution to the spin relaxation time may exceed that of previously studied contributions, such as the Rashba term, even for moderate concentrations of low-symmetry impurities.

[1]Work supported by ARO Grant No. W911NF-08-1-0317

1:15PM B15.00009 Modeling of diffusion of injected electron spins in spin-orbit coupled microchannels , LIVIU P. ZÂRBO, Institute of Physics ASCR, CZ, JAIRO SINOVA, Texas A & M University, USA, I. KNEZEVIC, University of Wisconsin-Madison, USA, J. WUNDERLICH, Hitachi Cambridge Laboratory, UK, T. JUNGWIRTH, Institute of Physics ASCR, CZ — Understanding of the collective electron spin dynamics under the influence of spin-orbit fields is a key requirement in the quest for all-electrical semiconductor spintronic devices. We investigate the spin dynamics of an ensemble of spin polarized electrons injected in the diffusive microchannel of a model device with linear Rashba and Dresselhaus spin-orbit coupling. Using a spin-dependent ensemble Monte Carlo method, we analyze the steady state spin density patterns dependence on channel dimension and orientation, spin-orbit coupling strengths and external magnetic fields. We show that in the persistent spin helix regime, the spin density patterns depend only on the system geometry and channel orientation. Magnetic fields of order of tesla are required to affect spin dynamics in the persistent spin helix regime. Our simulation results [PRB 82, 205320 (2010)] have been used to help understand the spin diffusion in the channel of the recently demonstrated spin Hall effect transistor [arXiv:1008.2844].

1:27PM B15.00010 Unitarity of scattering and edge spin accumulation in a ballistic and quasiballistic regimes , ALEXANDER KHAETSKII, University at Buffalo, SUNY, EUGENE SUKHORUKOV, University of Geneva, Switzerland — We consider a 2D ballistic structure with spin-orbit-related splitting of the electron spectrum. We calculated the edge spin density which appears in the presence of a charge current through the structure. Combined effect of the boundary scattering and spin precession leads to oscillations of the edge polarization. The problem is solved with the use of the method of scattering states. We clarified the important role of the unitarity of scattering for the problem of edge spin accumulation. For Rashba Hamiltonian, which is linear in momentum, and in the case of a straight boundary it leads to exact cancellation of long-wave oscillations of the spin density with a period order of spin precession length. However, this appears to be rather exceptional case. In general, the smooth spin oscillations recover, as it happens, e.g., for the wiggly boundary. For qubic Hamiltonian (2D holes) the unitarity scattering conditions are different, as a result, even in the case of a straight boundary the cancellation of the smooth oscillations in spin density does not occur. Similar problem is considered for the case when the sample size is large compared to the mean free path which in its turn is much larger than the spin precession length. For example, for the cubic Hamiltonian the "edge" contribution to the spin density can be larger than the "bulk" one which appears as a result of the spin flux from the bulk. This demands the reinterpretation of the experimental results [1]. [1]. J. Wunderlich et al., PRL 94, 047204 (2005).

1:39PM B15.00011 Visualizing zitterbewegung in spin-orbit coupled semiconductor quantum wires , MARKKU JAASKELAINEN, ULRICH ZULICKE — We study a spin-orbit coupled parabolic quantum wire in the ballistic regime and develop a method for visualizing zitterbewegung in phase space. We introduce a Husimi distribution on the transverse coordinate and calculate the distribution of spin by a decomposition into Bloch vector components. The Husimi distribution corresponds to the simultaneous, unsharp measurement of the transverse position and velocity in accordance with the uncertainty principle. In phase space, the distribution exhibits a combination of spin precession and coherent oscillation along the longitudinal coordinate, i.e. zitterbewegung. This behavior closely matches the semiclassical dynamics for small values of the spin-orbit coupling. For increasing spin-orbit coupling strength, the oscillation amplitude initially increases, whereas for very large values the oscillation amplitude is quenched.

1:51PM B15.00012 Theory of carrier dynamics in InSb parabolic quantum wells[1] , D. SAHA, G.D. SANDERS, C.J. STANTON, University of Florida, M. BHOWMICK, T. MERRITT, G.A. KHODAPARAST, Virginia Tech, T.D. MISHIMA, M.B. SANTOS, University of Oklahoma — InSb, with the narrowest gap among the III-V compound semiconductors, shows considerable promise as a quantum well material because its small conduction-band mass gives it a large room temperature electron mobility, and its large g-factor makes it attractive for spintronic devices. We present experiments and theoretical calculations for carrier dynamics in a strained 50-nm thick InSb/AlInSb parabolic quantum well. Our calculations are based on the 8-band Pidgeon-Brown model generalized to include the effects of the parabolic confinement potential as well as pseudomorphic strain. Optical properties are calculated within the golden rule approximation and compared with experiments. We model one and two color, time-resolved pump-probe differential transmission and reflectivity experiments. The change in the infrared probe pulse as a function of delay time provides information on carrier and spin relaxation dynamics. Both interband and intra-band dynamics are studied.

[1]Supported by NSF through grants DMR-0507866, DMR-0520550, DMR-0706313, and DMR-0846834.

2:03PM B15.00013 Imaging spin transport in a semiconductor with an iron-filled carbon nanotube , ANDREW BERGER, VIDYA BHALLAMUDI, DOMINIC LABANOWSKI, PALASH BANERJEE, CAMELIA MARGINEAN, DENIS PELEKHOV, DAVID STROUD, P. CHRIS HAMMEL, The Ohio State University, KATHY MCCREARY, ROLAND KAWAKAMI, University of California, Riverside, FRANZISKA WOLNY, THOMAS MUEHL, Leibniz Institue for Solid State and Materials Research, Dresden — There has been much recent progress in the field of spintronic device fabrication, creating a need for characterization tools. We are developing a low-temperature scanned probe microscope with the ability to position, with high precision, a magnetized iron-filled carbon nanotube above a spin-injected semiconductor device [1]. The inhomogeneous field of this unique magnetic probe will be experienced by spins in the sample. We have developed a technique for simulating the effects of such an inhomogeneous field [2]. Crucially, we find that our scanned probe technique can create highly localized spin density features on a length scale comparable to the nanotube diameter. This will allow for spatial mapping of the spin density with high resolution – a capability not possible in current electrical detection schemes. Such experiments may provide information about interface effects, scattering, and material properties which influence spin behavior.

[1] F. Wolny, et al. J. Appl. Phys. 104, 064908 (2008)
[2] V. Bhallamudi, et al. arXiv:1010.3747v1 [cond-mat.mes-hall]

Monday, March 21, 2011 11:15AM - 2:15PM –
Session B16 DMP GMAG: Focus Session: Magnetic Nanostructures II D173

11:15AM B16.00001 Electronic structure and electron spectroscopy of magnetic iron oxide nanoparticles , J. GAZQUEZ, J. SALAFRANCA, Universidad Complutense de Madrid, Spain, M. VARELA, S. PENNYCOOK, Oak Ridge National Lab, S.T. PANTELIDES, Vanderbilt University, P. MORALES, ICMM-CSIC, Spain, N. PEREZ, A. LABARTA, X. BATLLE, Univ. Barcelona, Spain — Magnetic iron oxide nanoparticles are good candidates for biomedical applications due to their low toxicity and easy functionalization. We synthesized magnetite (Fe3O4) nanoparticles by a high temperature decomposition method. They present some very desirable properties for applications: very high saturation magnetization, and excellent degree of crystallinity. Transmission electron microscopy images, and electron energy loss spectroscopy with atomic resolution allow a composition map that shows small variations in relative composition between the core and the surface, and subtle changes in the absorption spectra. Our density functional (DFT) calculations address different factors contributing to the magnetic properties. Changes in the electronic structure correlate with different features in the experimental absorption spectra, yielding a better understanding of the magnetic order. We study the role of structural defects, the organic surfactant, stoichiometry and the nominal oxidation state of iron, and their effect in determining the equilibrium magnetic state. This work is supported by DOE Materials Sciences and Engineering Division and the European Research Council Starting Investigator Award.

11:27AM B16.00002 Magnetic properties of Fe/Fe_3O_4 core/shell nanostructure , VIVEK SINGH, MOHINDAR SEEHRA, West Virginia University, S. BALI, E. EYRING, University of Utah, N. SHAH, F. HUGGINS, G. HUFFMAN, University of Kentucky — Magnetic properties of a core/shell nanostructure with spherical core of Fe/FeB and a shell of Fe_3O_4/γ-Fe_2O_3 are reported employing magnetometry, electron magnetic resonance (EMR) and Mössbauer spectroscopy. This nanostructure was produced by reducing $FeCl_3{\cdot}6H_2O$ with $NaBH_4$. Combining the results from XRD, TEM and Mössbauer spectroscopy showed the nanostructure to consist of a core of diameter D$\simeq$20 nm containing both α-Fe with D$\simeq$7 nm and amorphous Fe-B alloy and a shell of thickness 5 nm containing Fe_3O_4/γ-Fe_2O_3. Measurements of the magnetization M vs. temperature (2 K to 370 K) and in H upto 65 kOe show a blocking temperature T_B $\simeq$30 K associated with the oxide shell and ferromagnetism upto 370 K with nearly temperature-independent saturation M_S $\simeq$70 emu/g and coercivity H_C $\simeq$100 Oe. In EMR studies at 9.28 GHz, two lines are observed: a narrower line with linewidth ΔH$\simeq$600 Oe and g$\simeq$2 and a broader line with ΔH$\simeq$4200 Oe and g$\simeq$2.2. These parameters of the narrower line combined with its disappearance below 50 K suggests its origin to be the oxide shell whereas the broader line is due to Fe/FeB core. Research supported by U. S. Dept. of Energy, Contract #DE-FC26-05NT42456.

11:39AM B16.00003 Fe and Fe oxide nanoparticles ensembles with macroscopic anisotropy[1] , MIGUEL ANGEL GARCIA, Institute for Ceramic and Glass - CSIC — We report here the fabrication Fe and Fe oxide nanoparticles over glass substrates exhibiting macroscopic anisotropy. Fe thin films were deposited onto glassy substrates by thermal evaporation and were subsequently annealed in air and argon atmosphere. The difference of thermal expansion coefficient between the substrate and the metallic film induces stresses in the substrate-metal interface leading to hole nucleation, growing and percolation, and finally to the formation of a metallic a nanoparticles layer. Anisotropic nanoparticles can be obtained by applying mechanical stress during the thin the film deposition or the annealing process. The applied stress induce anisotropy axis for the NPs shape that lead to the formation of elongated nanoparticles with macroscopic texture. Anisotropy can be increased by applying a magnetic field during thermal annealing. We analyze here the magnetization and anisotropy of individual nanoparticles and nanoparticles interactions and their relationship with the processing parameters.

[1]This work was supported by the Spanish Ministry of Science and Education through the project FIS-2008-06249

11:51AM B16.00004 Magnetic Core-Shell Morphology of Structurally Uniform Magnetite Nanoparticles , KATHRYN KRYCKA, NIST Center for Neutron Research — Magnetic nanoscale structures are intriguing, in part, because of the exotic properties that emerge compared with bulk. The reduction of magnetic moment per atom in magnetite with decreasing nanoparticle size, for example, has been hypothesized to originate from surface disordering to anisotropy-induced radial canting, which are difficult to distinguish using conventional magnetometry. Small-angle neutron scattering (SANS) is ideal for probing structure, both chemical and magnetic, from nm to microns across an ensemble of particles. Adding polarization analysis (PASANS) of the neutron spin orientation before and after interaction with the scattering particles allows the magnetic structure to be separated into its vector components. Application of this novel technique to 9 nm magnetite nanoparticles closed-packed into face-centered crystallites with order of a micron revealed that at nominal saturation the missing magnetic moments unexpectedly interacted to form well-ordered shells 1.0 to 1.5 nm thick canted perpendicular to their ferrimagnetic cores between 160 to 320 K [1]. These shells additionally displayed intra-particle "cross-talk", selecting a common orientation over clusters of tens of nanoparticles. However, the shells disappeared when the external field was removed and interparticle magnetic interactions were negligible (300 K), confirming their magnetic origin. This work has been carried out in collaboration with Ryan Booth, Julie Borchers, Wangchun Chen, Liv Dedon, Thomas Gentile, Charles Hogg, Yumi Ijiri, Mark Laver, Sara Majetich, James Rhyne, and Shannon Watson.

[1] K.L. Krycka *et al.*, Phys. Rev. Lett. 104, 207203 (2010)

12:27PM B16.00005 Magnetic Characterization of Ferrite Nanoparticles , MATTHEW BRYAN, PAUL SOKOL, Department of Physics, indiana University, GREG GUMINA, LYUDMILA BRONSTEIN, BOGDAN DRAGNEA, Department of Chemistry, Indiana University — Magnetic nanoparticles (NPs) of different compositions (FeO/Fe_3O_4, g-Fe_2O_3, FePt, and $CoFe_2O_4$) have been synthesized using high temperature organometallic routes described elsewhere. NPs (16.6 nm in diameter) of a mixed FeO/Fe_3O_4 (wuestite/magnetite) composition were prepared by thermal decomposition or iron oleate in the presence of oleic acid as a surfactant in dodocane at 370C in argon atmosphere. After the thermal treatment of the reaction solution at 200 C under air for 2 hours these NPs are transformed into maghemite (g-Fe_2O_3), the magnetization of which is significantly enhanced. NPs of $CoFe_2O_4$ (8 nm) have been prepared by simultaneous decomposition of Co(II) and Fe(III) acetylacetonates in the presence of oleic acid and oleylamine. The X-ray diffraction profile of these NPs is characteristic of cobalt ferrite. Alternatively, alloyed 1.8 nm FePt NPs prepared by simultaneous decomposition of Fe and Pt acetylacetonates in the reductive environment demonstrate a completely disordered structure, which is reflected in their magnetic properties. SQUID magnetometry was used to measure the magnetization of NPs at high and low temperatures. Zero-field cooling and field-cooling measurements were taken to demonstrate superparamagnetic behavior and an associated blocking temperature.

12:39PM B16.00006 Magnetically Tunable Polymer Nanocomposites for RF and Microwave Device Applications , K. STOJAK, S. PAL, H. SRIKANTH, University of South Florida-Physics, C. MORALES, J. DEWDNEY, J. WANG, T. WELLER, University of South Florida-Electrical Engineering — There has been much interest in polymer nanocomposites (PNC) recently due to potential applications for EMI shielding, tunable electromagnetic devices and flexible electronics. We report synthesis, structural, magnetic and RF characterization on PNCs ranging from 20-80 wt-% loadings of Fe_3O_4 and $CoFe_2O_4$ nanoparticles ($\sim$8nm) in a thermosetting resin from the Rogers Corporation. Nanoparticles were synthesized by thermal decomposition and characterized by XRD and TEM. Magnetic properties were studied using a Quantum Design PPMS. PNCs displayed characteristic features of superparamagnetism at room temperature and blocking at low temperature. Microwave transmission/reflection studies were done using a microstrip resonator. Strong tunability in the microwave absorption was observed. We extend our study to include nanoparticle-filled multi-walled carbon nanotubes synthesized by CVD. These high-aspect ratio magnetic nanostructures, with tunable anisotropy, are of particular interest in enhancing magnetic and microwave responses in existing PNCs.

12:51PM B16.00007 Field dependence of T_B in NiO and (Ni, Zn)O Nanoclusters[1] , YUNG HUH, Department of Physics, South Dakota State University, Brookings, SD 57007, M. PECK, R. SKOMSKI, R. ZHANG, P. KHAREL, M. ALLISON, D. SELLMYER, M. LANGELL — Size dependence of magnetic properties of rocksalt NiO and Zn substituted NiO nanoparticles are investigated. Nanoparticle diameters are determined from 8 to 30 nm by XRD and AFM. Uncompensated spins at the nanoparticle surface contribute to superparametism at low temperatures and their blocking temperatures increase with stronger applied field. The field induced spin canting of the antiferromagnetic sublattices is a bulk effect and studied by the substitution of Zn with transition metal. Nanoparticles start exhibiting bulk magnetic behavior with size greater than 18 nm. Magnetization rotation of uncompensated spins under the magnetic field is mainly due to nanoscale size effect. The anisotropy of the nanoparticle is about four times larger than that of the bulk NiO.

[1]This research is supported by the NSF (CHE-1012366 and Nebraska MRSEC Grant DMR-0820521), the DOE Grant DE-FG02-04ER46152 (P. K. and D. J. S.) and NCMN.

1:03PM B16.00008 Interacting Superparamagnetic Brownian Particles in an Array of 2D Asymmetric Magnetic Traps[1] , GREGORY VIEIRA, AARON CHEN, R. SOORYAKUMAR, The Ohio State University Department of Physics — We report on the ordering and fluctuation of multiple superparamagnetic particles confined by a thin liquid layer in a two-dimensional array of asymmetric magnetic trapping potentials. The repulsive dipolar interaction between magnetic particles and their confinement by the trapping potential cause the particles to form a cluster with characteristic inter-particle spacing within each trapping site, while the particles undergo thermal fluctuations. Applying an external magnetic field offers a convenient way to control the strength of the dipolar interactions and change the trapping potential landscape. Results on (a) Brownian motion of individual particles in the cluster, (b) re-distribution of particles into new clusters driven by a change in the external field, and (c) hopping of particles between clusters under fluid flow will be presented.

[1]Support from ARO grant W911NF-10-1-0353 is acknowledged.

1:15PM B16.00009 Realization of a Bowl-like Potential and Its Confinement of Magnetic Microspheres[1] , AARON CHEN, THOMAS HENIGHAN, GREGORY VIEIRA, RATNASINGHAM SOORYAKUMAR — Field-induced self-assembly of fluid-borne superparamagnetic microspheres not only has its importance in nanotechnology, but it also serves as a model for studies of phase transitions at the nano- to micro-meter scale. In this report, we experimentally demonstrate and theoretically account for the dynamics and structural order of a two-dimensional cluster of microspheres in the presence of a bowl-like potential. The potential is derived from magnetic patterns imprinted on the surface together with externally applied magnetic fields. Due to competition between the repulsive dipolar interaction amongst the microspheres and the confining force provided by the bowl-like potential, a cluster of microspheres with characteristic inter-sphere spacing is stabilized within the potential. The role of external magnetic fields which provide a convenient means to tune the strength of the dipolar interactions, and thereby control the relative importance of the two competing interactions, will be presented.

[1]Support from ARO grant W911NF-10-1-0353 is acknowledged.

1:27PM B16.00010 Tailored Magnetostructural Transitions[1] , RADHIKA BARUA, FELIX JIMENEZ-VILLACORTA, DONALD HEIMAN, LAURA H. LEWIS, Northeastern University — Dominance of the surface atoms over the bulk atoms in nanoscaled magnetostructural systems may alter the ground state of the system and thereby change the transition character. Creation of a nanostructured magnetostuctural system was carried out via rapid solidification of $(FeRh)_5Cu_{95}$ to precipitate nanoscaled isolated FeRh precipitates in a Cu matrix upon annealing. Bulk FeRh has an abrupt antiferromagnetic - ferromagnetic transition around T =370 K. X-ray diffraction performed on the quenched $(FeRh)_5Cu_{95}$ alloy indicates only the presence of Cu of slightly expanded lattice parameter a=3.62 Å, with ferromagnetism confirmed at room temperature by SQUID magnetometry. Vacuum annealing at 200 °C causes a secondary phase to appear with an abrupt magnetic phase transition at T_t = 130 K. Details of the magnetic behavior of this nanostuctured phase will be discussed.

[1]Research performed under the auspices of the U.S. DOE BES under contrac [DE-FG02-10ER46711

1:39PM B16.00011 Synthesis of Ferrimagnetic Fe_3Se_4 Nanostructures with Giant Coercivity[1] , HONGWANG ZHANG, GEN LONG, DA LI, HAO ZENG, Department of Physics, SUNY at Buffalo — In this study, we present the synthesis of Fe_3Se_4 nanostructures by a one-pot high temperature organic solution-phase method. The size of these nanostructures can be tuned from 50 to 500 nm and their shapes can be varied from nanosheets and nano-cactus to faceted nanoparticles by changing the precursors and reaction conditions. These nanostructures exhibit hard magnetic properties, with giant coercivity values reaching 40 kOe at 10 K, and 4 kOe at room temperature. The estimated lower bound of the magnetocrystalline anisotropy constant is 6×10^6 erg/cm^3, comparable to that of hcp Cobalt. The large coercivity/anisotropy is rare for compounds without noble metal or rare-earth elements. If Fe_3Se_4 based phases can be doped to enhance their Curie temperature and magnetization, they can be a low cost, non-toxic alternative to noble metal or rare earth based advanced magnets.

[1]Work supported by NSF DMR-0547036.

1:51PM B16.00012 Synthesis and Magnetic Properties of FePt@MnO Nano-*hetero*-Particles , THOMAS SCHLADT, TANJA GRAF, OSKAR KOEHLER, KERSTIN SCHNEIDER, WOLFGANG TREMEL, Johannes Gutenberg-University Mainz, Germany, INSTITUTE FOR INORGANIC AND ANALYTICAL CHEMISTRY TEAM — Monodisperse FePt@MnO nano-*hetero*-particles with different sizes and morphologies were prepared by a seed-mediated nucleation and growth technique. Both, size and morphology of the individual domains could be controlled by adjustment of the synthetic parameters. As a consequence, different particle constructs, including dimers, dumbbells and flowers, could be obtained by changing the polarity of the solvent. The FePt@MnO nano-*hetero*-particles were thoroughly characterized by (HR-)TEM- and XRD analysis and SQUID magnetometry. Due to a sufficient lattice match, the MnO NPs preferentially grow on the (111) surfaces of the *fcc*-FePt seeds. Furthermore, the surface spins of the antiferromagnetic MnO domains pin the magnetic moments of the ferromagnetic FePt NPs which leads to an exchanged biased magnetic hysteresis.

2:03PM B16.00013 Electron-electron correlations and magnetic properties of small FePt clusters[1] , ALAMGIR KABIR, NEHA NAYYAR, VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Department of Physics and NSTC, University of Central Florida, Orlando, FL 32816 — We have applied the DFT+U and the Nanoscale Dynamical Mean-Field Theory (NDMFT) [1] approaches to study the magnetic properties of small FePt clusters. The role of correlation effects in determining the geometry and the magnetic properties of the clusters as a function of chemical composition and the effective local Coulomb repulsion energy U is examined. We find that the magnetization to decrease with increasing number of Pt atoms. Interestingly, contrary to the bulk case, Pt clusters have nonzero magnetization. The magnetic properties are found to be very sensitive to the value of U, as a result of the dependence of the single particle energy levels on this parameter. Dynamical correlation effects, which are taken into account in the DFT+DMFT approach and which lead to an increase of the average in time double occupancy of the d-orbitals, results in a significant decrease of magnetization as compared to the results from the DFT+U case.

[1] V. Turkowski et al, J. Phys.: Condens. Matt. 22, 462202 (2010)

[1]Work supported by DOE Grant DOE-DE-FG02-07ER46354.

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B17 GMAG DMP: Focus Session: Bulk Properties of Complex Oxides - Manganites II

D174

11:15AM B17.00001 Dynamics of bi-stripes and a colossal metal-insulator transition in the bi-layer manganite $La_{2-2x}Sr_{1+2x}Mn_2O_7$ $(x \sim 0.59)$, ZHE SUN, University of Colorado, Boulder — Electronic phases with stripe patterns have been intensively investigated for their vital roles in novel properties of correlated electronic materials. How these real-space patterns affect the conductivity and other properties of materials (which are usually described in momentum space) is one of the major challenges of modern condensed matter physics. By studying the electronic structure of $La_{2-2x}Sr_{1+2x}Mn_2O_7$ $(x \sim 0.59)$ and in combination with earlier scattering measurements, we demonstrate the variation of electronic properties accompanying the melting of so-called bi-stripes in this material. The static bi-stripes can strongly localize the electrons in the insulating phase above $T_c \sim 160$K, while mobile electrons grow up and coexist with a significant portion of localized electrons when the static bi-stripes melt below T_c. The presence of localized electrons below T_c suggests that the melting bi-stripes exist as a fluctuating counterpart. From static to melting, the bi-stripes lead to a "colossal" metal-insulator transition in this material. Work was done in collaboration with Q. Wang, A. V. Fedorov, H. Zheng, J. F. Mitchell, D. S. Dessau.

11:51AM B17.00002 Probing multiple magnetic transitions and phase coexistence in mixed phase manganites , M.H. PHAN, N.S. BINGHAM, H. SRIKANTH, University of South Florida, C.L. ZHANG, S.W. CHEONG, Rutgers University — $La_{5/8-y}Pr_yCa_{3/8}MnO_3$(LPCMO) manganites exhibit a complex phase diagram due to coexisting and competing magnetic and electronic phases. A complete understanding of the origin of phase coexistence and separation in this system has remained elusive. To resolve this, it is essential to employ experimental methods that allow detailed investigations of the temperature and magnetic field response of the different phases. In this study we introduce magnetocaloric effect (MCE) and radio-frequency transverse susceptibility (TS) experiments as being ideally suited for this purpose. While MCE is generally considered in the community as an "applied" measurement tool to characterize magnetic refrigerant materials, we demonstrate that it is actually a very useful probe of magnetic transitions and ground state magnetic properties in LPCMO. TS experiments probe a phase conversion between the charge-ordered and ferromagnetic phases and magnetic field-induced kinetic arrest. Our studies provide an important understanding of the phase coexistence and separation in mixed phase systems like LPCMO.

12:03PM B17.00003 Soft x-ray investigation on the spin and orbital states of $La_{1.4}Sr_{1.6}Mn_2O_7$, K.-T. KO, H. JANG, J.-H. PARK, Dept. Physics, POSTECH, B.-G. PARK, J.-Y. KIM, PAL, SUNG BAEK KIM, I-FEM & Dept. Physics, POSTECH, S-W. CHEONG, R-CEM & Dept. Physics and Astronomy, Rutgers University — The spin and orbital states of $La_{1.4}Sr_{1.6}Mn_2O_7$ was investigated by using the x-ray absorption spectroscopy (XAS) and the soft x-ray resonant scattering (SXRS) at Mn $L_{2,3}$-edge. The field induced spin reorientation transition was observed by SXRS. The polarization dependent analysis revealed that the AFM spin axis changes from out-of-plane to in-plane axis. Additionally, the orbital states were determined from the polarization dependent XAS and CI model calculation, where the orbital state were changed by cooling temperature and external magnetic field. Here, the orbital states of low temperature ferromagnetic and field induced ferromagnetic are identical. Finally, we discuss the magnetoelastic coupling including spin and orbital structure of $La_{1.4}Sr_{1.6}Mn_2O_7$.

12:15PM B17.00004 Optical Investigation on Collective Dynamics of Charge-Orbital Density Wave in Layered Manganites , JUN FUJIOKA, Multiferroics Project, ERATO, JST, YOSHIAKI IDA, Department of Applied Physics, University of Tokyo, YOUTAROU TAKAHASHI, NORIAKI KIDA, Multiferroics Project, ERATO, JST, RYO SHIMANO, Department of Physics, University of Tokyo, YOSHINORI TOKURA, Department of Applied Physics, University of Tokyo — We have investigated the broad band optical spectra on the layered manganites $R_{1-x}Sr_{1+x}MnO_4$ (R=Nd and La) to reveal the collective charge/orbital density wave dynamics by means of the terahertz time domain spectroscopy [1]. The collective charge/orbital density wave excitation is observed around 9 meV in the charge/orbital stripe phase, when the nominal e_g-electron filling (1-x) of Mn-ion is less than around 1/3. By contrast, such a collective mode almost vanishes at x=1/2, which is explained in terms of the enhanced Jahn-Teller interaction cooperative with the electron correlation effect.

[1] J. Fujioka *et al.*, Phys. Rev. B. **82**, 140409(R) (2010).

12:27PM B17.00005 Bilayer manganites: polarons in the midst of a metallic breakdown , MARK GOLDEN, FREEK MASSEE, SANNE DE JONG[1], YINGKAI HUANG, University of Amsterdam, ANDREW BOOTHROYD, D. PRABHAKARAN, University of Oxford, ROLF FOLLATH, ANDREI VARYKHALOV, HZB, LUC PATTHEY, MING SHI, PSI, JEROEN GOEDKOOP, University of Amsterdam — The exact nature of the low temperature electronic phase of the manganite materials family, and hence the origin of their colossal magnetoresistive (CMR) transition is still a flagship issue in emergent correlated matter research. By combining new photoemission and tunneling data, we show that in the bilayer (N=2) manganite $La_{2-2x}Sr_{1+2x}Mn_2O_7$ the lattice/spin/orbital polaronic degrees of freedom win out, all across the CMR region of the phase diagram. This means that the generic ground state is that of a system in which strong interactions result in vanishing coherent quasi–particle spectral weight at the Fermi level for all locations in k–space. The incoherence of the charge carriers offers a unifying explanation for the anomalous charge-carrier dynamics seen in transport, optics and electron spectroscopic data. The stacking number N is the key factor for true metallic behavior, as an intergrowth-driven breakdown of the polaronic domination to give a robust metal possessing a traditional Fermi surface is seen in the bilayer system.

[1]Now at SLAC

12:39PM B17.00006 Synthesis, Structure, and Physical Properties of $Ba_2Mn_2Sb_2O$ Single Crystals , JIANNENG LI, S. STADLER, A. KARKI, Y. XIONG, R. JIN, Louisiana State University — We have grown high-quality single crystals of $Ba_2Mn_2Sb_2O$, which possesses the hexagonal structure as determined by X-ray powder diffraction technique. The magnetic susceptibility (χ) is isotropic above $T_N \sim 60$ K, initially increasing with increasing temperature (T). After reaching the maximum at $T_{MAX} \sim 150$ K, χ decreases with increasing T and can be described by Curie-Weiss law with negative Curie-Weiss temperature. Below T_N, magnetic anisotropy is observed: χ_{ab} decreases sharply but χ_c increases with decreasing T, suggesting an antiferromagnetic type ordering at T_N. Interestingly, the temperature dependence of electrical resistivity along both *ab* plane and c direction changes from exponential dependence above T_{MAX} to logarithmic dependence below T_{MAX}, reflecting strong Kondo effect.

12:51PM B17.00007 Evaluating Born and local effective charges in nanoscale MnO[1] , Q.-C. SUN, X.S. XU, University of Tennessee, S.N. BAKER, A.D. CHRISTIANSON, Oak Ridge National Laboratory, J.L. MUSFELDT, University of Tennessee — Phonons are exquisitely sensitive to finite length scale effects in complex materials because they are intimately connected to charge, polarizability, and structure, and a quantitative analysis of their behavior can reveal microscopic aspects of chemical bonding. To investigate these effects in a model correlated oxide, we measured the infrared vibrational properties of 8 nm particles of MnO, compared the results with the analogous bulk material, and quantified the phonon confinement with a calculation of Born effective charge. Our analysis reveals that the Born effective charge decreases by ∼20% compared to the bulk material. This finding is important for understanding finite length scale effects in this simple binary oxide and the more complicated functional oxides that emanate from this parent compound.

[1]This work is supported by the U.S. DOE, the JDRD Program at UT, and the JIAM SEED funding at UT.

1:03PM B17.00008 Collective Phase Mode and the Role of lattice distortions at $T_N \sim T_C$ in XMn_2O_5 (X= Bi, Pr, Sm, Gd, Tb) , N.E. MASSA, LANAIS EFO-CEQUINOR, UNLP, La Plata, Argentina, A.F. GARCÍA FLORES, E. GRANADO, IFGW, UNICAMP, Campinas, Brazil, G.F.L. FABBRIS, G. DE M. AZEVEDO, LNLS, Campinas, Brazil, L. DEL CAMPO, D. DE SOUSA MENESES, P. ECHEGUT, CNRS-CEMHTI, Orleans, France , M.J. MARTÍNEZ-LOPE, J.A. ALONSO, ICMM-CSIC, Madrid, Spain — We report on detailed temperature dependent infrared reflectivity, Raman, local structure, and X-ray diffraction measurements of multiferroic XMn_2O_5 (X= Bi, Pr, Sm, Gd, Tb). While for $BiMn_2O_5$ there are weak but distinct spectroscopic changes that together with high resolution diffraction patterns suggest a lattice role at $T_N \sim T_C$, for the rare earth (R) replaced infrared spectra have as a main feature a broad band at meV energies in addition to progressive rotation of Mn-O polyhedra. That band, independent of the R^{3+} ion size and common to all, suggests hopping of carriers through fluctuations at a local scale. It partially condenses below 40 K, i.e., the collective electronic behavior changes from delocalized to one partially localized. We assimilate that condensate to a CDW-like phase mode. It might indicate induced orbital correlation of charge transfers between Mn sites.Frequency Raman phonon shifts are observed at T∼60 K, due to spin-phonon coupling, and at $T_N \sim T_C$. Below $T_N \sim T_C$ there is no a Raman soft mode that might be associated to a CDW amplitude mode.

1:15PM B17.00009 Korringa-like relaxation in A-site ordered manganites , S. SCHAILE, H.-A. KRUG VON NIDDA, A. LOIDL, J. DEISENHOFER, Experimentalphysik V, Center for Electronic Correlations and Magnetism, Institute for Physics, Augsburg University, D-86135 Augsburg, Germany, T. NAKAJIMA, Y. UEDA, Material Design and Characterization Laboratory, Institute for Solid State Physics, University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8581, J — Half doped manganites exhibiting charge- and orbital ordering transitions are paradigm materials for studying colossal magnetoresistance, the existence of ferroelectricity or Zener polaron-type features. We report on high-temperature electron spin resonance studies of A-site ordered and disordered ABaMn$_2$O$_6$ A =Y,Sm,La. We find a Korringa-like spin-relaxation above the charge-ordering transition and extending up to 1000 K in the A-site ordered antiferromagnetic systems A =Y,Sm, a unique feature for a truly metallic state not having been reported in manganites before. In agreement with the ESR intensity this finding suggests that the ESR signal stems from Mn^{4+} core spins which relax via the quasi-delocalized e_g electrons. In contrast in the disordered AFM and the ferromagnetic samples no Korringa relaxation is observed. Hence, the conductivity does not significantly influence the spin relaxation in those compounds.

1:27PM B17.00010 Magnetic order in $La_{1-x}Ca_xMnO_3$ nanopowder , CHETAN DHITAL, Boston College, CLARINA DELA CRUZ, High flux Isotope reactor, Oak Ridge Tennessee, KEFONG WANG, Boston College, Chestnut Hill, MA,02467, JUN-MING LIU, Nanjing University, ZHIFENG REN, STEPHEN WILSON, Boston College, Chestnut Hill, MA,02467 — Here we present neutron diffraction studies exploring the spin behavior in nanocrystalline $La_{1-x}Ca_xMnO_3$ (LCMO). Confinement effects and the influence of phase separation have long been key issues within the underlying electronic behavior of the manganites. The coexistence of competing electronic phases has been reported across length scales exceeding 100nm in bulk manganites in proximity of the first-order metal-to-insulator phase transition in their phase diagrams. When the grain size of manganite crystals approaches the size of intrinsically phase-separated domains, new magnetic phases can be stabilized and the resulting electronic behavior dramatically altered. In this talk, we present results from our recent investigations of the magnetism in LCMO samples whose grain-size has been reduced to the nanometer scale. Newly stabilized static spin order and its relevance to phase separation in this manganite system will be discussed.

1:39PM B17.00011 Density functional investigation of the spin frustration and the field-driven long-range ordering in the honeycomb lattice system $Bi_3Mn_4O_{12}(NO_3)$, JIA LIU, WON-JOON SON, MIKE WHANGBO, NCSU — $Bi_3Mn_4O_{12}(NO_3)$, consisting of the honeycomb lattices of Mn^{4+} (d^3) ions, has dominant antiferromagnetic interactions ($\theta_{CW} = -257$ K) but its spins do not order down to 0.4 K. However, applied magnetic fields induce a long-range magnetic order, which is believed to arise from the spin canting due to the Dzyaloshinskii-Moriya interaction. To explain these observations, we examined the spin exchanges between the Mn^{4+} ions (J_1, J_2, J_c) by DFT+U calculations and the preferred orientation of their spins by DFT+U+SOC calculations. The spin frustration is reproduced by U close to zero with $J_2/J_1 \approx 1/2$. The cause for the field-induced long-range magnetic ordering was explored on the basis of DFT+U+SOC calculations.

1:51PM B17.00012 New magnetic structures in novel and conventional manganites , AZIZ DAOUD-ALADINE, STFC Rutheford Appleton Laboratories, JUAN RODRÍGUEZ-CARVAJAL, CRISTIAN PERCA, LOREYNNE PINSARD-GAUDART — The determination of the magnetic structures of manganites has always been at the root of their fundamental understanding [1]. We studied the magnetic structures of half-doped charge ordered manganites that are either show the prototype [1] CE-type magnetic structure ($Pr_{1/2}Ca_{1/2}MnO_3$), or variants of this order ($YBaMn_2O_6$ [2] and $Pr_{0.6}Ca_{0.4}MnO_3$) with neutron diffraction. The study of $Pr_{1/2}Ca_{1/2}MnO_3$ (ILL, France) is the first ever done on a single crystal and it essentially confirms the pioneering picture [1], whereas the NPD studies of $YBaMn_2O_6$ [2] (PSI, Switzerland) and $Pr_{0.6}Ca_{0.4}MnO_3$ [3] (ISIS, UK), give two unprecedented results. The $YBaMn_2O_6$ magnetic structure corroborates the hotly debated ordering of Zener Polarons [4], and high resolution NPD data evidence a new spin reorientation transition around T$\sim$20K far below its TN$\sim 170K$ in $Pr_{0.6}Ca_{0.4}MnO_3$ [3] that has so far only been vaguely observed. We will discuss the consequences that these results have on the still hotly debated understanding of the connection between charge/orbital and spin orderings in the manganites. [1] Wollan, E.O. and Koehler, W.C. Rev. 100, 545 (1955) [2] A. Daoud-Aladine et al., Phys. Rev. Lett.: 101 166404 (2008) [3] A. Daoud-Aladine et al., unpublished [4] M. Coey Nature 430, 155-157 (8 July 2004)

2:03PM B17.00013 ABSTRACT WITHDRAWN –

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B18 GMAG DMP: Focus Session: Low D/Frustrated Magnetism - Quantum Magnetism D172

11:15AM B18.00001 Abelian and Non-Abelian Height Models , R. ZACH LAMBERTY, STEFANOS PAPANIKOLAOU, CHRIS HENLEY, Cornell University — We present Monte Carlo simulations on a new class of lattice models in which the degrees of freedom are elements of an abelian or non-abelian finite group G, placed on directed edges of a two-dimensional lattice. The group product around any plaquette is constrained to be the group identity, as in a discrete gauge model, but in contrast a "height model" only allows a certain subset of group elements to appear on edges. These models often realize a classical form of topological order, in that the ensemble breaks up into sectors labeled by loop products (group products taken around topologically non-trivial loops). Our implementation uses a non-local Monte Carlo update, whereby a pair of topological defects is created and later recombined after one diffuses; this allows the simulation to visit different topological sector. We measured two quantities as diagnostics of topological order (i) The relative probabilities of different sectors, which were found to converge to unity with increasing system size L. (ii) The probability distribution of the separation R of a defect pair, which should approach a constant (be deconfined). Both results show exponential decay as a function of L or R, as expected for a liquid-like phase having only topological order. As a check, we measured the same two quantities in a model equivalent to the 6-vertex model, known to be a critical state, and confirmed the algebraic decay in that case.

11:27AM B18.00002 Application of DFT+U for calculating magnetic parameters for manganese based molecular magnets , SHRUBA GANGOPADHYAY, NanoScience Technology Center, Department of Chemistry, University of Central Florida, Orlando, FL, 32826, ARTEM MASUNOV, NanoScience Technology Center, Department of Chemistry, Department of Physics, University of Central Florida, Orlando, FL, 32826 — Single-molecule magnets are promising materials for molecular spintronics and quantum computing applications. Two methods feasible to predict the exchange coupling parameters of molecular magnets, broken symmetry Density Functional Theory and DFT with empirical Hubbard U parameter (DFT+U). In this contribution we apply DFT+U to study magnetic coupling for two Mn12-based molecular magnetic wheel using Vanderbilt Ultrasoft Pseudopotential plane wave DFT method implemented in Quantum ESPRESSO. Unlike most previous studies, we adjust U parameters for both metal and ligand atoms using five dineuclear organometallics as the benchmarks. Our study finds antiparallel spin alignment of the weakly interacting fragments of Mn_{12}, while the magnetic coupling inside the fragments are much stronger, both are in agreement with experimental observations.

11:39AM B18.00003 ABSTRACT WITHDRAWN –

11:51AM B18.00004 DMRG Study of Anisotropic Triangular Heisenberg Lattice

, ANDREAS WEICHSELBAUM, Ludwig Maximilians University, Munich, Germany, STEVEN R. WHITE, UC Irvine, USA — The anisotropic antiferromagnetic two-dimensional triangular Heisenberg lattice for spin $1/2$ describes certain classes of transition-metal oxides (TMOs) and chalcogenides (TMCs) supported by experimental data. The understanding of the ground state properties of this frustrated system from a theoretical point of view, however, has remained an extraordinary challenge. In the model under consideration, quasi-one-dimensional Heisenberg chains of uniform intrachain coupling strength J interact with their neighboring chains via the triangular interchain coupling J'. By varying the anisotropy ratio $j = J'/J$ from $j = 0$ (decoupled Heisenberg chains) to $j = 1$ (uniform triangular lattice with finite Neel order like local magnetization), it was pointed out [1,2] that spin liquid properties up to remarkably high values of j of about 0.85 exist. We present in detail our results on the incommensurable correlations using DMRG with special care given to finite size effects. We argue that incommensurable correlations persist throughout the entire range of $j \in [0, 1]$.

[1] S. Yunoki et al., PRB 74, 014408 (2006).
[2] D. Heidarian et al., PRB 80, 012404 (2009).

12:03PM B18.00005 Interacting antikinks on a diamondback ladder I

, MAYRA TOVAR, KIRILL SHTENGEL, University of California at Riverside — Recently introduced "antikinks" are spin $1/2$ excitations of the Heisenberg antiferromagnet on a sawtooth lattice. The idea is that they mimic spinons of the kagome antiferromagnet. Antikinks are triangles of spins which are not in their ground state. Treating antikinks as free non- interacting particles (a good approximation for the sawtooth chain), their energy was found to be substantially reduced by delocalization. We study antikinks on a "diamondback" ladder in which all spins are shared between two triangles. Consequently, in a uniform case the concentration of antikinks becomes $1/4$ and they strongly interact, making such a model a much better approximation for the kagome case. We treat these effects perturbatively by allowing different Heisenberg couplings on the up- and downward oriented triangles, the two limiting cases being the sawtooth and uniform diamondback ladder. We find a non-monotonic, power-law decay of induced interactions between the antikinks with their separation. The consequences of these interactions will be discussed in this talk.

12:15PM B18.00006 Interacting antikinks on a diamondback ladder II

, KIRILL SHTENGEL, MAYRA TOVAR, UC Riverside — Recently introduced "antikinks" are spin $1/2$ excitations of the Heisenberg antiferromagnet on a sawtooth lattice [1]. The idea is that they mimic spinons of the kagome antiferromagnet. Antikinks are triangles of spins which are not in their ground state. Treating antikinks as free non-interacting particles (a good approximation for the sawtooth chain), their energy was found to be substantially reduced by delocalization [1]. We study antikinks on a "diamondback" ladder in which all spins are shared between two triangles. Consequently, in a uniform case the concentration of antikinks becomes $1/4$ and they strongly interact, making such a model a much better approximation for the kagome case. We treat these effects perturbatively by allowing different Heisenberg couplings on the up- and downward oriented triangles, the two limiting cases being the sawtooth and uniform diamondback ladder. We find a non-monotonic, power-law decay of induced interactions between the antikinks with their separation. The consequences of these interactions will be discussed in this talk.

[1] Z. Hao and O. Tchernyshyov, Phys. Rev. Lett. **103**, 187203 (2009)

12:27PM B18.00007 Partial Kondo screening in geometrically frustrated Kondo lattice systems

, YUKITOSHI MOTOME, KYOYA NAKAMIKAWA, University of Tokyo, YOUHEI YAMAJI, Rutgers University, MASAFUMI UDAGAWA, University of Tokyo — One of the most important concepts in Kondo lattice systems is competition between the Kondo coupling and the RKKY interaction. The competition leads to a quantum critical point between a magnetically-ordered state and a Fermi liquid state, and furthermore, it is the origin of novel phenomena around the quantum critical point, such as a non-Fermi liquid behavior and a superconductivity. To explore a new quantum phase resulting from the competition, we investigate the ground state of geometrically-frustrated Kondo lattice systems by employing a high-precision variational Monte Carlo simulation. We find that a partially-ordered state, in which a magnetic order and a Kondo spin singlet coexists, emerges between a magnetically-ordered state stabilized by the RKKY interaction and a Kondo spin liquid state stabilized by the Kondo coupling. We clarified that this new quantum phase is stabilized by quantum fluctuations as well as magnetic anisotropy, and that it is accompanied by a charge disproportionation. Ref. Y. Motome *et al.*, Phys. Rev. Lett. **105**, 036403 (2010).

12:39PM B18.00008 Study of SU(N) magnets on the cubic lattice[1]

, HAO SONG, MICHAEL HERMELE, Department of Physics, University of Colorado at Boulder — We consider a class of $SU(N)$ magnets that have the same spin on every lattice site, which is obtained as the completely antisymmetric tensor product of $m < N$ fundamental representations. These models, which can be realized in ultracold gases of alkaline earth atoms in optical lattice potentials, have the remarkable property that more than two spins must be combined to form a singlet. A recent study of this model on the square lattice in the large-N limit found a chiral spin liquid ground state with topological order. Inspired by this result, we have studied the three-dimensional version of this model, solving it on the cubic lattice in the large-N limit, which addresses the competition among a variety of non-magnetic states, including some with exotic order. We present results on the phase diagram as the fraction m/N is varied.

[1]This work is supported by the U.S. Department of Energy, under grant no. DE-SC0003910

12:51PM B18.00009 Trial wave function for the quantum Ising model at zero temperature

, JULIO F. FERNÁNDEZ, Universidad de Zaragoza, Spain — A trial wavefunction for the ground state of the transverse field Ising model is proposed. It is a product of pair wavefunctions, which is exact for up to three spins, and is amenable to Monte Carlo calculations. We study the phase transition that occurs at zero temperature as the transverse field varies. Results for the Ising ferromagnet and some spin-glass models will be given.

1:03PM B18.00010 Thermodynamics of deconfined bosonic spinons in two dimensions[1]

, VALERI KOTOV, University of Vermont, ANDERS SANDVIK, OLEG SUSHKOV, Boston University — We consider the quantum phase transition between a Neel antiferromagnet and a valence-bond solid (VBS) in a two-dimensional system of $S = 1/2$ spins. Assuming that the excitations of the critical ground state are linearly dispersing deconfined spinons obeying Bose statistics, we derive expressions for the specific heat and the magnetic susceptibility at low temperature T. Comparing with quantum Monte Carlo results for the J-Q model, which is a candidate for a deconfined Neel–VBS transition, we find excellent agreement, including a logarithmic correction in the susceptibility. In our treatment, this is a direct consequence of a confinement length scale $\Lambda \propto \xi^{1+a} \propto 1/T^{1+a}$, where ξ is the correlation length and $a > 0$ (with $a \approx 0.2$ in the model).
Reference: A. W. Sandvik, V. N. Kotov, and O. P. Sushkov, arXiv:1010.2522 (2010).

[1]AS is supported by NSF Grant No. DMR-0803510.

1:15PM B18.00011 Properties of Resonating-Valence-Bond Spin Liquids and Critical Dimer Models[1] , YING TANG, ANDERS W. SANDVIK, Boston University, CHRISTOPHER L. HENLEY, Cornell University — We use Monte Carlo simulations to study properties of resonating-valence-bond (RVB) spin liquid states for $s = 1/2$ spins on 2D square lattices. It is well known that the spin-spin correlations decay exponentially in these states, but we find that the four-spin (valence-bond-solid, VBS, type) correlations are critical [1]. We compare various properties of the RVB with those of the classical dimer model (CDM), i.e., the exact ground state wavefunction of the critical Rokhsar-Kivelson quantum dimer model. It is well known that the CDM maps to a height model with a gradient-squared elasticity governed by a stiffness constant K. We show that also the RVB has such an effective classical field theory description, namely its (i) four-spin (dimer) correlations (ii) probabilities of different winding number sectors, and (iii) separation of monomer defect pairs, are all consistent with the same value of K (which is higher than in the CDM, i.e., the RVB is closer to an ordered VBS state). In addition to the short-bond RVB we also consider systems with longer bonds, and again find consistency with the height-model description. We discuss implications of the critical fluctuations of the RVB states.

[1] Y. Tang, A. W. Sandvik, and C. L. Henley, arXiv:1010.6146.

[1]NSF No. DMR-0803510 (AWS) and DMR-1005466 (CLH)

1:27PM B18.00012 Quantum spin liquid in two-dimensional Kagome lattice spin-1/2 XY model with 4-site ring exchange[1] , LONG DANG, ROGER MELKO, University of Waterloo — We have studied the 2D Kagome lattice spin-1/2 XY model with 4-site exchange. The ground state properties are investigated within the framework of the Stochastic Series Expansion quantum Monte Carlo (QMC) technique. We have found a featureless insulating phase in the regime of large 4-site exchange interaction. This novel phase is a potential candidate for a the Z_2 quantum spin liquid phase proposed by Balents, Girvin and Fisher [Phys. Rev. B, **65**, 224412 (2002)] in a related model. Our efforts to characterize this phase using large-scale QMC simulations are also discussed.

[1]SHARCNET and NSERC of Canada

1:39PM B18.00013 Linear independence of nearest neighbor valence bond states on several 2D lattices[1] , JULIA WILDEBOER, ALEXANDER SEIDEL, Washington University in St. Louis — We show for several two-dimensional lattices that the spin-$1/2$ nearest neighbor valence bond states are linearly independent. To do so, we utilize and further develop a method recently introduced [1] for the kagome lattice. This method relies on the identification of an appropriate cell for the respective lattice, for which a certain local linear independence property can be demonstrated. Whenever this can be achieved, linear independence follows for arbitrarily large lattices that can be covered by such cells, for open or periodic boundary conditions. We report that this method is applicable to a number of 2D lattices including the kagome, honeycomb, square, pentagonal I and II, and the star lattice. Applications of general linear independence properties, such as the derivation of effective quantum dimer models, are discussed. Furthermore, motivated by a spin-$1/2$ Hamiltonian on the kagome lattice that has Anderson's resonating-valence-bond (RVB) spin liquid wave function(s) as ground state(s) [1], we mention possibilities to study the properties of this RVB wave function for the kagome and other frustrated lattices using Monte Carlo techniques. [1] A. Seidel, Phys. Rev. B **80,** 165131 (2009).

[1]This research was supported by the National Science Foundation under Grant No. DMR-0907793.

1:51PM B18.00014 Symmetry Fractionalization in Two Dimensions , HONG YAO, Department of Physics, University of California Berkeley, LIANG FU, Department of Physics, Harvard University, XIAO-LIANG QI, Department of Physics, Stanford University — Topologically ordered states are often characterized by topological properties, such as braiding statistics and fusion rules, of their excitations. However, excitations also carry symmetry quantum number, namely a representation of a symmetry group, when a topologically ordered state respects the symmetry. If an excitation's symmetry quantum number cannot be obtained from a finite integer number of fundamental constituents of the system, we propose to call such phenomena "symmetry fractionalization." We introduce a solvable SO(3) spin-rotational and time reversal invariant spin-1 model on the honeycomb and decorated honeycomb lattices. We show that the ground state is the equal-weight superposition of all valence loops, which we call "resonating valence loop" (RVL) state and which is a quantum spin liquid respecting all the symmetries of the model. Ends of broken loops are excitations with spin-$1/2$, which are deconfined spinons. Since spin-$1/2$ cannot be obtained from an integer numbers of spin-1, the system exhibits symmetry fractionalization (specifically the "SO(3) symmetry fractionalization"). Moreover, for time-reversal T, a spinon has $T^2 =$ -1, while integer spins have $T^2 = +1$. Consequently, the system also has "time-reversal fractionalization."

2:03PM B18.00015 Defect-driven phase transitions out of the Coulomb phase , HYEJIN JU, UCSB, SIMON TREBST, Microsoft Station Q, UCSB, CHRISTOPHER HENLEY, Cornell University — Lattice models constrained by a local "conservation law," such as close-packed dimer models on 3D bipartite lattices, exhibit an emergent "Coulomb phase" with characteristic power-law correlations. We have studied, by Monte Carlo simulations, phase transitions out of the Coulomb phase induced by introducing a finite fugacity of defect excitations in dimer models. We report two cases. (1) In the simple cubic dimer covering, we admit non- bipartite dimers (connecting sites in the same sublattice), which appear as effective charges with Coulomb-like interactions. Non- bipartite defects induce a transition immediately out of the Coulomb phase, exponentially damping the critical correlations via Debye screening. We characterize this transition by extracting the screening length from our numerical calculation of the dimer structure factor.(2) In the diamond lattice, we initially restrict the dimers to a 2D layer forming a (bipartite) honeycomb lattice, and then admit interlayer dimers. These bipartite dimers appear as dipoles and do not destroy the Coulomb phase, but induce an immediate transition from a 2D to 3D Coulomb phase.

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B19 GMAG DMP: Focus Session: Spin Transport & Magnetization Dynamics in Metals II D170

11:15AM B19.00001 Effects of disorder on magnetic vortex dynamics[1]

, HONGKI MIN, Condensed Matter Theory Center, Department of Physics, University of Maryland — Experimental measurements of domain wall propagation are typically interpreted by comparison to reduced models that ignore both the effects of disorder and the internal dynamics of the domain wall structure. Using micromagnetic simulations, first we study vortex wall propagation in magnetic nanowires induced by fields or currents in the presence of disorder. We show that the disorder leads to increases and decreases in the domain wall velocity depending on the conditions. These results can be understood in terms of an effective damping that increases as disorder increases. As a domain wall moves through disorder, internal degrees of freedom get excited, increasing the energy dissipation rate [1]. Next we study the effect of disorder on vortex gyration in a magnetic disc. A vortex gyrating in a magnetic disc has two regimes of motion in the presence of disorder. At large gyration amplitudes, the vortex core moves quasi-freely through the disorder potential. As the amplitude decreases, the core can become pinned at a particular point in the potential and precess with a significantly increased frequency. In the pinned regime, the amplitude of the gyration decreases more rapidly than it does at larger precession amplitudes in the quasi-free regime. In part, this decreased decay time is due to an increase in the effective damping constant and in part due to geometric distortion of the vortex. A simple model with a single pinning potential illustrates these two contributions [2].

[1] Hongki Min, Robert D. McMichael, Michael J. Donahue, Jacques Miltat, and M. D. Stiles, Phys. Rev. Lett. **104**, 217201 (2010).
[2] Hongki Min, Robert D. McMichael, Jacques Miltat, and M. D. Stiles (unpublished).

[1]This work has been supported in part by the NIST-CNST/UMD-NanoCenter Cooperative Agreement.

11:51AM B19.00002 Spin-torque-driven excitations in magnetic thin films[1]

, C. WANG, H. SEINIGE, T. STAUDACHER, M. TSOI, Physics Department, University of Texas at Austin — Spin transfer torque (STT) refers to a novel method to control and manipulate magnetic moments using an electrical current. For the past decade it has proven to be a fascinating domain of research with a number of manifestations in various systems interesting both from fundamental science's point of view as well as for technological applications. In ferromagnetic/nonmagnetic (F/N) multilayers a dc electrical current can switch and/or drive its constituent F parts into high-frequency precession which is of interest for microwave and magnetic recording technologies. Interestingly, application of high-frequency currents can also drive the multilayer, e.g., into ferromagnetic resonance (STT-FMR) precession. In our experiments we use point contacts to inject high microwave currents into a variety of magnetic thin films including NiFe/Cu/NiFe/IrMn and NiFe/Cu/Co spin valves, and single ferromagnetic (NiFe or Co) films. The resulting magnetodynamics are detected electrically when a small rectified dc voltage appears across the contact at resonance. We find that in addition to a standard FMR, the microwave currents can excite other resonance modes in our point contacts. We study the behavior of the excitations as a function of applied magnetic field, dc bias current, and microwave frequency.

[1]Supported in part by NSF grants DMR-06-45377

12:03PM B19.00003 Minimization of Ohmic losses for domain wall motion in ferromagnetic nanowires[1]

, ARTEM ABANOV, OLEG TRETIAKOV, YANG LIU, Texas A&M University — We study current-induced domain-wall motion in a narrow ferromagnetic wire. We propose a way to move domain walls with a resonant time-dependent current which dramatically decreases the Ohmic losses in the wire and allows driving of the domain wall with higher speed without burning the wire. For any domain wall velocity we find the time-dependence of the current needed to minimize the Ohmic losses. Below a critical domain-wall velocity specified by the parameters of the wire the minimal Ohmic losses are achieved by dc current. Furthermore, we identify the wire parameters for which the losses reduction from its dc value is the most dramatic.

[1]This work was supported by the NSF Grant No. 0757992 and Welch Foundation (A-1678).

12:15PM B19.00004 Equilibration in All-Perpendicular Spin Valves Subject to Short Current Pulses *

, DANIEL BEDAU, HUANLONG LIU, JONATHAN SUN, JORDAN KATINE, ERIC FULLERTON, STEPHANE MANGIN, ANDREW KENT, NEW YORK UNIVERSITY, NEW YORK, NY TEAM, IBM T.J. WATSON RESEARCH CENTER, P.O.BOX218 NY TEAM, HITACHI-GST, SAN JOSE, CA TEAM, UNIVERSITY OF CALIFORNIA,SAN DIEGO,CA TEAM, NANCY-UNIVERSITY, NANCY, FRANCE TEAM — Our recent experiments have shown that all-perpendicular spin valves can be switched by short current pulses (<5 ns) [1]. In this limit we found that the switching probability only depends on the spin-angular momentum in the pulse [1]. However, such studies do not directly resolve the magnetization dynamics and relaxation. To study equilibration of spin valves driven out of equilibrium by short current pulse we have developed a pump-probe method, capable of 50 ps resolution. A probe pulse, a variable delay after the pump pulse, is used to determine the magnetization relaxation rate. When the delay between the pump and probe pulses is less than 1 ns the net switching probability differs from that at longer delays. An analysis of this difference shows that the free layer angular-momentum decays exponentially with time after the pump pulse. From these studies we obtain a lifetime, which we use to estimate the free layer damping. [1] Bedau et. al. Appl. Phys. Lett. 96, 022514 (2010) & ArXiv:1009.5240 *supported by: USARO Grant No. W911NF0710643

12:27PM B19.00005 Enhanced magnetization drift velocity and current polarization in $(CoFe)_{1-x}Ge_x$ alloys[1]

, ROBERT MCMICHAEL, NIST, MENG ZHU[2], NIST and Maryland Nanocenter, BRIAN SOE, NIST and Harvey Mudd College, MATT CAREY, STEFAN MAAT, JEFF CHILDRESS, Hitachi Global Storage Technologies — We present measurements of current spin polarization and magnetization drift velocity in $(CoFe)_{1-x}Ge_x$ alloys ($x \leq 0 \leq 0.3$), using a spin wave Doppler technique where spin wave transmission is measured between fixed-wavevector antennas coupled to current-carrying wires [1,2]. In a current density J, the transmission resonance frequency is shifted by $\Delta f = kv/2\pi$, where $v = Jg\mu_B P/(2eM_s)$ is a magnetization drift velocity. Measurement of Δf allows calculation of v and current spin polarization P. With increasing Ge concentration, v increases dramatically from (3.1 $\pm$ 0.2) m/s for CoFe to (8.2 $\pm$ 0.6) m/s for $(CoFe)_{0.7}Ge_{0.3}$ ($J = 10^{11}$ A/m^2). We attribute this increase in drift velocity primarily to decreased magnetization. The current polarization increases from 0.84 $\pm$ 0.04 for CoFe and reaches a maximum of 0.95 $\pm$ 0.05 at approximately 25% Ge.

[1] V. Vlaminck and M. Bailleul, Science, 322, 410 (2008)
[2] M. Zhu, C. L. Dennis and R. D. McMichael, Phys. Rev. B. 81, 140407R (2010).

[1]This work is supported in part by NIST-CNST/UMD-NanoCenter Cooperative Agreement and the National Science Foundation.
[2]Current affiliation: Seagate Technology

12:39PM B19.00006 Planar spin-transfer device with dynamical polarizer and analizer

, YAROSLAW BAZALIY, ANTON KRAVCHENKO — The behavior of the planar spin-transfer devices with monodomain magnetic layers can be described by the macrospin Landau-Lifshitz-Gilbert (LLG) equation with spin-transfer terms. The LLG description of a device with two layers is simplified after applying the overdamped, large easy-plane anisotropy approximation. A decrease of the magnetic layer thickness asymmetry creates a transition from the conventional polarizer-analizer ("fixed layer – free layer") operation regime to the regime of the nearly identical magnets. Here electric current leads to a "Slonczewski windmill" dynamic state, rather than producing the magnetic switching. The "windmill" precession state of a device with two free layers was investigated by numerical solution of the LLG equation.

12:51PM B19.00007 Optimal field sweep rate in magnetic switching of a single-domain particle , SHU YAN, YAROSLAW BAZALIY, University of South Carolina, ANDRZEJ STANKIEWICZ, NVE Corporation — The speed of magnetic switching is an important parameter of memory cells. We consider a magnetic moment with an easy axis anisotropy switched by an external field applied at a small angle to the axis. By solving the Landau-Lifshitz-Gilbert(LLG) equation numerically, it is found that the switching time of the magnet is not monotonically increasing with the field sweep rate of the applied field. The dependence has a minimum, i.e., there exists an optimal field sweep time. Analytic approximations are derived for the dependence of the switching time on the field sweep rate and for the value of the optimal field sweep time. Our results have important implications for the optimization of magnetic memory devices.

1:03PM B19.00008 Ballistic (precessional) contribution to the conventional magnetic switching[1] , ANDRZEJ STANKIEWICZ, NVE Corporation, YA. B. BAZALIY[2], SHU YAN, University of South Carolina — We consider a magnetic moment with an easy axis anisotropy energy, switched by an external field applied along the axis. Additional small constant bias field is applied perpendicular to the axis. It is found that the magnet's switching time is a non-monotonic function of the rate at which the field is swept from "up" to "down". Switching time exhibits a minimum at a particular optimal sweep time. This unusual behavior is explained by the admixture of a ballistic (precessional) rotation of the moment caused by the perpendicular bias field in the presence of a variable switching field. Analytic approximations are derived for the dependence of the switching time on the field sweep rate and for the value of the optimal field sweep time. The existence of the optimal field sweep time has important implications for the optimization of magnetic memory devices.

[1]supported by NSF DMR-0847159
[2]also at the Institute of Magnetism, Kyiv, Ukraine

1:15PM B19.00009 ABSTRACT WITHDRAWN –

1:27PM B19.00010 AC Magnetic Susceptibility and μSR Study of Spin Dynamics and the Onset of Magnetic Correlations in $LiHo_xY_{1-x}F_4$[1] , R.C. JOHNSON, Boston College, B.Z. MALKIN, Kazan Federal University, A. LASCIALFARI, Univ. of Milan, A. AMATO, C. BAINES, Paul Scherrer Institute, J.S. LORD, S.R. GIBLIN, Rutherford Appleton Laboratory, B. BARBARA, Néel Institute, M.J. GRAF, Boston College — The onset of correlation effects in the magnetic Ho^{3+}-subsystem in $LiHo_xY_{1-x}F_4$ single crystals is studied by comparing measurements and simulations of the field and frequency dependent magnetic AC susceptibility at 1.8 K and field and temperature dependent muon depolarization rates (μSR) for the concentrations x=0.0017, 0.0085, 0.041 and 0.0855. Specific features in the field and frequency dependence of in-phase and out-of-phase susceptibilities, in particular, broadening of peaks (dips) in χ' (χ") that indicate enhanced relaxation processes at field induced avoided level crossings, can be associated with x-dependent changes of cross relaxation rates and the phonon bottleneck effect in the spin-lattice relaxation. The observed peak in the measured temperature dependent muon relaxation rate appears to be related to a maximum at the frequency 60 cm^{-1} in the acoustic phonon density of states.

[1]Work supported by NSF grant DMR-0710525.

1:39PM B19.00011 Temperature dependence of the effective exchange and biquadratic coupling in ferromagnets: Calculation in the disordered local moment method , PAUL LARSON, KIRILL BELASHCHENKO, University of Nebraska — We have implemented the disordered local moment (CPA-DLM) method within the tight-binding linear muffin-tin orbital (LMTO) basis. This implementation self-consistently determines the angular distribution function of the generalized Heisenberg model and the angular-dependent local potentials in the symmetry-broken state; the CPA procedure involves numerical integration over the polar angle of the spin. We present benchmark calculations for several materials including Fe, Co, FePd, FePt, and CoPt. We further extract the temperature dependence of the effective exchange and biquadratic coupling parameters from the angular dependence of the single-site grand potential. We find that the effective exchange parameter in Fe is almost temperature-independent, while the biquadratic interaction is entirely negligible at all temperatures. In FePd the effective exchange varies noticeably as a function of temperature, while the biquadratic coupling is somewhat more pronounced but still relatively small.

1:51PM B19.00012 Effect of occupation numbers on exchange coupling in low dimensional magnetic nanostructures[1] , D. TERRADE, H. X. YANG, A. KALITSOV, L. NISTOR, M. CHSHIEV, B. DIENY, SPINTEC, CEA/CNRS/UJF, Grenoble, France — Interlayer exchange coupling (IEC) has been of great interest for spintronic community and has been shown directly related to equilibrium spin current (ESC). Here we present a study of the influence of the electronic occupation numbers on the angular dependence of the IEC in magnetic layered nanostructures with finite thickness ferromagnetic (FM) layers. The calculations were performed within the tight-binding model using the nonequilibrium Green function technique both within perturbation theory and exact diagonalization approaches. We found that the period of IEC oscillations as a function of FM layer thickness has nonmonotonic variation with electronic states occupation numbers (Fermi level position). In the limit of 2-site model it is found that perturbation theory fails to describe correctly exchange coupling angular dependence always giving sinusoidal behavior for the ESC while the exact solution alternates between sinusoidal and strongly nonsinusoidal behavior as a number of electrons in the system is varied.

[1]This work was supported by Nanosciences Foundation, Grenoble, France.

2:03PM B19.00013 Spin and phase coherence times in lithographically defined bismuth wires , MARTIN RUDOLPH, J.J. HEREMANS, Virginia Tech — We performed low temperature magnetotransport measurements on lithographically defined semimetal thin film bismuth wires and used the weak-antilocalization effect to determine spin and phase coherence times. Purpose-made Bi mesoscopic structures have not been extensively studied, yet are of interest due to the strong spin-orbit coupling in the material and its surface states. The spin and phase coherence times in mesoscopic Bi wires are here studied as function of temperature and wire width. The phase coherence time saturates at temperatures below 2 K, and appears limited by electron-phonon interactions above 2 K. The spin coherence time shows a dependence on width unexpected in Bi thin films. The spin coherence time increases as the width is reduced, similar to the dependence observed in wires fabricated on spin-orbit coupled semiconductor two-dimensional systems. The similarity may be an indication that the weak-antilocalization signature is dominated by two-dimensional strongly spin-orbit coupled Bi surface states (DOE DE-FG02-08ER46532).

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B20 FIAP/DMP GERA/DCOMP: Focus Session: Physics of Energy Storage Materials II – Anodes and Capacitors D168

11:15AM B20.00001 Anode-electrolyte double-layer of Li-ion batteries: Structure and Li-ion intercalation[1] , DAVID O. WIPF, Department of Chemistry, Mississippi State University, IBRAHIM ABOU HAMAD, PER ARNE RIKVOLD, Department of Phsics, Florida State University, MARK A. NOVOTNY, Department of Phsics & Astronomy, Mississippi State University — The electrochemical double-layer structure plays an important role in Li-ion intercalation during charging of Li-ion batteries with a graphite anode. In our recent Molecular Dynamics studies of a proposed accelerated charging method [I. Abou Hamad *et al.*, Phys. Chem. Chem. Phys. **12**, 2740-2743 (2010)], we notice that ethylene carbonate and propylene carbonate molecules of the electrolyte assemble themselves in a preferred orientation at the electrode-electrolyte interface. On the other hand, they are randomly oriented in the bulk electrolyte. We show that the structure of the double layer is affected by the intercalating Li-ion: while the dipole moments of double-layer molecules far from the intercalating Li-ion point toward the graphite sheets of the anode, they point away from the intercalation site close to the intercalating Li-ion. This observation should contribute to a better understanding of the intercalation process.

[1]This work was supported in part by NSF Grant No. DMR-0802288

11:27AM B20.00002 High Throughput Computational Discovery of Intermetallic Anodes for Li Batteries[1] , SCOTT KIRKLIN, Northwestern University, CHRIS WOLVERTON — We have developed a framework to perform high-throughput computational screening of intermetallic compounds as candidates for Li battery anodes. We have used our method to calculate, from density functional theory (DFT), more than 5000 anode lithiation reactions, based on more than 100 intermetallic compounds. We have specifically focused on the 3d-transition metal silicides, nidtrides and phosphides. Given the set of DFT total energies for all compounds, the reaction path upon lithiation is predicted using the recently-developed grand canonical linear programming (GCLP) method. The anode performance is then characterized by the cell potential vs lithium metal, energy density and volume expansion. The accuracy of this approach is first validated for pure silicon, and then extended to binary intermetallic compounds. Based on the results of these calculations, future experimental study can be guided toward systems with promising thermodynamic properties.

[1]Center for Electrical Energy Storage, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

11:39AM B20.00003 Li and Si diffusion in Si anodes in Li-ion batteries: An *ab-initio* molecular-dynamics-based study , PRIYA JOHARI, VIVEK B. SHENOY, Division of Engineering, Brown University, Providence RI 02912, USA. — Several studies have been carried out in the past few years to understand the dynamics of Li diffusion in Si anodes of Li-ion batteries, however, most of these studies are restricted to the diffusion of a single Li atom in crystalline Si. While, it is well known that crystalline Si becomes amorphous on lithiation, this phenomenon has not been considered in previous computational work. Here, we report the results of molecular dynamics simulations that were carried out to study the diffusion of Li atoms in crystalline as well as amorphous Si for the LiSi phase. We have also analysed the dynamics of the Si atoms during lithiation to understand its role in stress generation/relaxation. We find that Li diffuses faster in amorphous Si as compared to crystalline Si, while the diffusivity of Si is around two orders of magnitude lesser than Li.

11:51AM B20.00004 Li-ion Battery Electrode Materials Design from First-Principles Calculations , KRISTIN PERSSON, Lawrence Berkeley National Laboratory — First-principles calculations can provide a powerful tool for investigating and optimizing electrode materials. While the strength of computations lies in the ability to control what is being calculated, the challenge is to ensure that the calculation is relevant for the physical processes that dominate the performance of the material. We will discuss this balance and show examples of how computations can aid in the design of current Li-ion rechargeable battery electrode materials by identifying and understanding the performance bottlenecks on the atomistic level. As the most commonly used anode in today's Li-ion batteries, graphite shows poor rate capability at lower temperatures, leading to over-potential and Li plating. Using first-principles calculations, coupled with a cluster expansion of Li interactions and kinetic Monte Carlo we were able to show that *intrinsic* Li diffusion in graphite can be very fast, providing guidance towards designing higher-rate carbonaceous anode materials. On the cathode side, we have studied the layered $Li(Ni_{1/3},Mn_{1/3},Co_{1/3})O_2$ material, which is an interesting candidate if Co is partially substituted by the cheaper Al. Li migration in this material is influenced by several factors such as Li slab space, cation ordering and interlayer mixing. We present ab initio calculations of Li diffusivity as a function of Al content and slab spacing in the layered material, which elucidates the intrinsic rate performance effect of the Al substitution in the bulk material.

12:27PM B20.00005 Crystalline-amorphous interfaces in Li-ion batteries[1] , MARIA K. CHAN, JEFFREY GREELEY, Argonne National Laboratory, CENTER FOR ELECTRICAL ENERGY STORAGE, DOE ENERGY FRONTIER RESEARCH CENTER COLLABORATION — Amorphous and crystalline materials are associated with fast ionic transport and long term structural stability, respectively, both desirable properties in lithium ion battery materials. It is therefore no surprise that amorphous-crystalline interfaces are ubiquitous in Li-ion batteries. Using first principles density functional theory (DFT), and primarily Si as an example, we study models of crystalline-amorphous interfaces in Li-ion batteries. We will discuss the structure of such an interface and its energetic and mechanical effects on lithium insertion, as well as the kinetics of Li ion transport near and across the interface. The mechanism of solid state amorphization will also be discussed.

[1]Work funded by Center for Electrical Energy Storage, DOE Energy Frontier Research Center

12:39PM B20.00006 Li Diffusion Characteristics and Energetics in TiO_2 , H. YILDIRIM, SUBRAMANIAN SANKARANARAYANAN, JEFF GREELEY, Argonne National Laboratory — We present the results of density functional theory-based calculations for the activation energies of Li diffusion in TiO_2 crystalline and amorphous structures. Additionally, molecular dynamics simulations using shell potential models are used to investigate the Li ion diffusion mechanisms for various titania morphology. The diffusion pathways and the corresponding energetics for each diffusion mechanism are further probed using the DFT-based Nudged Elastic Band Method. We will report the calculated diffusion energetics (MD and DFT) for each (Li-TiO_2) system and compare the atomic scale Li transport characteristics on crystalline and amorphous TiO_2 structures. We also discuss the effect of Li concentration on the diffusion energetics.

12:51PM B20.00007 Composite MnO2-Carbon Electrodes for High Energy Density Storage , BRAD CORSO, ISRAEL PEREZ, PHILIP COLLINS, Department of Physics and Astronomy, Univ. of California at Irvine, Irvine, CA 92697 — The development of batteries with ever higher power densities is challenged by fundamental materials limitations that might be solved with hybrid combinations of materials. For example, metal oxides with high lithium ion capacities lack the conductivity to be good battery anodes, but composites that add graphitic carbon can achieve both capacity and conductivity. In this case, fast interfacial electron transfer between the materials is critical to achieving high performance. Here, we describe an electrochemical synthesis that achieves precise, conformal MnO2 films on graphitic surfaces. Furthermore, by using single-walled nanotubes as the carbon support, we can control defect densities with single defect resolution. Charge-discharge cycling of these electrodes, combined with control over point defects, directly distinguishes the enhanced charge transfer of defects and illuminates the structure-function relationship in interfacial electron transfer. This research is supported by the NEES Energy Frontier Research Center of the U.S. DOE Office of Basic Energy Sciences (#DESC0001160).

1:03PM B20.00008 Charge-Driven Structural Transformation and Valence Versatility of Boron Sheets in Magnesium Borides[1] , YUFENG ZHAO, National Renewable Energy Laboratory, CHUNMEI BAN, QIANG XU, SUHUAI WEI, ANNE C. DILLON, NATIONAL RENEWABLE ENERGY LABORATORY TEAM — We show here that boron sheets exhibit highly versatile valence and the layered boron materials may hold the promise for a high energy-density magnesium-ion battery. Practically, boron is superior to previously known multi-valence materials, especially transition metal compounds, which are heavy, expensive, and often not benign. Based on Density Functional Theory simulations, we have predicted a series of stable magnesium borides MgBx with a broad range of stoichiometries, $2 < x \leq 16$, by removing magnesium atoms from MgB2. The layered boron structures are preserved through an in-plane topological transformation between the hexagonal lattice domains and triangular domains. The process can be reversibly switched as the charge transfer changes with Mg insertion/extraction. The mechanism of such a charge-driven transformation originates from the versatile valence state of boron in its planar form. The discovery of these new physical phenomena suggests the design of a high-capacity magnesium-boron battery.

[1]Funded by the U.S. Department of Energy under subcontract number DE-AC36-08GO28308 through: DOE Office of Energy Efficiency and Renewable Energy Office of the Vehicle Technologies Program.

1:15PM B20.00009 Nanostructured Mg Thin Film Electrodes for Mg-Air Batteries , TAHA DEMIRKAN, Department of Applied Science, University of Arkansas at Little Rock, Little Rock, AR 72204, WISAM KHUDHAYER, Department of Applied Science, Engineering Science and Systems, University of Arkansas at Little Rock, AR, 72204, FATIH CANSIZOGLU, TANSEL KARABACAK, Department of Applied Science, University of Arkansas at Little Rock, Little Rock, AR 72204 — Over the past decades, primary Mg-air batteries got the attention of several researchers due to their low cost, non-toxicity, and theoretically expected high terminal voltage and high specific capacity values. However, corrosion and formation of a passivation layer around the electrode have been among the major challenges resulting in low columbic efficiencies compared to theoretically expected values. In this study, we utilized a glancing angle deposition (GLAD) method for fabricating nanostructured Mg thin film electrodes with unique physical properties to overcome these problems. Electrodes were prepared using a thermal evaporation GLAD system. Magnesium coatings in various forms ranging from conventional dense thin films to highly porous nanoblades were prepared through the control of deposition angle from normal to oblique angles, respectively. We show that the properties of Mg-air batteries can be significantly improved using nanostructured Mg thin film electrodes and lead to enhanced terminal voltage and specific capacity values.

1:27PM B20.00010 1-pyrenecarboxylic acid Functionalization of Graphene: Effect on Capacitive Energy Storage , SUJOY GHOSH, RAKESH SHAH, Department of Physics, Southern Illinois University Carbondale, IL-62901, XIAOHONG AN, Department of Physics, Northeastern University, Boston, MA 02115, DINESH RAWAT, Department of Physics, Southern Illinois University Carbondale, IL-62901, SWASTIK KAR, Department of Physics, Northeastern University, Boston, MA 02115, SAIKAT TALAPATRA, Department of Physics, Southern Illinois University Carbondale, IL-62901, DEPARTMENT OF PHYSICS, SOUTHERN ILLINOIS UNIVERSITY CARBONDALE, IL-62901 COLLABORATION, DEPARTMENT OF PHYSICS, NORTHEASTERN UNIVERSITY, BOSTON, MA 02115 COLLABORATION — We will present a comparison of Electrolytic Double Layer Capacitance (EDLC) performance of membrane electrodes fabricated using pure and 1-pyrenecarboxylic acid (PCA)-functionalized graphene flakes. A significant increase in specific capacitance as well as energy and power density values in PCA graphene electrodes indicates that surface functionalization (that affects the hydrophilicity) of graphene-based materials is crucial for improving capacitive energy storage ability of these materials.

1:39PM B20.00011 Electrochemical Double Layer Capacitors Using Few Layers of Graphene Grown on Nickel Foil. , R. SHAH, U. PHILIPOSE, J.M. PEREZ, Department of Physics, University of North Texas, Denton, TX, 76203, S. TALAPATRA, Department of Physics, Southern Illinois University Carbondale, IL, 62901 — We report on the properties of Electrochemical Double Layer Capacitors (EDLCs) fabricated using few layers of graphene synthesized on Nickel (Ni) foil by Chemical Vapor Deposition (CVD). The graphene films were characterized by Raman spectroscopy and showed that the film comprised more than one layers of graphene. The capacitive behavior of the fabricated EDLCs was examined using cyclic voltammetry, constant current charge/discharge, and impedance spectroscopy. These measurements show that the charge storage phenomenon is non-Faradic in nature. The capacitance of graphene on Ni electrodes was then compared to blank Ni foil electrodes and it was found that the capacitance of graphene on Ni foil is substantially higher than the blank Ni foil electrode. These results show that the few layers of graphene film grown on Ni foil could be promising material to function as electrodes for electrochemical energy storage device applications.

1:51PM B20.00012 First-principles study of the structure of $RuO_2 \cdot x\mathbf{H_2O}$, FEI ZHOU, YONGDUO LIU, UCLA, MARK ASTA, UC Berkeley, VIDVUDS OZOLINS, UCLA — Hydrous ruthenia, $RuO_2 \cdot xH_2O$, is a high-performance electrode material for electrochemical supercapacitors. Two different structural models of hydrous ruthenia had been proposed. In one of them, hydrogen is incorporated in metal vacancies inside the oxide host (("bulk model"), while in the other model structural water associated with Ru-O occupies the region between rutile nanograins ("core + grain-boundary model"). We present a theoretical examination of the validity of the bulk model by optimizing hydrogen positions within RuO_2 with proton-compensated Ru vacancies using a combination of a systematic search algorithm based on electrostatics, database searching and density-functional theory calculations. We find that all the considered bulk model structures are unstable by $\sim 0.3 - 0.4$ eV per H_2O molecule with respect to phase separation into anhydrous RuO_2 and water. Structures with hydroxyl groups or aggregate H_2O are significantly lower in energy (though still unstable with respect to phase separation), demonstrating that the water prefers to agglomerate outside RuO_2. Our results strongly disfavor the bulk model with hydrogen inside RuO_2 and support the core+grain-boundary model of hydrous ruthenia.

2:03PM B20.00013 Ab initio study of the charge storage mechanism of ruthenium dioxide as an electrochemical ultracapacitor , YONGDUO LIU, FEI ZHOU, VIDVUDS OZOLINS, University of California, Los Angeles — The charge storage mechanisms of ruthenium dioxide were investigated by first principles calculations. Both H-injected bulk and H-adsorbed RuO2(110) surface have been studied in order to obtain a whole picture of the discharging process of ruthenium dioxide as a supercapacitor. We have predicted the crystal structure of ruthenium-oxy-hydroxide (ROOH). By ab-inito voltage calculations, we also found that the RuO2(110) surface is completely hydrated before the usual voltammagram measurements, which suggests that the redox reactions happen in deep layers and should be diffusion dominated processes.

Monday, March 21, 2011 11:15AM - 1:15PM –
Session B21 DCOMP: General Theory D161

11:15AM B21.00001 Optimization of Elastic Constant Values in Non-cubic Crystals using Computational Image Matching , MADELEINE MSALL, Bowdoin College, TIMOTHY HEAD, Abilene Christian University — Point excitation in ultrasound or heat pulse experiments excites non-equilibrium phonons that carry energy along the group velocity direction. Phonon images map the sharp boundaries between high and low flux regions, called caustics, which are directly related to folds in the acoustic wave surface. Computational simulations show that caustic positions are extremely sensitive to the values of the elastic constants. We explore methods of determining the elastic constants using image matching techniques. Given the dependence of single image features on a constellation of constants, there are many local minima encountered in the search. This talk will present quantifiable criteria for image matching in this context and discuss potential heuristic or stochastic methods to deal with the problem of local minima.

11:27AM B21.00002 Entropic sampling without windows[1] , RONALD DICKMAN, ANTÔNIO CUNHA-NETTO, UFMG — We describe an entropic sampling method that permits estimation of the number of configurations over the full range of energies, with dividing the latter into subsets or "windows." Our method involves progressive refinement of an initial approximation for the density of states, using a set of random walks that span the energy range. Applied to the two-dimensional Ising model the method yields the critical temperature to an accuracy of about 0.01%, and critical exponents to 0.5% or better. Predictions for system sizes $L = 10$ - 160, for the temperature of the specific heat maximum, and the specific heat at the critical temperature, are in very good agreement with exact results. The antiferromagnetic transition is well represented. Excellent results are also obtained for the three-dimensional Ising model (simple cubic lattice) and the lattice gas with nearest-neighbor exclusion. We observe that attempts to restrict the sampling to a subset of the full energy range lead to distortions in the density of states, even if the restriction is imposed in a smooth manner, rather than with a sharp barrier.

[1]We thank CNPq, Brazil for financial support.

11:39AM B21.00003 Nearly exact calculations of small atomic and molecular systems using explicilty correlated gaussians[1] , SERGIY BUBIN, KALMAN VARGA, Vanderbilt University, LUDWIK ADAMOWICZ, University of Arizona — We demonstrate how very precise (virtually exact) solutions of various quantum mechanical problems can be obtained using the variational method with explicitly correlated Gaussian basis functions (ECGFs). As examples we consider several benchmark systems, such as few-electron atoms and molecules, as well as Coulomb systems containing exotic particles. We also discuss the evaluation of relativistic corrections in the framework of ECGFs.

[1]This work has been partially supported by NSF

11:51AM B21.00004 Metallic Phase of Water Ice Predicted at Megabar Pressures[1] , BURKHARD MILITZER, HUGH WILSON, University of California, Berkeley — We predict water ice to attain two new crystal structures with Pbca and Cmcm symmetry at 7.6 and 15.5 Mbar, respectively [Phys. Rev. Lett. 105 (2010) 195701]. With density functional calculations, we analyze the structural and electronic properties of these phases at zero temperature. The Pbca phase, like the known high-pressure ice phases VII, VIII, X and Pbcm, is insulating and consists of two interpenetrating hydrogen bonded networks, but the Cmcm phase is metallic and consists of corrugated sheets of H and O atoms. The H atoms are squeezed into octahedral positions between next-nearest O atoms while they occupy tetrahedral positions between nearest O atoms in lower-pressure phases. Our predictions may be testable with ramp compression experiments that can reach megabar pressures at lower temperatures than conventional shock wave experiments. The predicted insulator-to-metal transition would lead to an increase in reflectivity that can be measured with spectroscopic techniques.

[1]Supported by NSF and NASA.

12:03PM B21.00005 Supersymmetric Quantum Mechanics in Multiple Dimensions Applied to Variational Monte Carlo - A Proof of Principle Study[1] , THOMAS MARKOVICH, KAUSHIK MAJI, ERIC BITTNER, DON KOURI, University of Houston — We present a new approach to variational monte carlo using our N-Dimensional generalization of Supersymmetric Quantum Mechanics. We do this by introducing a *vector* superpotential in an orthogonal hyperspace. In the case of N distinguishable particles in three dimensions this results in a vector superpotential with $3N$ orthogonal components. The original scalar Schrödinger operator can be factored into vector "charge" operators: $\vec{Q}_1$ and $\vec{Q}_1^\dagger$. Using these operators, we can write the original (scalar) Hamiltonian as $H_1 = \vec{Q}_1^\dagger \cdot \vec{Q}_1 + E_0^{(1)}$. The second sector Hamiltonian is a tensor given by $H_2 = \vec{Q}_1 \vec{Q}_1^\dagger + E_0^{(1)}$ and is isospectral with H_1. The vector ground state of sector two, $\vec{\psi}_0^{(2)}$, can be used with the charge operator $\vec{Q}_1^\dagger$ to obtain the excited state wave functions of the first sector. We demonstrate the approach with examples of a pair of separable 1D harmonic oscillators and the example of a non-separable 2D anharmonic oscillator (or equivalently a pair of coupled 1D oscillators).

[1]Supported by R.A. Welch Foundation Grant E-0608.

12:15PM B21.00006 Electromagnetic and gravitational signatures of black hole and neutron star mergers , STEVEN LIEBLING, Long Island University — Astrophysical binary systems composed of some combination of compact objects (black holes(BH) and neutron stars(NS)) are extremely interesting dynamical systems. Such systems are generally extremely good radiators of gravitational waves, and, in at least some cases, they should be excellent electromagnetic sources. As such, they hold great promise for concurrent detection from both recently completed gravitational wave observatories and from conventional telescopes. I describe recent results achieved with a fully relativistic adaptive code for the merger of BH-BH, BH-NS, and NS-NS systems with magnetic fields.

12:27PM B21.00007 Quantification of Partially Ordered Sets with Application to Special Relativity , NEWSHAW BAHREYNI, KEVIN H. KNUTH, Department of Physics, University at Albany, Albany NY — A partially ordered set is a set of elements ordered by a binary ordering relation. We have shown that a subset of a partially ordered set can be quantified by projecting elements onto a pair of chains where the elements of each chain are quantified by real numbers. This results in a quantification based on pairs of real numbers (pair). Intervals, defined by pairs of elements, can be quantified similarly. A pair can be decomposed into a sum of a symmetric pair and an antisymmetric pair and mapped to a unique scalar which results in the Minkowskian form. Changing the basis of quantification from one pair of chains to another, under special conditions, leads to the generalized Lorentz transformation for pairs. We apply these results to a causally-ordered set of events by identifying a chain of events with an observer equipped with a clock in an inertial frame. We obtain the Minkowski metric of flat space-time as well as Lorentz transformations, which results in there being a maximum invariant speed. We find that the mathematics of special relativity arises from quantifying causal relationships among events, and requires neither the principle of relativity nor the fact that the speed of light is constant.

12:39PM B21.00008 Lunar Orbit Anomaly and GM=tc^3 Cosmology , LOUISE RIOFRIO, University of Houston Clear Lake — Studies of the Moon at Johnson Space Center have confirmed a large anomaly in lunar orbital distance, with possible applications to Relativity. Our Lunar Laser Ranging Experiment has reported the Moon's semimajor axis increasing at 3.82 ± .07 cm/yr, anomalously high. If the Moon were gaining angular momentum at this rate, it would have coincided with Earth less than 2 Gyr ago. The Mansfield sediment (Bills, Ray 2000) measures lunar recession at 2.9 ± 0.6 cm/yr. Additional observations independently measure a recession rate of 2.82 ± .08 cm/yr. LLRE differs from independent experiments by 10 sigma. A cosmology where speed of light c is related to time t by GM=tc^3 has been suggested to predict the redshifts of Type Ia supernovae, and a 4.507034% proportion of baryonic matter (Riofrio 2004). If c were changing in the amount predicted, lunar orbital distance would appear to increase by an additional 0.935 cm/yr. An anomaly in the lunar orbit may be precisely accounted for, shedding light on puzzles of "dark energy." In Planck units this may be summarised as M=R=t.

12:51PM B21.00009 On a Broken Formal Symmetry between Kinetic and Gravitational Energy

, ARMIN NIKKHAH SHIRAZI, University of Michigan — Historically, the discovery of symmetries has played an important role in the progress of our fundamental understanding of nature. This paper will demonstrate that there exists in Newtonian theory in a spherical gravitational field a formal symmetry between the kinetic (KE) and gravitational potential energy (GPE) of a test mass. Put differently, there exists a way of expressing GPE such that the form of the mathematical expression remains invariant under an interchange of KE and GPE. When extended to relativity by a suitable assumption, it leads to a framework that bridges the general relativistic and Newtonian conceptions of gravitational energy, even though the symmetry is broken except in the infinitesimal limit. Recognizing this symmetry at infinitesimal scales makes it possible to write a relativistic equation of an individual graviton, the properties of which under under one interpretation may be unexpected.

1:03PM B21.00010 The Relativistic Quantized Force: Newton's Second Law, Inertial and Gravitational; Generalization of Schwarzschild Metric for Strong and Weak Gravitational Field

, AZZAM ALMOSALLAMI, SCSR — In this paper we derived the relativistic Quantized force, where the force given as a function of frequency[1]. Where, in this paper we defined the relativistic momentum as a function of frequency equivalent to the energy held by a body, and time, and then the quantized force is given as the first derivative of the momentum with respect to time. Subsequently we introduce in section one Newton's second law as it is relativistic quantized, and in section two we introduce the relativistic quantized inertial force, and then the relativistic quantized gravitational force, and the quantized gravitational time dilation. At the end we shall generalize the Schwartzschild metric to describe the weak and strong gravitational field.

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B22 DCMP: Correlated Electrons Including "115" Materials D163

11:15AM B22.00001 Quantum critical point in $UCo_{1-x}Fe_xGe$[1]

, NORAVEE KANCHANAVATEE, KEVIN HUANG, JAMES HAMLIN, RYAN BAUMBACH, DIEGO ZOCCO, M. BRIAN MAPLE, Department of Physics, University of California, San Diego, La Jolla, California 92093, USA — We have carried out a comprehensive study of the $UCo_{1-x}Fe_xGe$ series across the entire range of compositions $0 \leq x \leq 1$, and report the results of x-ray diffraction, magnetization, specific heat, and electrical resistivity measurements to uncover the magnetic and superconducting phase diagram. Substitution of Fe into UCoGe initially results in an increase in the Curie temperature and a rapid destruction of the superconducting state. Near $x = 0.2$, the ferromagnetic transition is suppressed to zero temperature at an apparent quantum critical point, and the temperature dependences of the electrical resistivity and specific heat suggest non-Fermi liquid behavior.

[1]DOE: DE-FG02-04ER46105, NSF: DMR-0802478

11:27AM B22.00002 Non Fermi liquid properties of Ni-V close to the ferromagnetic quantum critical point[1]

, ALMUT SCHROEDER, SARA UBAID-KASSIS, BRENDAN WYATT, Kent State University, Kent OH, THOMAS VOJTA, Missouri University of Science and Technology, Rolla MO — Resistivity (ρ) and magnetization (M) data of the d-metal alloy $Ni_{1-x}V_x$ are presented in the vicinity of the critical vanadium concentration $x_c \approx 11\%$ where the onset of long-range ferromagnetic (FM) order is suppressed to zero temperature. Above x_c the temperature (T) dependence of the magnetic susceptibility is best described by simple nonuniversal power laws (e.g. $M/H(T,H\to 0) \sim T^{\alpha-1}$). Also the resistivity displays power laws ($\Delta\rho \sim T^n$). Both exponents α(x) and n(x) vary with x displaying signatures of a disordered quantum phase transition in a metal very different than of a clean 3D FM.

[1]Supported by NSF (DMR-0306766, DMR-0339147, DMR-0906566) OBR-440653 and Research Corporation.

11:39AM B22.00003 Non-Fermi Liquid behavior in Itinerant Ferromagnet, $HfMnGa_2$

, CARLOS MARQUES, Brookhaven National Laboratory and Department of Physics and Astronomy, Stony Brook University, YURI JANSSEN, Brookhaven National Laboratory, MOO SUNG KIM, Brookhaven National Laboratory and Department of Physics and Astronomy, Stony Brook University, LIUSUO WU, Department of Physics and Astronomy, Stony Brook University, MEIGAN ARONSON, Brookhaven National Laboratory and Department of Physics and Astronomy, Stony Brook University — Single crystals of $HfMnGa_2$, space group Pnma, were grown using a Ga self flux technique. A sharp peak in the AC susceptibility χ_{AC} shows a phase transition at $T_C \approx 26K$, followed by Curie-Weiss behavior at higher temperatures. Arrott plot analysis confirms this transition is ferromagnetic with a spontaneous moment of $\mu_0 \cong 0.3\mu_B$/Mn. $HfMnGa_2$ has a coercive field of ~ 0.1 T as well as a large magnetic anisotropy that restricts the moments to point in the [010] direction. Both a large Rhodes-Wohlfarth parameter $\mu_{\text{fluct}}/\mu_0 \cong 3.6$ and low T_C suggest $HfMnGa_2$ is comparable to other itinerant ferromagnets MnSi, $ZrZn_2$ and Ni_3Al. Resistivity $\rho(T)$ shows $HfMnGa_2$ to be metallic with $\rho(T) - \rho_0$ having a $T^{5/3}$ dependance in the ordered state. This non-Fermi liquid relationship was also observed in Ni_3Al and $ZrZn_2$ over a more limited range of temperatures.

11:51AM B22.00004 Electronic, magnetic and structural properties of $Cr_{1-x}V_xN$

, CAMILO QUINTELA, Department of Applied Physics, University of Santiago de Compostela, Spain, FRANCISCO RIVADULLA, Departament of Physical Chemistry, University of Santiago de Compostela, Spain, JOSE RIVAS, Department of Applied Physics, University of Santiago de Compostela, Spain — We report a systematic study on the electronic, magnetic and structural properties of stoichiometric and hole-doped CrN and present the magnetic and electronic phase diagram for the $Cr_{1-x}V_xN$ series. Stoichiometric CrN is a narrow gap, correlation-induced, semiconductor that orders antiferromagnetically below 286 K. The changes in the chemical bond associated to the magnetic order result in a non-activated behavior of the resistivity in the antiferromagnetic state, showing some similarities with other materials proposed to be itinerant-AF, like $CaCrO_3$. Doping this state with holes drives the system towards itinerant electron behavior through a series of inhomogeneous magnetic/electronic states. Given the chemical and structural simplicity of this system, it could provide an interesting place to study the evolution from an antiferromagnet with a non-thermally activated charge transport to a paramagnetic metal in a non-oxide material.

12:03PM B22.00005 Magnetic Correlations in Yb_4LiGe_4: A μSR and ^{7}Li NMR Study[1]

, S. DISSELER, M.J. GRAF, Boston College, P. CARRETTA, University of Pavia, S. PETER, Northwestern University, N. SVENSSON, Boston College, S.R. GIBLIN, Rutherford Appleton Lab, A. AMATO, C. BAINES, Paul Scherrer Institute — We present results from zero and longitudinal μSR and ^{7}Li NMR together along with magnetization and dynamic susceptibility on the multivalent, intermetallic compound Yb_4LiGe_4. A magnetic transition at 1.4K in dynamic susceptibility is observed, corresponding to a rapid increase in the quasi-static relaxation component of the ZF MuSR spectra. The strong magnetic field dependence exhibited in these measurements demonstrates a non-trivial criticality, and suggests a close relation to the quantum critical phenomenon observed in other Yb and Ce based systems. Based on support from NMR spectra, we discuss the potential of competing low temperature phases, and the importance of the spin fluctuations in describing the observed phenomena.

[1]This research was sponsored by NSF grant DMR-0710525.

12:15PM B22.00006 Low-temperature specific heat of $Nd_{1-x}Ca_xB_6$ single crystals[1] , JOLANTA STANKIEWICZ, MARCO EVANGELISTI, ICMA, CSIC-Universidad de Zaragoza, ZACHARY FISK, Department of Physics, University of California, Irvine — We measured the heat capacity on random alloys of $Nd_{1-x}Ca_xB_6$ ($x < 0.4$) in the 0.4 to 40 K temperature range. We calculated the lattice contribution to the specific heat, arising from the Debye-type phonons of the boron framework and Einstein-type oscillators of the cation sublattice. To this end, we used data obtained for the heat capacity of a LaB_6 single crystal which we measured in the same temperature range. Subtracting lattice and Schottky-type contributions from the measured heat capacity, we find that the electronic portion, linear in temperature, decreases sharply upon doping with Ca, most likely owed to changes in the Fermi surface.

[1]We acknowledge support from grant MAT2008/03074, of MICINN-Spain, and from grant NSF-DMR-0801253.

12:27PM B22.00007 High-pressure resistivity of $CeCoIn_5$ at low temperatures using four-point probe technique and finite element analysis[1] , NATHANIEL BRADY, GEORGIY TSOI, University of Alabama at Birmingham, TESFAYE GEBRE, National High Magnetic Field Lab, YOGESH VOHRA, DAVID HILTON, University of Alabama at Birmingham — We performed high-pressure electronic characterization of the heavy fermion superconductor, $CeCoIn_5$. Using a designer diamond anvil four-point probe system, we measured the temperature-dependent resistivity up to 25 GPa and found evidence for a decrease in the effective mass at high pressures. We determined the resistivity using Van Der Pauws method and a finite element analysis approach. Room temperature resistivity with increasing pressure was also measured and a maximum in resistivity was observed near $\sim$8 GPa. These data suggest the existence of a pressure-dependent modification of the $4f$ hybridization at the highest pressures

[1]Nathaniel Brady acknowledges support from the Department of Education Grant No. P200A090143.

12:39PM B22.00008 Exploring the antiferromagnetic superconducting phase in $CeCoIn_5$, ELIZABETH BLACKBURN, TED FORGAN, University of Birmingham, PINAKI DAS, MORTEN RING ESKILDSEN, University of Notre Dame, MARK LAVER, CHRISTOF NIEDERMAYER, JONATHAN WHITE, Paul Scherrer Institut, CEDOMIR PETROVIC, Brookhaven National Laboratory — $CeCoIn_5$ is a heavy fermion type-II superconductor showing clear signs of Pauli-limited superconductivity. $CeCoIn_5$ is also very close to a magnetically ordered ground state; this can be achieved by, for instance, doping with Cd. A variety of measurements give evidence for a transition at high magnetic fields inside the superconducting state, when the field is applied either parallel to or perpendicular to the c axis. In the latter case, antiferromagnetic order develops on the high-field side of the transition, with a magnetic wavevector of (q q 0.5), where $q = 0.44$ reciprocal lattice units [1]. We show that this order remains as the field is rotated out of the basal plane, but that the associated moment eventually disappears above 17°, indicating that anomalies seen with the field parallel to the c axis are not related to this magnetic order [2]. Our measurements emphasise the fragility of this magnetic order.

[1] M. Kenzelmann et al., Science 321, 1652 (2008).
[2] E. Blackburn et al., Phys. Rev. Lett. 105, 187001 (2010).

12:51PM B22.00009 Electronic inhomogeneity in heavy Fermions[1] , ZACHARY FISK, Department of Physics and Astromony, University of California, Irvine, Irvine, CA 92697, ERIC BAUER, YI-FENG YANG, Los Alamos National Laboratory, Los Alamos, NM 87545, CIGDEM CAPAN, Physics and Astronomy, Washington State University, PO Box 642814, Pullman, WA 99164-2814, FILIP RONNING, JOE THOMPSON, ROMAN MOVSHOVICH, Los Alamos National Laboratory, Los Alamos, NM 87545, ANDREA BIANCHI, Department de Physique, Universite de Montreal, Montreal H3C 3J7, RICARDO URBANO, National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32306, HIRONORI SAKAI, Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Ibarakai 319-1195 — The experimentally determined superconducting condensation energy of La-doped $CeCoIn_5$ is interpreted to show that the superconducting fraction decreases linearly with La concentration, consistent with the measured residual normal fraction seen in the electronic specific gamma remaining in the superconducting state as T $\rightarrow$ 0K. The In NQR data is also discussed. Our result points to an electronically inhomogeneous state that appears to be common to doped heavy Fermion materials near a quantum critical point.

[1]NSF-DMR-0801253

1:03PM B22.00010 Cooperative Intermediate Valence and Anomalous Stability of the Kondo Lattice in $Ce_{1-x}Yb_xCoIn_5$[*1] , R.E. BAUMBACH, L. SHU, M. JANOSCHEK, E. GONZALES, K. HUANG, T.A. SAYLES, J.J. HAMLIN, D.A. ZOCCO, C.A. MCELROY, M.B. MAPLE, University of California, San Diego, J. PAGLIONE, University of Maryland, P.-C. HO, California State University, Fresno, J.R. O'BRIEN, Quantum Design — We have investigated the chemical substitution series $Ce_{1-x}Yb_xCoIn_5$ ($0 \leq x \leq 1.0$) by means of X-ray diffraction, energy dispersive X-ray, specific heat, electrical resistivity, and magnetic susceptibility measurements. As Yb is substituted for Ce, the lattice constants remain roughly constant up to $x = 0.775$, contrary to Vegard's law, after which phase separation is observed for $0.8 \leq x < 1$. The superconducting transition temperature shows only a weak linear suppression with increasing x, while the coherence temperature remains constant up to $x = 0.775$. We also observe non-Fermi-liquid behavior for $0 \leq x \leq 0.775$ which is sensitive to the exact value of x, although there is no indication for a quantum critical point in the $T - x$ phase diagram. These results suggest that the Ce and Yb ions adopt cooperative intermediate valence states which preserve the Kondo lattice behavior and SC, while the associated valence fluctuations lead to strong modifications in the non-Fermi-liquid behavior as a function of x.

[1]Supported by grants U.S. DOE DE-FG02-04ER46105 and NSF 0802478.

1:15PM B22.00011 Scanning tunneling microscopy and spectroscopy measurements of heavy fermion compound $CeCoIn_5$[1] , EDUARDO DA SILVA NETO, PEGOR AYNAJIAN, COLIN PARKER, Princeton University, PAUL TOBASH, ERIC BAUER, Los Alamos National Laboratory, ALI YAZDANI, Princeton University — The heavy fermion compound $CeCoIn_5$ has a rich electronic phase diagram as a function of doping, pressure, and magnetic field. The interaction between Ce's f-electrons and the conduction bands is expected to form Kondo screening of the spins starting at relatively high temperatures. Below 2.3 K $CeCoIn_5$ is known to exhibit an unconventional superconducting ground state. We present scanning tunneling microscopy and spectroscopy (STM/S) as a function of temperature on $CeCoIn_5$. The in-situ cleaved samples show three different layer terminations. Acquiring structural information from STM topographies we identify the chemical character of each layer. STS measurements, on all surfaces, performed over a wide range of temperature show the rapid development of an energy gap in the tunneling density of states near the onset of coherence ($\sim$ 40 K). The origin of the observed energy gap and its relation to heavy band hybridization is addressed.

[1]Work primarily supported by DOE-BES. Infrastructure at Princeton Nanoscale Microscopy Laboratory also supported by NSF-DMR, NSF-MRSEC programme through PCCM, and the W. M. Keck foundation.

1:27PM B22.00012 Electron-spectroscopy of the heavy fermion alloy $Ce_{1-x}Yb_xCoIn_5$[1] , L. DUDY, J.W. ALLEN, University of Michigan, J. DENLINGER, Advanced Light Source, Lawrence Berkeley National Laboratory, L. SHU, M. JANOSCHEK, R.E. BAUMBACH, M.B. MAPLE, University of California, San Diego — $Ce_{1-x}Yb_xCoIn_5$ (YbCe115) is a new 115 alloy series with long range magnetic order suppressed in the whole substitution range. Measurements reveal a rich phase diagram in which the Kondo lattice is robust against Yb substitution, superconductivity persists to high values of x, and the non-Fermi-liquid behavior is enhanced by Yb substitution [1].We have characterized the electronic structure of this new alloy by x-ray and angle resolved photoemission spectroscopy (XPS and ARPES) performed at the Advanced Light Source (ALS). Yb 4f XPS spectra vary with increasing x from dominantly Yb^{3+} to a mix of Yb^{3+} and Yb^{2+}, in agreement with inferences from the magnetic susceptibility [1]. We will present ARPES data to show the x-dependence of the Fermi surface and discuss the relation of the electronic structure to the transport properties. The effect of surface contributions to the XPS and ARPES data will be assessed.

[1] Lei Shu et al, to be published

[1]Work supported by the U.S. Dept. of Energy under Contract No. DEFG02-07ER46379 at UM, DE-AC02-05CH11231 at the ALS and DEFG02-04ER46105 at UCSD.

1:39PM B22.00013 The Fermi surface of $CePt_2In_7$: a two-dimensional analog of $CeIn_3$, MOAZ ALTARAWNEH, MPA-CMMS. Los Alamos National Laboratory, NEIL HARRISON, ROSS MCDONALD, FEDOR BALAKIREV, CHARLES MIELKE, PAUL TOBASH, JIAN-XIN ZHU, JOE THOMPSON, FILIP RONNING, ERIC BAUER — We report magnetic quantum oscillations in magnetic fields extending to ∼60 T in single crystals of the body-centered tetragonal antiferromagnetic $CePt_2In_7$ recently discovered to exhibit pressure- induced superconductivity at T_c = 2.1 K. Despite two-dimensionality of its Fermi surface, the microscopic electronic properties of layered $CePt_2In_7$ are revealed to be more similar to cubic $CeIn_3$ than layered $CeRhIn_5$. A significant field-induced change in the Fermi surface occurs at H_m around 45 T in both $CePt_2In_7$ and $CeIn_3$, below which it is broken into small pockets with field-dependent effective masses -signaling 4f-electron involvement in the Fermi surface for $H < H_m$. Our findings suggest that $CePt_2In_7$ and $CeIn_3$ differ solely by the dimensionality of their Ce sublattices, thus realizing an ideal pair of compounds for investigating the effect of dimensionality on boosting superconductivity.

1:51PM B22.00014 Tuning the Quantum Critical Points in $CeCoIn_5$ and $CeRhIn_5$ Through Pt Doping: Synthesis, Single Crystal and Physical Property Studies , PAUL TOBASH, KRZYSZTOF GOFRYK, FILIP RONNING, JOE THOMPSON, Los Alamos National Laboratory, STANISLAV STOYKO, ARTHUR MAR, Department of Chemistry, University of Alberta, ERIC BAUER, Los Alamos National Laboratory — The well known $CeCoIn_5$ and $CeRhIn_5$ compounds provide an excellent opportunity for understanding the physics of heavy fermion superconductivity as well as quantum criticality in correlated electron intermetallics. Besides using hydrostatic pressure as a means to tune the physics of these materials, chemical doping has also proved essential for moving through the superconducting/magnetic boundary in these materials. We extend chemical substitution in $CeCoIn_5$ and $CeRhIn_5$ to another transition metal, Pt, and report on the synthesis, structure, and physical properties of single crystals of $CePt_xCo_{1-x}In_5$ and $CePt_xRh_{1-x}In_5$. Single crystal X-ray diffraction confirmed the tetragonal structure of both systems which crystallize with the $P4/mmm$ space group and are derivatives of the parent compounds $CeCoIn_5$ and $CeRhIn_5$, respectively. We report the physical property measurements, which include magnetic susceptibility, heat capacity, and electrical resistivity.

2:03PM B22.00015 Quantum criticality and Fermi surface topology in $CeRhIn_5$, H.Q. YUAN, L. JIAO, J.L. ZHANG, Department of Physics, Zhejiang University, Y. KOHAMA, M. JAIME, J. SINGLETON, E.D. BAUER, HAN-OH LEE, T. PARK, J.D. THOMPSON, Los Alamos National Laboratory — In the heavy fermion compound $CeRhIn_5$, superconductivity occurs upon partially suppressing the antiferromagnetic state via applying pressure. At the quantum critical point (p_c=2.3GPa), observations of a Fermi surface change from a small Fermi volume to a large one [1] seems to favor the scenario of local quantum criticality [2]. In this talk, we will present the first experimental evidence of a magnetic field induced quantum phase transition in $CeRhIn_5$ by measuring the ac specific heat and the de Hass van Alphen effect using the facilities of pulsed magnetic field at Los Alamos. The antiferromagnetic transition of $CeRhIn_5$ is eventually suppressed at a critical field of $H_c \simeq 50$ T. A dramatic change of the Fermi surface is found close to H_c, but still on the antiferromagnetic side. At sufficiently low temperatures, the Fermi surface in the antiferromagnetic state undergo a topological change from a small Fermi volume to a large one with increasing magnetic field, the latter being kept unchanged in the paramagnetic state at fields above H_c. These findings seem to support a different scenario for the field induced quantum phase transition in $CeRhIn_5$, e.g., the spin-density-wave-type quantum criticality. [1] H. Shishido et. al., J. Phys. Soc. Jpn. 74, 1103 (2005). [2] Q. Si et al., Nature 413, 804 (2001).

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B23 DCOMP DMP: Focus Session: Iron Based Superconductors – Electronic Structure, Theory and Spectroscopy D165

11:15AM B23.00001 Point contact spectroscopy (PCS) on the Fe122 pnictides and Fe11 chalcogenides , H.Z. ARHAM, C.R. HUNT, W.K. PARK, L.H. GREENE, U. Illinois, U-C, J. GILLETT, S. SEBASTIAN, U. Cambridge, Z.J. XU, J.S. WEN, Z.W. LIN, Q. LI, G. GU, BNL, A. THALER, S.L. BUDKO, P.C. CANFIELD, Ames Lab., ISU — We present PCS results on $Ba(Fe_{1-x}Co_x)_2As_2$ and $Fe_{1+y}Te$. The superconducting (S) crystals (x=0.08) show multigap like Andreev peaks. The non-S crystals (x=0.015, y=0.03) also show a conductance enhancement with split peaks at low temperatures (T). This conductance enhancement does not match with the bulk antiferromagnetic (AFM) transition T and survives up to 90 K for y=0.03 (T_N ∼69 K) and 130 K for x=0.015 (T_N ∼115 K). For the S samples in the coexisting regime (x=0.05 & 0.055), in addition to the Andreev peaks below T_C, a zero bias conductance enhancement develops and survives for ∼5K above T_C. PCS detects conductance changes due to quasiparticles scattering off charge or spin ordering. These conductance enhancements may arise from orbital ordering as detected by photoemission spectroscopy[1] and AFM ordering (Q-scattering), respectively.[2] [1]Yi et.al, arXiv:1011.0050. [2]Bobkova et.al, PRL 94, 037005 (2005). UIUC work supported by NSF-DMR-0706013, U.S. DOE Award No.DE-AC02-98CH10886, BNL work by DOE Award No.DE-AC0298CH10886, Cambridge work by EPSRC, Trinity College, the Royal Society, the Commonwealth Trust. Ames Lab operated by ISU under DOE Contract No.DE-AC02-07CH11358.

11:27AM B23.00002 Point Contact Andreev Reflection Studies on Iron Pnictide Superconductors[1] , XIAOHANG ZHANG, S.R. SAHA, N.P. BUTCH, K. KIRSHENBAUM, J. PAGLIONE, R.L. GREENE, I. TAKEUCHI, Center for Nanophysics and Advanced Materials (CNAM), University of Maryland, Y.-S. OH, Y. LIU, L.Q. YAN, K.-H. KIM, Seoul National University — We have systematically investigated the temperature, doping and the directional dependence of the gap structure for various types of single crystal iron pnictide superconductors by point contact Andreev reflection spectroscopy. Our studies were performed on highly transparent junctions evidenced by sharp and dramatic conductance enhancements at low temperatures. For the 122 family, despite some small features occasionally observed on the spectroscopy curves which may originate from the multiband superconductivity, a more conclusive characteristic of our obtained spectra is the presence of one predominant superconducting gap. By applying the BTK model, we find that the determined gap size scales well with the transition temperature, resulting in the $2\Delta/k_BT_C$ value of ~ 3.1 for both potassium doped and cobalt doped single crystals. Directional studies suggest that this gap is highly isotropic. Results on chalcogenide and nickel doped 122 superconductors will also be discussed. [X. H. Zhang et al., Phys. Rev. B 81, 024518 (2010)].

[1]Supported by CNAM and NSF DMR-0653535

11:39AM B23.00003 Point contact spectroscopy of Co-doped pnictide superconductors[1] , JOHN TIMMERWILKE, ALESSANDRA GALLASTEGUI, J.S. KIM, G.R. STEWART, AMLAN BISWAS, Department of Physics, University of Florida, Gainesville, Florida 32611, N.H. SUNG, M.S. KIM, B.K. CHO, School of Materials Science and Engineering, Gwangju Institute of Science and Technology (GIST), Gwangju 500-712, Korea — Iron pnictides are an interesting material for superconductivity research, since they provide a contrasting system for high temperature superconductivity to the cuprates. Point-contact spectroscopy is a unique method which has been used for investigating the density of states of cuprate superconductors and can help shed light on the pnictide superconductors as well. Point-contact measurements have an advantage over tunneling spectroscopy since they are less sensitive to sample surface quality and the dimensionless barrier parameter Z, can be varied with contact pressure. We have performed point contact measurements using an apparatus with a capacitive displacement sensor which enables us to systematically vary Z. We will present point contact spectra obtained on single crystal $Ba(Fe_{0.926}Co_{0.074)2}As_2$ samples and other cobalt doped iron pnictide samples at various temperatures, magnetic fields, and Z.

[1]NSF DMR-0804452, DE-FG02-86ER45268, KOSEF R15-2008-006-01002-0

11:51AM B23.00004 First-principles studies for understanding diverse high-T_c[1] , HAI-PING CHENG, University of Florida — In this talk, I survey results and insights gained from first-principles calculations on materials that exhibit superconducting behavior at temperatures higher than those characteristic of conventional BCS superconductors. These range from highly correlated cuprate Mott insulators as represented by the bismuth-strontium-calcium-copper-oxides (BSCCOs) to border-line itinerant-Mott systems such as the recently discovered 1111 and 122 pnictides. ultimate goal of our studies is to correlate T_c with specific material composition using detailed first-principles calculations in conjunction with many-body physics techniques via the critical step of constructing real-materials model Hamiltonians. By manipulating impurity doping, which plays a crucial role in the phase diagrams of high T_c materials, we hope to find guidance for designing candidate systems with T_c higher than ones currently known. BSCCO material, density functional calculations using a good generalized-gradient approximation (GGA) yield structural information that is correlated to the experimentally observed (STM) super-modulation and impurity peak in the high energy regime ($\sim$1 eV), even though the Kohn-Sham bands from such functionals fail to have a band gap. For FeAs-based high-T_c systems, DFT band-structure calculations provide a very good starting point for constructing model Hamiltonians for studies of spin fluctuation and electron pairing mechanisms. Fermi sheets that have been constructed using Wannier transformed Kohn-Sham states have provided critical information for understanding this family of superconducting materials. Analysis of the details of magnetic ordering, density of states, and 2D vs. 3D features in both the 1111 and 122 materials have been valuable in understanding sometimes perplexing experimental findings. Effects of Co impurities have been studied and fully analyzed as well., I will discuss persistent challenges related to calculations on the structure of the non-magnetic state $Ba_1Fe_2As_2$ system. Both further examination of the underlying physics and development of new approximate functionals are needed.

[1]Supported by DOE/BES and NSF/DMR, computed at NERSC and UF/HPC.

12:27PM B23.00005 Point-Contact Andreev Reflection Spectroscopy of Iron-Based Superconductors[1] , YI-TANG YEN, J.Y.T. WEI, University of Toronto and Canadian Institute for Advanced Research, S.R. SAHA, T. DRYE, K. KIRSHENBAUM, J. PAGLIONE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, RONGWEI HU*, C. PETROVIC, Brookhaven National Laboratory, K.W. YEH, M.K. WU, Institute of Physics, Academia Sinica, Taiwan — We carry out point-contact Andreev reflection spectroscopic studies at cryogenic temperatures on single crystals of Fe-chalcogenide and Fe-pnictide superconductors, including $FeS_{1-x}Te_x$, $FeSe_{1-x}Te_x$, $SrFe_{1.84}Pt_{0.16}As_2$ and $BaFe_{1.9}Pt_{0.1}As_2$. Our data are analyzed using current theoretical models involving multiband superconductivity. Further interpretations will be made in comparison with scanning tunneling spectroscopy measurements on Fe-chalcogenides and $NbSe_2$. *Present address: Ames Laboratory, Iowa State University

[1]Work supported by NSERC, CFI/OIT, Taiwan National Science Council, AFOSR-MURI Grant FA9550-09-1-0603, U.S. D.O.E. and Brookhaven Science Associates (No.DE-Ac02-98CH10886), and Center for Emergent Superconductivity

12:39PM B23.00006 Observation of multiple superconducting gaps in $Fe_{1+y}Se_xTe_{1-x}$ through Andreev reflection , DEBTANU DE, CARLOS DIAZ-PINTO, ZHENG WU, PEI-HERNG HOR, HAIBING PENG, Department of Physics and Texas Center for Superconductivity, University of Houston — Iron-based superconductors have been under intensive study because of the high transition temperature and the intriguing physical mechanisms involving the superconductivity and magnetic orders. Theoretical studies on the role of spin fluctuation suggest unconventional S wave pairing and multiple superconducting (SC) gaps due to the five disjoint Fermi surfaces. However, this multiple SC-gap scenario has yet to be confirmed in experiments. Here we report the experimental observation of five SC gaps in $Fe_{1+y}Se_xTe_{1-x}$ from Andreev reflection spectra, along with negative differential conductance dips due to the pair breaking related to the largest SC gap. The evolution of the multiple SC gaps is further investigated as a function of both temperature and magnetic field. For the largest SC gap, the Andreev reflection signal persists above bulk Tc, suggesting the existence of phase incoherent Cooper pairs.

12:51PM B23.00007 Scanning Tunneling Microscopy/Spectroscopy study on Optimally Potassium Doped Single Crystal $BaFe_2As_2$, JIHUA MA, Department of Physics and Texas Center for Superconductivity, University of Houston/Department of Physics, Boston College, ANG LI, Department of Physics and Texas Center for Superconductivity, University of Houston, CHENGLIN ZHANG, PENGCHENG DAI, Department of Physics and Astronomy, University of Tennessee, SHUHENG PAN, Department of Physics and Texas Center for Superconductivity, University of Houston — The iron pnictide parent compound material can be brought into superconducting state by chemical doping. It is worthwhile to study and compare the hole- and electron-doped iron pnictides. Among the well-known family of $AEFe_2As_2$ (AE=Ca, Sr, Ba), the scanning tunneling microscopy/spectroscopy study on hole-doped samples is insufficient. In this talk we will present high resolution STM/STS results on (001) surface of the optimally doped single crystal $Ba_{0.6}K_{0.4}Fe_2As_2$ (Tc$\sim$37K). With the data we will discuss the spatial variation of the superconducting energy gap.

1:03PM B23.00008 STM Studies on the Surface Structure of Ba122 iron pnictides cleaved at Low Temperature , ANG LI, Department of Physics and Texas Center for Superconductivity, University of Houston, JIHUA MA, Department of Physics and Texas Center for Superconductivity, University of Houston/Department of Physics, Boston College, A. SEFAT, M. MCGUIRE, B. SALES, D. MANDRUS, Oak Ridge National Laboratory, R. JIN, Department of Physics and Astronomy, Louisiana State University, CHENGLIN ZHANG, PENGCHENG DAI, Physics Department, University of Tennessee, SHUHENG PAN, Department of Physics and Texas Center for Superconductivity, University of Houston — We have performed scanning tunneling microscopy/spectroscopy (STM/STS) studies on electron- and hole-doped $BaFe_2As_2$ iron pnictides ($Ba(Fe_{1-x}Co_x)_2As_2$ and $Ba_{1-x}K_xFe_2As_2$). Two types of surface topography are always found when the samples are cleaved at low temperature. One has a square-like structure and the other shows a dimerization into rows. Details of these two surfaces, particularly at their boundaries, will be utilized to argue about the surface termination. We also show the impacts of these two surface structures and some topographic features on the tunneling spectrum.

1:15PM B23.00009 STM Studies of the Lattice Distortion at the Surface of $Ba(Fe_{1-x}Co_x)_2As_2$, SHUHENG PAN, ANG LI, Department of Physics and Texas Center for Superconductivity, University of Houston, JIHUA MA, Department of Physics and Texas Center for Superconductivity, University of Houston/Department of Physics, Boston College, A. SEFAT, M. MCGUIRE, B. SALES, D. MANDRUS, Oak Ridge National Laboratory, R. JIN, E. PLUMMER, Department of Physics and Astronomy, Louisiana State University — At low temperatures the bulk of the iron pnictides such as $Ba(Fe_{1-x}Co_x)_2As_2$ goes from an orthorhombic structure phase to the tetragonal phase with doping. This phase transition is also accompanied by a magnetic phase transition. These phenomena have been discussed in the context of the mechanism of superconductivity in the iron pnictides. With careful examination of our low temperature STM topographic images on the single crystals of $Ba(Fe_{1-x}Co_x)_2As_2$, we found thatthe lattice distortions of the two observed surface structures, namely "Root 2" and "1×2", evolve with doping concentration x across the superconducting dome. Starting from parent compound, the orthorhombic "Root 2" structure evolves towards rhombic, while the "1×2" structure evolves from rhombic to orthorhombic. We will discuss the implications of such doping dependent lattice distortion.

1:27PM B23.00010 Observation of multiple gaps and vortex bound states in Ba0.6K0.4Fe2As2 by Scanning Tunneling Microscopy/Spectroscopy , LEI SHAN, YONG-LEI WANG, BING SHEN, BIN ZENG, JING GONG, YAN HUANG, HUAN YANG, CONG REN, HAI-HU WEN, Institute of Physics and National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, Beijing 100190, China, ANG LI, SHUHENG PAN, Department of Physics and Texas Center for Superconductivity, University of Houston, Houston, Texas 77204-5002, USA, DA WANG, QIANG-HUA WANG, National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, China — We report on low-temperature scanning tunneling microscopy/spectroscopy studies of the electronic structure in single crystalline Ba0.6K0.4Fe2As2. Multiple superconducting gaps were observed in the density of states (DOS) and the sizes of the two dominant gaps are 7.6 meV and 3.3 meV, respectively. The flat bottom of the DOS spectra near zero bias indicates the nodeless feature of the gaps, while the global fitting to the spectra requires definitely the anisotropy. By applying magnetic fields, we observed ordered vortices with Andreev bound states in vortex cores. The bound states and their spatial evolution can be qualitatively explained by our numerical calculations when considering the multiband s-wave superconductivity.

1:39PM B23.00011 Quasiparticle Interference in Iron-Based Superconductors , JOHANNES KNOLLE, Max Planck Institute for the Physcis of Complex Systems, D-01187 Dresden, Germany, ALIREZA AKBARI, ILYA EREMIN, Ruhr-Universitat Bochum, D-44801 Bochum, Germany, RODERICH MOESSNER, Max Planck Institute for the Physcis of Complex Systems, D-01187 Dresden, Germany — The phase diagram of iron-based superconductors exhibits an anti ferromagnetic phase at low doping, an unconventional superconducting phase at larger carrier concentration, and possibly a coexistence regime of both orders in between. What are the signatures of the different orders in the electronic spectrum and how can phase sensitive measurements distinguish between different order parameter symmetries? To address these questions we systematically calculate quasiparticle interference (QPI) signatures for the relevant candidate phases of iron-based superconductors. Experimentally, QPI can be probed through spectroscopic imaging-scanning tunneling microscopy (SI-STM) thanks to impurities unavoidably present in the sample. We show that in the anti ferromagnetic phase the rotational symmetry of the electronic structure is broken, signatures of which are also seen in the coexistence regime with both superconducting and magnetic order. In the superconducting regime the different scattering behavior for magnetic and non-magnetic impurities allows us to verify the $s\pm$ symmetry of the order parameter. Furthermore, we discuss the effect of possible gap minima or nodes.

1:51PM B23.00012 Cryogenic Scanning Tunneling Spectroscopy of Superconducting Iron Chalcogenide Single Crystals[1] , J.Y.T. WEI, IGOR FRIDMAN, University of Toronto and Canadian Institute for Advanced Research, KUO-WEI YEH, MAW-KUEN WU, Institute of Physics, Academia Sinica,Taiwan, RONGWEI HU[2], C. PETROVIC, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory — We report scanning tunneling spectroscopy measurements on the iron-based superconductors of the "11" family including $Fe_{1-y}Te_{1-x}Se_x$ and $Fe_{1-y}Te_{1-x}S_x$. Conductance spectra and atomically-resolved images are obtained on single crystals down to 300 mK. A gap-like structure is observed, showing an asymmetric spectral background, non-trivial spatial variation and temperature dependence. We discuss our data in terms of possible gap anisotropy and doping inhomogeneities, and in relation to other recent spectroscopic measurements on iron-based superconductors.

[1]Work supported by NSERC, CFI/OIT, CIFAR, Taiwan National Science Council, U.S. DOE and Brookhaven Science Associates (No. DE-Ac02-98CH10886), and in part by the Center for Emergent Superconductivity, an Energy Frontier Research Center.

[2]Present address: Ames Laboratory and Iowa State University

2:03PM B23.00013 Surface lattice dynamics of the 122-type iron pnictides[1] , JING TENG, CHEN CHEN, GUORONG LI, AMAR KARKI, JIANDI ZHANG, RONGYING JIN, WARD PLUMMER, Louisiana State University — We present a systematic High Resolution Electron Energy Loss Spectra (HREELS) study of the surfaces lattice dynamics of the cleaved single crystals of the parent compounds AFe_2As_2 (A=Ba, Ca) as a function of temperature and sample treatment. The different phonon signatures on the competing surface reconstructions 1×2 phase and $(\sqrt{2}\times\sqrt{2})R45^\circ$ phase are studied. For Ba there are two optical phonon modes are observed at 18 and 29 meV, which can be identified as the A_{1g} and B_{1g} vibrations of the As and Fe atoms, respectively. A detailed discussion is given in terms of the interplay between the spin and lattice in this novel system

[1]Supported by NSF DMR-1002622.

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B24 DCOMP DMP: Focus Session: Multiscale Modeling - Methodology and applications D167

11:15AM B24.00001 Recent Advances in Accelerated Molecular Dynamics Methods[1] , ARTHUR VOTER, Los Alamos National Laboratory — Many important materials processes take place on time scales that vastly exceed the nanoseconds accessible to molecular dynamics simulation. Typically, this long-time dynamical evolution is characterized by a succession of thermally activated infrequent events involving defects in the material. Over the last 14 years, we have been developing a new class of methods, accelerated molecular dynamics, in which the known characteristics of infrequent-event systems are exploited to make reactive events take place more frequently, in a dynamically correct way. For certain processes, this approach has been remarkably successful, offering a view of complex dynamical evolution on time scales of microseconds, milliseconds, and sometimes beyond. Examples include metallic surface diffusion and growth, radiation damage annealing, and dynamics of nanotubes and nanoscale clusters. After an introduction to these methods, I will present some recent advances and results, and then describe the major ongoing challenges and our current thinking on how to overcome them.

[1]This research has been supported by DOE/BES, DOE/ASCR, DOE/SciDAC, and by the Los Alamos LDRD program.

11:51AM B24.00002 Multiscale (atomistic to mesoscopic) modeling of carbon nanotube materials[1] , LEONID ZHIGILEI, University of Virginia — A principal challenge in the development of computational models for investigation of collective dynamic phenomena in multi- component molecular systems or nanocomposites is presented by the gap between the atomistic description of the elementary structural units and the effective material behavior and properties. We approach this challenge through the development of computational models for dynamic simulations at intermediate (mesoscopic) length and time scales. An example of a mesoscopic model that is being currently designed in our group for carbon nanotube (CNT)-based materials and nanocomposites will be discussed in the presentation. The mesoscopic dynamic model for CNT materials is based on a coarse-grained representation of individual CNTs as chains of stretchable cylindrical segments [1] and a computationally- efficient "tubular potential" method describing the van der Waals interactions among the CNT segments [2]. Mesoscopic descriptions of CNT buckling and fracture are developed based on the results of atomistic simulations and incorporated into the model. Mesoscopic simulations performed for a system composed of randomly distributed and oriented CNTs predict a spontaneous self-assembly of CNTs into a continuous network of bundles with partial hexagonal ordering of CNTs within the bundles [2]. The structures produced in the simulations are similar to the structures of CNT films and mats observed in experiments. The first results illustrating the applications of the model for investigation of the response of CNT materials to dynamic mechanical loading, analysis of the structural dependence of the thermal transport properties [3] and gas permeability in CNT films will be briefly discussed in the presentation. Challenges and possible future directions in the development of a realistic mesoscopic description of nanocomposite materials will be outlined.

[1] L.V. Zhigilei, C. Wei, D. Srivastava, Phys. Rev. B 71, 165417, 2005.
[2] A.N. Volkov, L.V. Zhigilei, J. Phys. Chem. C 114, 5513, 2010; ACS Nano 4, 6187, 2010.
[3] A.N. Volkov, L.V. Zhigilei, Phys. Rev. Lett. 104, 215902, 2010.

[1]This work is supported by AFOSR (Grant No. FA9550-10-1-0545) and NSF (Grant No. CBET-1033919).

12:27PM B24.00003 Toward Distinct Element Method Simulations of Carbon Nanotube Systems[1] , EVGENIYA AKATYEVA, TYLER ANDERSON, ILIA NIKIFOROV, University of Minnesota, DAVID POTYONDY, Itasca Consulting Group, ROBERTO BALLARINI, TRAIAN DUMITRICA, University of Minnesota — We propose distinct element method modeling of carbon nanotube systems. The atomic-level description of an individual nanotube is coarse-grained into a chain of spherical elements that interact by parallel bonds located at their contacts. The spherical elements can lump multiple translational unit cells of the carbon nanotube and have both translational and rotational degrees of freedom. The discrete long ranged interaction between nanotubes is included in a van der Waals contact of nonmechanical nature that acts simultaneously with the parallel bonds. The created mesoscopic model is put into service by simulating a realistic carbon nanotube ring. The ring morphology arises from the energy balance stored in both parallel and van der Waals bonds.

[1]We thank NSF CAREER under Grant No. CMMI-0747684, NSF under Grant No. CMMI 0800896.

12:39PM B24.00004 Coarse-Grained Monte Carlo Simulations of Continuous Systems , XIAO LIU, WARREN SEIDER, TALID SINNO, University of Pennsylvania — Various types of Monte Carlo simulations are used extensively to simulate an enormous range of material properties. Restricting particle positions to fixed lattice sites can substantially increase the computational efficiency of a simulation, and this benefit increases as the lattice becomes coarser. However, the confinement of particle positions to a rigid lattice necessarily reduces the available configurational degrees of freedom in a system and this constraint can become very important at elevated temperatures. In this presentation, we discuss a new framework for performing Metropolis Monte Carlo and kinetic Monte Carlo (KMC) simulations of continuous systems on coarse, rigid lattices, while preserving the phase-space contributions of the missing degrees-of-freedom. The approach relies on the pre-computation of coarse-grained interaction potentials using equilibrium sampling of small systems. The coarse-grained simulation methodologies are shown to reproduce both equilibrium (e.g. phase diagram), and non-equilibrium (e.g. aggregation dynamics) features in the corresponding fully resolved systems. In the latter case, the coarse potential is used to compute rates for moves in a coarse-grained KMC system.

12:51PM B24.00005 Quantum-mechanical and QM/MM simulations of proton dissociation free energies in solution , NOAM BERNSTEIN, Naval Research Laboratory, CSILLA VARNAI, University of Cambridge, MONIKA FUXREITER, Hungarian Academy of Sciences, GÁBOR CSÁNYI, University of Cambridge — Chemical reactions often occur in the presence of a solvent, in particular water for biological systems. To describe such processes a quantum mechanical (QM) description of the reaction site is needed, combined with a large number of solvent molecules that affect the reaction via their electrostatic fields and free energy effects of their long-range structure. We have simulated the dissociation of a proton from the side chain of a tyrosine molecule, as a realistic model system. We compute a free energy difference, using umbrella integration, from the average restraint force as a function of O^{-}-H^{+} distance as the proton is transferred from the side-chain to nearby water molecules to form H_3O^{+}. We use a combination of periodic QM calculations using DFT and force-mixing QM/MM simulations implemented in QUIP and CP2K. The pure QM calculations are used for reference values and for determining appropriate restraint conditions for the free energy calculations. The force-mixing QM/MM method, which gives accurate forces throughout the system, is used to evaluate free energies for comparison with experiment. We extrapolate the free energy for the initial transfer of the proton to the bulk solvated proton regime by analytically computing electrostatic and entropy contributions.

1:03PM B24.00006 Understanding Vibrational Spectra of Silicon Nanocrystals , DUNDAR YILMAZ, CEM SEVIK, Texas A&M University, CEYHUN BULUTAY, Bilkent University, TAHIR CAGIN, Texas A&M University — After the discovery of light emission from porous Si, nanostructured Si became a promising material for opto-electronic applications. For two decades lots of both experimental and theoretical works done in order to understand mechanisms behind the interaction of light with low dimensional forms of Si. In this work we employed MD simulation technique. The simulation details are similar to our earlier work except we used Large Scale Atomistic Molecular Modeling Package Software (LAMMPS) with ReaxFF package as an integrator. We used constant pressure constant temperature (NPT) ensemble with a simulation box size around 4.2 nm. We inserted silicon nanocrystals into amorphous silicon dioxide matrix with diameter ranging from 2 nm to 3.2 nm using a scheme defined in our previous work7. We also simulated free standing hydrogen passivated nanocrystals with same diameters to compare effects of oxide matrix on the nanocrystals. The effect of strain on vibrational spectra of Silicon Nanocrystals is studied as a function of nanocrystal diameter using reactive molecular dynamics simulations technique for both embedded and hydrogen passivated nanocrystals. With use of refined parameters our calculations reproduce the redshift of the Raman active transverse optical peak of Si-Si vibrations with decreasing the nanocrystal size.

1:15PM B24.00007 *Ab initio* study of the *thermodynamic properties and the* phonon calculations of Zircon and Reidite , MRUNALKUMAR CHAUDHARI, JINCHENG DU, University of North texas — Zircon and Reidite are the polymorphs of Zirconium Silicate which find its importance geologically, because of its natural hosting to various radioactive elements in the crust of the earth. High permittivity also makes it a promising material for the gate dielectric material in metal-oxide semiconductors. Knowledge of the thermodynamic properties and the phonon based calculations is very critical to understand the high temperature and high pressure properties in order to consider its application as an effective natural storage for the radioactive wastes. These properties are thoroughly studied both computationally and experimentally for zircon, while significantly less attention was paid to reidite in the literature. The thermodynamic properties and phonon calculations of Zircon and Reidite were studied using ab initio based periodic density-functional theory (DFT) based calculations using the generalized gradient approximation (GGA). Various properties such as free energy, internal energy, entropy, heat capacity and thermal displacement as a function of temperature is calculated using the PHONON software. Various phonon based density of states and dispersion curves are calculated and compared with the experimental data. No first principles based computational results were reported up to now. Calculated bulk properties agree very well with the experimental data in the literature.

1:27PM B24.00008 One-dimensional model of interacting-step fluctuations on vicinal surfaces: Analytical formulas and kinetic Monte-Carlo simulations[1] , PAUL PATRONE, T.L. EINSTEIN, U. of Maryland, College Park, DIONISIOS MARGETIS, Math Dept., U. of Maryland, College Park — We study a 1+1D, stochastic, Burton-Cabrera-Frank (BCF) model of interacting steps fluctuating on a vicinal crystal. The step energy accounts for entropic and nearest-neighbor elastic-dipole interactions. Our goal is to formulate and validate a self-consistent mean-field (MF) formalism to approximately solve the system of coupled, nonlinear stochastic differential equations (SDEs) governing fluctuations in surface motion. We derive formulas for the time-dependent terrace width distribution (TWD) and its steady-state limit. By comparison with kinetic Monte-Carlo simulations, we show that our MF formalism improves upon models in which step interactions are linearized. We also indicate how fitting parameters of our steady state MF TWD may be used to determine the mass transport regime and step interaction energy of certain experimental systems.[2]

[1]PP and TLE supported by NSF MRSEC under Grant DMR 05-20471 at U. of Maryland; DM supported by NSF under Grant DMS 08-47587.
[2]P. Patrone, T. L. Einstein, D. Margetis, Phys. Rev. E, in press.

1:39PM B24.00009 Real-time visualization of excited-state dynamics in molecular chains[1] , YONGHUI LI, CARSTEN ULLRICH — Time-dependent density-functional theory allows one to calculate excitation energies and the associated transition densities in principle exactly. The transition density matrix (TDM) provides additional information on electron-hole localization and coherence of a specific excitation. We have extended the TDM concept into the real-time domain in order to visualize the excited-state dynamics in conjugated molecules. Our computational scheme is based on solving the time-dependent Kohn-Sham equations with the OCTOPUS code and then calculating the time-dependent Kohn-Sham TDM using a spatial partitioning scheme. The method is applied to show in real time how locally created electron-hole pairs spread out over neighboring conjugated molecular chains. The coupling mechanism, electron-hole coherence, and the possibility of charge separation are discussed.

[1]This work is supported by NSF Grants DMR-0553485 and DMR-1005651

1:51PM B24.00010 Thermal conductivity of bulk crystals from first-principles lattice dynamics[1] , KEIVAN ESFARJANI, MIT, JUNICHIRO SHIOMI, University of Tokyo, GANG CHEN, MIT — Based on first-principles density-functional calculations, we have developed and tested a force field for Silicon, which can be used for Molecular dynamics simulations and the calculation of its thermal properties. This force field uses the exact Taylor expansion of the total energy about the equilibrium positions up to 4th order. In this sense, it becomes systematically exact for small enough displacements, and can reproduce the thermodynamic properties of Si with high fidelity. Having the harmonic force constants, one can easily calculate the phonon spectrum of this system. The cubic force constants, on the other hand, will allow us to compute phonon lifetimes and scattering rates. Results on equilibrium Green-Kubo molecular dynamics simulations of thermal conductivity as well as an alternative calculation of the latter based on the relaxation-time approximation will be reported. The accuracy and ease of computation of the lattice thermal conductivity using these methods will be compared. Results on other non-trivial materials such as Heuslers will also be presented. This approach paves the way for the construction of accurate bulk interatomic potentials and force constants database, from which lattice dynamics and thermal properties can be calculated and used in larger scale simulation methods such as Monte Carlo.

[1]Support from the S3TEC center funded by DOE-EFRC, and JSPS Excellent Young Researchers Overseas Visit Program is acknowledged.

2:03PM B24.00011 Optimizing laser pulses for controlled excitation of materials and molecules[1] , ROLAND ALLEN, Texas A&M University — This talk extends the ideas of recent papers, including [1] Zhou et al., Phys. Rev. B 82, 075433 (2010); [2] Lin et al., J. Phys. Cond. Mat. 21, 485503 (2009); and [3] Allen, Phys. Rev. B 78, 064305 (2008). There are three basic points: (1) A combination of analytical models and density-functional-based simulations provides guidance for tailoring laser pulses to achieve optimum vibrational and electronic excitation. In [1] it was found that the maximum relative response of a specific vibrational mode with period T is achieved when the FWHM duration of a pulse is equal to 0.42 T, and later work by Jiang et al. provided a similar criterion for the duration and delay times in a series of pulses. (2) It is possible for microscopic (density-functional-based) simulations to provide input for larger-scale simulations, in the form of stresses etc. (as demonstrated in [2]) and excitation-dependent interatomic potentials. (3) It is possible to extend current techniques for simulations of the coupled dynamics of electrons, nuclei, and the radiation field in highly-excited materials, using for example nonequilbrium Green's functions.

[1]Work supported by Robert A. Welch Foundation, Grant A-0929.

Monday, March 21, 2011 11:15AM - 2:15PM –
Session B25 DCMP: Superconductivity: Spin properties, Structure and Dynamics D166

11:15AM B25.00001 Structure, spin-stripe order, and superconductivity in $La_{1.905}Ba_{0.095}CuO_4$ with and without 1% Zn substitution of Cu[1] , JINSHENG WEN, UC Berkeley/BNL, Z. XU, G. XU, Q. JIE, M. HUCKER, BNL, A. ZHELUDEV, W. TIAN, B. WINN, J. ZARESTKY, ORNL, D. SINGH, NCNR, T. HONG, ORNL, Q. LI, G. GU, J. TRANQUADA, BNL — We have performed susceptibility, thermal transport, and neutron scattering measurements to study the effect of Zn and magnetic field on the structure, spin-stripe order and superconductivity, and the interplay between them in $La_{1.905}Ba_{0.095}CuO_4$ with and without 1% Zn. It is shown that the bulk superconductivity is depressed by either the Zn doping or the magnetic field, spin stripe order is enhanced, and the structure is unaffected. For a range of magnetic field, the spin stripe order appears to stabilize a quasi-two-dimensional vortex glass phase.

[1]Supported by Office of Basic Energy Sciences, US DOE, under Contract No. DE-AC02-98CH10886.

11:27AM B25.00002 Electron-Spin Excitation Coupling in an Electron Doped Copper Oxide Superconductor Pr0.88LaCe0.12CuO4-δ[1] , JUN ZHAO, Department of Physics, University of California, Berkeley, FRANCIS C. NIESTEMSKI, SHANKAR KUNWAR, Department of Physics, Boston College, SHILIANG LI, Institute of Physics, Chinese Academy of Sciences, PAUL STEFFENS, ARNO HIESS, Institut Laue Langevin, Grenoble, France, HYE JUNG KANG, NIST Center for Neutron Research, STEPHEN D. WILSON, ZIQIANG WANG, Department of Physics, Boston College, PENGCHENG DAI, Department of Physics and Astronomy, The University of Tennessee, Knoxville, VIDYA MADHAVAN, Department of Physics, Boston College — We use polarized and unpolarized inelastic neutron scattering to study the magnetic excitations of the electron doped copper oxide superconductors Pr0.88LaCe0.12CuO4-δ (PLCCO, Tc =21 K, 24 K) over a wide energy range. We found the energy dependence of the imaginary part of the dynamic susceptibility displays two distinct energy scales in both samples. Interestingly, the STS measurements on the same samples reveal two modes that evolve with T_c in a similar manner as neutron modes. A comparison of the spatial and temperature dependence of the neutron and STS modes suggests that the low energy mode is associated with antiferromagnetism while the high energy mode is connected with superconductivity. These results suggest that spin excitations are the mediating glue for the electron pairing in PLCCO.

[1]J.Z is supported by a fellowship from the Miller Institute for Basic Research in Science

11:39AM B25.00003 Fluctuating stripes at the onset of the pseudogap in the high-Tc superconductor Bi2Sr2CaCu2O8+x[1] , COLIN PARKER, PEGOR AYNAJIAN, EDUARDO H. DA SILVA NETO, AAKASH PUSHP, Princeton University, SHIMPEI ONO, CRIEPI, Japan, JINSHENG WEN, ZHIJUN XU, GENDA GU, Brookhaven National Laboratory, ALI YAZDANI, Princeton University — A long standing question in high-T_c cuprates has been the interplay between pseudogap, which is generic to all hole-doped cuprates, and stripes, whose static form occurs in only one family of cuprates over a narrow range of the phase diagram. I will present new data [1] on the spatial reorganization of electronic states at the onset of the pseudogap state ($T*$) in the high-temperature superconductor $Bi_2Sr_2CaCu_2O_8 + x$ taken with a scanning tunneling microscope (STM). The onset of the pseudogap phase coincides with the appearance of electronic patterns whose doping and energy dependence has the predicted characteristics of fluctuating stripes. While demonstrating that the fluctuating stripes emerge with the onset of the pseudogap state and occur over a large part of the cuprate phase diagram, these experiments indicate that they are a consequence of pseudogap behavior rather than its cause.

[1] C. V. Parker, et al, Nature 2010 (in press) doi:10.1038/nature09597

[1]Work supported by DOE-BES, NSF-DMR, NSF-MRSEC through PCCM, and the W. M. Keck Foundation.

11:51AM B25.00004 Manipulating stripes in $La_{2-x}Ba_xCuO_4$ in extreme environments[1] , MARKUS HUECKER, GENDA GU, ZHIJUN XU, JINSHENG WEN, JOHN M. TRANQUADA, Brookhaven National Laboratory, MARTIN VON ZIMMERMANN, HASYLAB at DESY, Hamburg, Germany — Competing magnetic and electronic interactions in the copper-oxide high temperature superconductors often result in nanoscale inhomogeneity of the charge and spin density. Such observations motivated a proposal that dynamic electronic inhomogeneities are intrinsic to the copper-oxide planes, and can result in electronic states that break their four-fold symmetry. We have performed high-energy single-crystal X-ray diffraction in high magnetic fields and at high pressure to show that the charge and spin stripe phase in $La_{2-x}Ba_xCuO_4$ constitutes such a state. In particular, our results provide strong evidence that charge stripe correlations in the cuprates are electronically driven and are enhanced within vortices.

[1]The work at Brookhaven was supported by the Office of Science, U.S. Department of Energy under Contract No. DE-AC02-98CH10886.

12:03PM B25.00005 Hidden itinerant-spin extreme in heavily-overdoped LSCO revealed by dilute Fe doping: A combined neutron scattering and ARPES study , RUIHUA HE, Stanford & ALS, M. FUJITA[1], M. ENOKI, Tohoku, M. HASHIMOTO, Stanford, S. IIKUBO, Tohoku, S.-K. MO, ALS, H. YAO, Berkeley, T. ADACHI, Y. KOIKE, Tohoku, Z. HUSSAIN, ALS, Z.-X. SHEN, Stanford, K. YAMADA, Tohoku — Fluctuations of the localized spins on Cu and the itinerant spins of doped holes have been theoretically conceived to be both essential for high-Tc superconductivity. While the former clearly leads to an antiferromagnetic order in the undoped Mott phase (the localized-spin extreme), it has remained open whether the latter has an inherent tendency towards the formation of some magnetic order at very high dopings where it becomes dominant (the itinerant-spin extreme). By perturbing the non-magnetically-ordered heavily-overdoped LSCO with 1% Fe doping, we found by elastic neutron scattering an incommensurate magnetic order induced below 20 K, which cannot be ascribed to the localized spins on Cu or doped Fe. ARPES study of the itinerant doped holes suggests that this order is driven by a strong Fermi surface nesting, which is inherent in the pristine LSCO but has so far eluded a clean revelation. Our finding presents the first experimental example of the long-sought itinerant-spin extreme for cuprates and supports its important fluctuations that should be considered along with its localized counterparts for HTSC at intermediate dopings.

[1]Equally contributed to this work.

12:15PM B25.00006 Two distinct electronic sites in the Cu-O plane of the (La, Sr)CuO(4) pseudogap state , ROBERT SMITH, PHILIP KUHNS, ARNEIL REYES, GREGORY BOEBINGER, NHMFL/FSU — At intense magnetic fields (30 T) ^{17}O NMR exhibits two distinct signatures for planar oxygen sites instead of the singular site expected from the identical lattice symmetry at oxygen sites in the copper-oxygen plane for underdoped, orthorhombic $La_{2-x}Sr_xCuO_4$. Analysis of Knight shift, linewidth, quadrupolar splitting and spectral asymmetry indicates that roughly 75% of the planar oxygens evidence antiferromagnetically- correlated nearest neighbor Cu moments at temperatures below ∼30 K, consistent with previous reports. A second planar oxygen site first observed in this study shows that there are mobile holes on roughly 25% of the planar oxygen sites that (a) suppress magnetism for all T<300K and (b) show a Knight shift that drops to zero below ∼60 K, evidencing pair formation at a temperature well above the superconducting transition temperature (∼4 K at 30 T) and more than twice the superconducting transition temperature at zero magnetic field.

12:27PM B25.00007 Oxygen staging in phase separated La2-xSrxCuO4+y , HASHINI MOHOTTALA, University of Hartford, 200 Bloomfield Avenue, LINDA UDBY, e-Science and Nanoscience Centres, Niels Bohr Institute, Universistetsparken 5, 2100, SAMUEL EMERY, B.O. WELLS, J. I. BUDNICK, University of Connecticut, 2152, Hillside road, Storrs CT-06269, CHRISTOF NIEDERMAYER, Laboratory for Neutron Scattering, ETHZ & PSI, CH-5232 Villigen PSI, Switzerland, KIM LEFMANN, e-Science and Nanoscience Centres, Niels Bohr Institute, Universistetsparken 5, 2100, N.H. ANDERSON, Materials Research Division, Risø DTU, Frederiksborgvej 399, 4000 Roskilde, Denmark, F.C. CHOU, Center for Condensed Matter Sciences, National Taiwan University, Taipei 10617, Taiwan — We studied oxygen staging in a series of La2-xSrxCuO4 (LSCO) samples using neutron scattering. The samples were oxidized using electrochemistry. Electronic phase separation was previously reported in the oxygen rich LSCO system with two stable phases identified as optimally doped superconducting phase and a magnetic phase (1/8th like) with the same ordering temperatures at 40 K [1]. Our present studies show staging in this system. Although staging was observed and extensively studied in the samples with no Sr [2], it has not been reported or systematically studied in the systems with both Sr and oxygen. We do find staging in the oxygenated LSCO system, but the staging peaks evolve as Sr concentration increases and excess oxygen concentration decreases. [1] H Mohottala et al. Nature Materials **5**, 377 - 382 (2006), [2] B.O. Wells et al., Z. Phys. B 100, 535 (1996).

12:39PM B25.00008 Tunable High Q Superconducting Microwave Resonator[1] , Z. KIM, JQI/UMD, C.P. VLAHACOS, CNAM/NASA, J.E. HOFFMAN, J.A. GROVER, JQI/UMD, B.K. COOPER, J.R. ANDERSON, A.J. DRAGT, C.J. LOBB, JQI/CNAM/UMD, L.A. OROZCO, S.L. ROLSTON, JQI/UMD, J.M. TAYLOR, JQI/NIST/UMD, F.C. WELLSTOOD, JQI/CNAM/UMD — We have developed a frequency tuning system for a "lumped-element" thin-film superconducting Nb microwave resonator on sapphire intended for coupling to cold trapped ^{87}Rb atoms. ^{87}Rb has hyperfine ground states, $|^5S_{1/2}, F = 1\rangle$ and $|^5S_{1/2}, F = 2\rangle$, which are separated by about 6.83 GHz and available as a two-level system for a qubit. The resonator consists of a meandering inductor and an interdigitated capacitor coupled to a transmission line. At T=12 mK and on resonance at 6.863 GHz, the loaded quality factor is 40,000. We employ an Al pin as a frequency tuner by placing it above the inductor using a piezo stage so that one can effectively change the inductance of the resonator.

[1]Work supported by NSF through the PFC at JQI.

12:51PM B25.00009 Nanomechanical Torque Magnetometry of Individual Mesoscopic Superconductors[1] , ABDUL SUHEL, University of Alberta, DOUG VICK, National Institute of Nanotechnology, MARK R. FREEMAN, University of Alberta and National Institute of Nanotechnology, JOHN P. DAVIS, University of Alberta — We have developed an extremely sensitive form of torque magnetometry based on thin nanomechanical resonators [1]. Previously, we applied this technique to study single magnetic vortices in nanomagnetic samples [2]. One advantage of this technique is that it has good time resolution, and each measurement can be performed quickly enough to gather significant statistics on such events [2]. We are now applying this technique to study single mesoscopic superconducting samples. We intend to measure the magnetic moment associated with superconducting vortices, as well as other magnetic effects that occur in mesoscopic superconductors [3,4]. We will discuss our progress towards this goal. [1] J.P. Davis, et al. Appl. Phys. Lett. **96**, 072513 (2010). [2] J.P. Davis, et al. New Journal of Physics **12**, 093033 (2010). [3] A.K. Geim, et al. Nature **396**, 144 (1998). [4] A.K. Geim, et al. Nature **407**, 55 (2000).

[1] MRF acknowledges support from NSERC, iCORE, CIFAR, NINT, and CRC. The Integrated Nanosystems Research Facility is supported through CFI and nanoAlberta.

1:03PM B25.00010 Strong disorders in cuprate superconductors in d-density wave state , HONG-YI CHEN, National Taiwan Normal University, CHUNG-PIN CHOU, Academia Sinica — The local density of states on strong disordered d-wave superconductor in d-density wave state is studied. Recently, E.W. Hudson et al [Nature Physics 4, 108 (2008)], reported a method to investigate the pseudogap. We explore the selfconsistent Bogoliubov-de Genns' equations with strong disorders. The quantum interference leading to definitive quasipartical spectra has also been considered. Without d- density wave state, the numerical results are in satisfactory agreement with the observations from STM experiments. With d- densitywave state, a new result can be used to determine the properties of pseudogap.

1:15PM B25.00011 Resonant Inelastic X-Ray Studies on the Cu-L edge in 1-Dimensional Cuprate Chains[1] , JAMES LEE, M. YI, W.S. LEE, Stanford University, K. ZHOU, C. MONNEY, Swiss Light Source, PSI, S. JOHNSTON, J. VAN DEN BRINK, IFW Dresden, T. SCHMITT, L. PATTHEY, Swiss Light Source, PSI, T.P. DEVEREAUX, Stanford University, K. KUDO, Y. KOIKE, Tohoku University, Z.X. SHEN, Stanford University — Resonant Inelastic X-ray Scattering (RIXS) is a photon-in, photon-out spectroscopy technique with the capability of seeing many-body interactions in great detail. The recent achievement of sub-eV resolution in RIXS has opened up a new avenue for experiments to study these effects quantitatively. Here we present high-resolution RIXS data at the Cu L-edge on the quasi-one-dimensional edge-sharing chain compound, $Ca_{2+x}Y_{2-x}Cu_5O_{10}$, which is the only known dopable quasi-1D chain compound. Charge excitations corresponding to doped holes can be clearly resolved when the photon energy is tuned to the resonance at the hole band. In addition, we find that the d-d excitations appear to disperse with incident photon energy and momentum, and have a nontrivial intensity modulation. Effects of hole doping on these excitations will be discussed.

[1]Work supported by DOE Office of Basic Energy Science, Division of Materials Science and Engineering, under contract DE-AC02-76SF00515 and the Stanford Graduate Fellowship.

1:27PM B25.00012 High-resolution RIXS measurement at O K-edge on the edge-shared chain cuprates, $Ca_{2+x}Y_{2-x}Cu_5O_{10}$, W.S. LEE, SIMES, SLAC National Accelerator Lab., J. LEE, M. YI, Stanford University, K. ZHOU, Swiss Light Source, PSI, S. JOHNSTON, IFW Dresden, T. SCHMITT, Swiss Light Source, PSI, JEROEN VAN DEN BRINK, IFW Dresden, T.P. DEVEREAUX, SIMES, SLAC National Accelerator Lab., K. KUDO, Y. KOIKE, Tohoku University, L. PATTHEY, Swiss Light Source, PSI, Z.X. SHEN, SIMES, SLAC National Accelerator Lab. — Quasi one dimensional copper oxides have been model systems in the field of correlated electron physics, because of rich phenomena exhibited in a relatively simple geometry. Its magnetic ground states, fluctuations, and excitations have been investigated extensively by theorists and experimentalists. Among the known quasi 1-D spin-chain compounds, $Ca_{2+x}Y_{2-x}Cu_5O_{10}$ is the only compound that can be hole-doped in a wide doping range, providing a unique opportunity to study the dynamics of hole in the quasi-1D environment. Here, we report ultrahigh resolution resonant inelastic soft x-ray scattering experiment at the O K-edge. With an energy resolution of $\sim$50 meV, we resolved rich charge excitations in the sub-eV range that has not been observed in the previous RIXS measurement on the same materials. In particular, we have resolved clear multi-phonon excitations near the elastic peak, suggesting a strong electron-phonon coupling in this quasi-1D system. Doping dependence of these excitations will also be demonstrated.

1:39PM B25.00013 Suppression of superconductivity in the fully frustrated Josephson junction array with site dilution[1] , BRUNA DE OLIVEIRA, University of Southern California, TOMMASO ROSCILDE, Ecole Normale Superieure de Lyon, STEPHAN HAAS, University of Southern California — We study the effects of geometric randomness on the ordered phases and phase transitions of frustrated classical Josephson junction (JJ) arrays. In particular, we consider a square lattice array with maximal frustration (one half flux quantum through each plaquette) and with site dilution. The homogeneous model is known to feature two phase transitions: an Ising transition for the ordering of vortices into a crystalline state, and a Kosterlitz-Thouless transition for the appearance of superconductivity. A detailed Monte Carlo study shows a strong effect of disorder on the separation of the ordering temperatures. In particular, superconductivity is completely suppressed well before one reaches the percolation threshold of the lattice. We hence suggest that diluted JJ arrays with magnetic frustration are strong candidates for the experimental observation of a vortex crystal in the normal state.

[1]This work was supported by a Chateaubriand Fellowship, awarded by the French Embassy in Washington D.C., USA.

1:51PM B25.00014 Dynamical Spectral weight transfer in the cuprates is described by the Hubbard model , PHILIP PHILLIPS, university of illinois, MARK JARRELL, Louisiana State University — Recently, Peets and colleagues [1] measured the x-ray intensity at the oxygen K-edge in overdoped $La_{2-x}Sr_xCuO_{4\pm\delta}$ (LSCO) and $Tl_2Ba_2CuO_{6+\delta}$. They concluded that, unlike the underdoped samples of LSCO and $YBa_2Cu_3O_x$ in which the integrated intensity increases at least linearly with doping, it saturates abruptly for a hole count exceeding $x_c \approx 0.23$. They interpreted the saturation as a breakdown of the 1-band Hubbard model in the cuprates. We analyse all the available data and show that they are completely described by the 1-band Hubbard model. The purported saturation is shown to occur at the doping level at which the dynamical contribution to the spectral weight turns off.

[1] D. C. Peets, Phys. Rev. Lett. **103**, 087402 (2009).

2:03PM B25.00015 Superstructure and Magnetism in Na0.825CoO2 - A NMR study , P.Y. CHU, B.-L. YOUNG, J.Y. JUANG, G.J. SHU, M.-W. CHU, F.C. CHOU — We report our NMR study of the Na ordering and magnetism in the single crystal of Na0.825CoO2, as follows. 1. The atomic order of Na is observed from the well- resolved 23Na NMR peaks, which suggests 6 Na inequivalent sites. The 59Co NMR also suggests 4 distinct Co sites due to Na ordering. 2. The magnetic field-induced transition from antiferromagnet to ferromagnet is verified by our 23Na spectra at different temperatures and fields. A slow spin dynamic of glassy-like behavior is observed near the AFM and FM boundary. 3. We observed the NMR frequency shift anomaly near 50K, the same temperature where the susceptibility shows the curvature. The anomaly suggests the onset of the magnetic correlation in prior to magnetic ordering.

Monday, March 21, 2011 11:15AM - 1:39PM –

Session B26 DMP DCOMP: Focus Session: Iron Based Superconductors – Growth D162/164

11:15AM B26.00001 Influences of material processing on the microstructure and intergranular current of polycrystalline Sm1111 iron-pnictides , A. YAMAMOTO, Univ. of Tokyo, J. JIANG, F. KAMETANI, A. POLYANSKII, J. WEISS, E. HELLSTROM, D. LARBALESTIER, NHMFL, A. MARTINELLI, A. PALENZONA, M. TROPEANO, M. PUTTI, Univ. of Genova, CNR-SPIN — We have prepared polycrystalline Sm1111 bulk samples by sintering and hot isostatic pressing (HIP) and studied the influence of processing on the microstructure and intergranular current. After sintering and HIPping, samples are denser with much less impurity SmOF and grain boundary wetting FeAs. They then show significantly larger hysteresis loops than as- prepared samples. But Tc of HIPed samples is lower than samples with optimal doping, indicating loss of fluorine during later processing. Nevertheless, even after the fluorine loss and its associated carrier density reduction produced by the HIP treatment, both Magneto-Optical and remanent magnetization analyses showed that the intergranular current was enhanced. We conclude that the denser microstructure and smaller impurity phase content of HIPped samples enhances their connected fraction, even as the doping state of the sample is degraded by F loss. Our study emphasizes that current transport in polycrystalline pnictides is a complex balance involving the need to control carrier density, especially at grain boundaries, while densifying the microstructure and avoiding normal-state grain boundary wetting phases like FeAs.

11:27AM B26.00002 Synthesis and superconducting properties of FeTe1-xSe Single Crystals under high magnetic fields , TESFAYE GEBRE, G. LI, J. WHALEN, National High Magnetic Field Laboratory, Tallahassee, FL 32310, B. CONNER, National High Magnetic Field Laboratory,Tallahassee, FL 32310, M. KOSTOV, Department of Chemical and Biomedical Engineering, FSU, Tallahassee, FL 32310, T. SIEGRIST, Department of Chemical and Biomedical Engineering, FSU, and National High Magnetic Field Laboratory, Tallahassee, FL 32310, L. BALICAS, National High Magnetic Field Laboratory,Tallahassee, FL 32310 — Single crystals of superconductor $FeTe_{1-x}Se_x$ ($0.1 \leq x \leq 0.5$) were synthesized using optical floating zone, Bridgeman technique, and solid stat reaction. The samples were synthesized under various temperature gradients and cooling rates. Crystals were characterized via EDX, X-ray scattering, magnetization and transport measurements. Upper critical fields Hc_2as estimated through the Werthamer-Hohenberg-Helfand (WHH) formalism indicate that these materials strongly surpass the weak coupling Pauli limiting field indicating that the shape of their phase diagram under field is essentially controlled by the Pauli effect. Annealing, leads to a metallic temperature dependence of the resistivity, and to sharper superconducting transitions. Despite the relatively small increase in single crystallinity, as quantified by single crystal x-ray diffraction measurements, we observe a different phase diagram under high magnetic fields when compared to non-annealed samples.

11:39AM B26.00003 Single crystal growth and superconducting properties of LiFeAs , BUMSUNG LEE, SEUNGHYUN KHIM, JAE WOOK KIM, SNU, EUN SANG CHOI, NHMFL, JUNG SOO KIM, G. R. STEWART, UF, KEE HOON KIM, SNU — LiFeAs, a representative compound for '111' system of Fe-based superconductors, has a tetragonal Cu_2Sb-type structure and possesses a single Fe-As tetrahedral layer sandwiched by the double Li layers. This structural characteristic provides a unique opportunity to realize homogeneous Li terminating surface upon cleaving, and this possibility makes LiFeAs attractive for investigating the intrinsic properties of Fe-based superconductors with various spectroscopic tools. In this sense, growing a large LiFeAs single crystal is a necessary step for studying intrinsic properties of the Fe-based superconductors. We report the successful growth of high quality LiFeAs single crystal by Sn-flux. Electrical resistivity studies reveal the superconducting onset temperature is 18.2 K with a transition width less than 1.1 K and RRR is about 24. Bulk superconductivity is supported by perfect shielding in the magnetic susceptibility and a clear jump in the specific heat. Upper critical field slopes of $dH_{c2}^{c}/dT \approx$-1.39 and $dH_{c2}^{ab}/dT \approx$-2.99 T/K near T_c predict $H_{c2}^{c}(0)\approx$17.2 and $H_{c2}^{ab}(0)\approx$36.9 T, and it points to a modest superconducting anisotropy about 2.3 near T_c. This observed modest anisotropy is a bit smaller than the band calculation results based on the GGA approximation but larger than the prediction considered effects of electron correlation through the dynamic mean field theory.

11:51AM B26.00004 ABSTRACT WITHDRAWN –

12:03PM B26.00005 Superconductivity and wire fabrication of FeSe family , TOSHINORI OZAKI, KEITA DEGUCHI, YOSHIKAZU MIZUGUCHI, HIROAKI KUMAKURA, YOSHIHIKO TAKANO, National Institute for Materials Science, NATIONAL INSTITUTE FOR MATERIALS SCIENCE TEAM — The 11 family is an fascinating iron-based superconducting system for not only elucidation of superconducting mechanism but also technological applications because of the simplest crystal structures, the less toxic and high critical field. Recently, we found that the superconductivity appears in the specimen immersed in alcoholic beverages. Focused on the pressure dependence of Se height from Fe layer in FeSe, we found that the Tc is correlated to Se height. Moreover, the anion height dependence of T_c for all FeAs-based superconductor obeyed a universal curve with a peak around 1.38 Å. We succeeded in observing the transport J_c in the single- and 7-core wires of $FeTe_xSe_{1-x}$ superconductor using an in-situ powder-in-tube (PIT) method. The J_c values in single- and 7-core wire are as high as 159 A/cm^2 and 100 A/cm^2 at 4.2 K, respectively. It is considered that the optimization of the composition, together with the improvement of the grain boundary in $FeTe_xSe_{1-x}$ superconducting wires, will lead to higher J_c.

12:15PM B26.00006 Synthesis of Large Single Crystals of LaMnPO[1] , GREG SMITH, JACK SIMONSON, CARLOS MARQUES, Stony Brook University, VICTOR LEYVA, Rice University, MEIGAN ARONSON, Stony Brook University — The compound LaMnPO is isostructural with LaFeAsO, a recently discovered high-temperature superconductor, but optical spectroscopy and transport measurements of this compound have been heretofore limited by small crystal size. Accordingly, crystal syntheses from Sn, Pb and molten salt fluxes (including NaCl/KCl, LiCl/NaCl, KCl, $CaCl_2$, $BaCl_2/CaCl_2$ and $KCl/CaCl_2$) were investigated. Fluorine doping was explored; concentrations less than 30 at.% (nominal) had no effect on crystal size; concentrations greater than 40 at.% (nominal) did not yield crystals. Once growth parameters were optimized, the crystals grew in a flat rectangular shape with black luster; their composition was verified with powder and single crystal x-ray diffraction. Successful growths yielded crystals with dimensions up to 3.2 mm by 1 mm by 10 μm, a significant improvement upon previously reported growths in the literature. These large crystals enabled our group to perform a wide range of experiments that were previously restricted to polycrystalline materials. It may be feasible to extend these methods to the synthesis of similar compounds.

[1]Research supported by a DOD National Security Science and Engineering Fellowship via the AFOSR

12:27PM B26.00007 ABSTRACT WITHDRAWN –

12:39PM B26.00008 Faceted nanocrystalline growth of FeTe on $SrTiO_3(001)$, YI LI, ZHAOLIANG LIAO, LINA CHEN, JIANNENG LI, AMAR KARKI, RONGYING JIN, WARD PLUMMER, JIANDI ZHANG, LOUISIANA STATE UNIVERSITY TEAM — The new class of iron based superconductors has ignited the materials community. Of all of these new superconductors, the Fe chalcogenide system is probably the simplest at least in structure. One of most interesting questions is how the properties of these systems change as the structure is manipulated. We have studied ultra thin films of FeTe grown on a $SrTiO_3$(001) surface by using Pulsed Laser Deposition (PLD) and characterized with surface techniques. We observe the formation of faceted nanocrystalline islands at the surface of thin films. The structure of the islanded surface, including the faceting angle of nanostructures, has been studied by Low Energy Electron Diffraction (LEED) as well as scanning tunneling microscope (STM). The correlation of such a 3D-type growth with growth conditions and substrate-induced strain in the ultra-thin films are discussed. *Supported by NSF-DMR1005562

12:51PM B26.00009 Superconducting Iron-Chalcogenide Thin Films and Coated Conductors , QIANG LI, WEIDONG SI, Brookhaven National Laboratory — Superconducting iron-chalcogenide superconducting films have been grown on a variety of substrates, including single crystalline and metallic substrates. In this presentation, we will report transport and structural properties of these films. The superconducting transition temperature of these films is significantly higher than that of the corresponding bulk materials. Analytical electron microcopy analysis indicates substantial structural difference between thee films and single crystals at atomistic level. Detailed measurement of the angular dependence of upper critical field and critical current density demonstrated that iron chalcogenide superconductors have lower anisotropy factor in comparison to the high Tc cuprates, that presents the unique opportunity for this class of materials in high field application.

1:03PM B26.00010 Superconducting properties of $FeSe_{0.5}Te_{0.5}$ and $FeTe{:}O_x$ thin films , WEIDONG SI, Brookhaven National Laboratory, AYAN BHATTACHARYA, SU JUNG HAN, IVO DIMITROV, LIJUN WU, QIANG LI — High quality superconducting thin films of $FeSe_{0.5}Te_{0.5}$ and $FeTe{:}O_x$ have been grown by pulsed laser deposition on various substrates including coated conductor. Thin films of $FeSe_{0.5}Te_{0.5}$ have a higher superonducting transition temperature Tc (onset start around 20K and zero resistance about 16 17K) than that of bulk. High resolution transmission electron microscopy has identified a microstructure only in thin films, which may be associated with the higher Tc. Magneto-transport measurement has been carried out to check the angular dependence of upper critical field Hc2 and the critical current density of the films with the direction of magnetic field. Both have shown a weak anisotropy. These films have a special high dHc2/dT at Tc, especially for $FeTe{:}O_x$ film.

1:15PM B26.00011 Maze-like surface reconstruction on pure $SrFe_2As_2$ observed by STM/STS[1] , MICHAEL DREYER, MARK GUBRUD, HUI WANG, SHANTA SAHA, NICK BUTCH, KEVIN KIRSHENBAUM, JOHNPIERRE PAGLIONE, University of Maryland — We measured undoped $SrFe_2As_2$ samples using a low temperature scanning tunneling microscope. Similar samples showed superconductivity in up to 15% of its volume in measurements of the diamagnetic screening although being undoped as confirmed by energy dispersive x-ray spectroscopy. The samples where cleaved at room temperature at a pressure $P < 10^{-8}$ mbar before introducing them into the low temperature scanning tunneling microscope (LTSTM) operating at a temperature of $T = 4.2$ K. Beside the usual striped surface reconstruction and disordered regions we observed areas showing a maze like reconstruction. Atomically resolved images strongly suggest that the maze structure is formed by adatoms and thus, by inference, is the striped phase. Scanning tunneling spectroscopy (STS) measurements showed a superconducting gap on both the striped and maze phase of the sample, similar to the spectra on a cobalt doped sample. The results will be discussed in detail.

[1]Funded in part by the Laboratory for Physical Sciences.

1:27PM B26.00012 Cleavage behavior and surface states in iron pnictides , KLAUS KOEPERNIK, ALEXANDER LANKAU, HELMUT ESCHRIG, JEROEN VAN DEN BRINK, SERGEY BORISENKO, IFW Dresden, Germany, ERIK VAN HEUMEN, MARK S. GOLDEN, Zeeman institute, University of Amsterdam, Netherlands — We present a density functional study of the surface electronic structure and the cleavage behavior of LiFeAs and Co-doped $BaFe_2As_2$. The results are discussed together with angle resolved photo emission (ARPES) and low energy electron diffraction (LEED) data. The two systems behave rather differently and we conclude that LiFeAs will be the ideal system for surface sensitive probes among the iron pnictide familly.

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B27 GQI: Focus Session: Superconducting Qubits - Measurement C155

11:15AM B27.00001 Quantum Noise in a Chirped Superconducting Nonlinear Resonator , KATER MURCH, R. VIJAY, QNL, UC Berkeley, IDO BARTH, LAZAR FRIEDLAND, Racah Institute of Physics, Hebrew University, IRFAN SIDDIQI, QNL, UC Berkeley — A nonlinear Josephson junction oscillator driven near resonance can exhibit bistability, forming the basis for sensitive, digital quantum state readout. We consider the case of a high-Q resonator embedded with a Josephson junction excited with a chirped frequency signal. For sufficient drive amplitude, the resonator phase locks with the drive signal and enters the high amplitude oscillation state, a phenomenon known as autoresonance. The probability of capture in a given chirped pulse depends on the initial phase difference between the drive signal and of the fluctuation induced oscillations of the resonator. We find that the width of this threshold is in agreement with recent theoretical predictions and is set by zero-point fluctuations of the resonator. Autoresonant capture forms the basis for fast readout of a superconducting qubit coupled to a high-Q resonator.

11:27AM B27.00002 Measurement backaction and the quantum Zeno effect in a superconducting qubit , DANIEL H. SLICHTER, R. VIJAY, IRFAN SIDDIQI, Quantum Nanoelectronics Laboratory, Dept. of Physics, UC Berkeley — Strong measurement of a quantum system can inhibit quantum state evolution, a phenomenon known as the quantum Zeno effect. If the measurement is not perfectly quantum non-demolition, it can also cause spurious transitions between states. We study these effects in a transmon qubit dispersively coupled to a superconducting microwave readout cavity. We use a fast, ultralow-noise parametric amplifier to amplify the microwave photons used to probe the qubit state, enabling continuous high-fidelity monitoring of the qubit. This arrangement allows us to observe quantum jumps between the qubit states in real time. We examine the dependence of the jump times on measurement strength and the qubit excitation protocol.

11:39AM B27.00003 Investigation of the measurement dynamics of a flux qubit inductively coupled to a readout dc-SQUID , PETER GROSZKOWSKI, JAY GAMBETTA, FRANK WILHELM, IQC, University of Waterloo — In this paper we investigate the measurement dynamics of a flux qubit inductively coupled to a capacitively shunted, readout dc-SQUID. We study how the measurement induced dephasing and relaxation rates scale as a function of the qubit operation point and measurement strength. We find analytical solutions when the measurement is quantum-non-demolition (QND) and provide a numerical investigation for non-QND operation. This is of importance as the measurement of the flux qubit when operated at its sweet spot is inherently non-QND. We conclude this with a discussion of the measurement efficiency and signal-to-noise ratio.

11:51AM B27.00004 Optimization of SQUID-based microwave parametric amplifiers for qubit readout , CHRIS MACKLIN, R. VIJAY, E. LEVENSON-FALK, D. SLICHTER, Z. MINEV, I. SIDDIQI, QNL, UC Berkeley — We present recent experimental and theoretical results on the optimization of SQUID-based parametric microwave amplifiers for ultra low noise readout of superconducting and spin-based qubits. The devices consist of an unshunted two-junction SQUID in parallel with an on-chip capacitor, forming a non-linear microwave resonator. The SQUID is operated in a non-linear regime below the critical current, thus producing no local dissipation. These amplifiers have gain exceeding 20 dB, 10 MHz of broadly tunable bandwidth, and quantum-limited noise performance. We present measurements on amplifiers with tunnel type and weak link Josephson junctions. We discuss the use of array structures to optimize dynamic range as well as a resonant flux-coupled input capable of operation in a transmission configuration and potentially suitable for on-chip integration.

12:03PM B27.00005 Fluxonium qubit readout with the Josephson parametric converter[1] , M. HATRIDGE, B. ABDO, A. KAMAL, N. MASLUK, F. SCHACKERT, M.H. DEVORET, Applied Phyics Dept., Yale University — Rapid, single shot quantum-non demolition readout is a prerequisite for proposed active quantum feedback and error correction experiments in superconducting qubit systems. The fluxonium qubit, an artificial atom comprised of a Josephson junction array inductively shunting a Cooper-pair box, is a non- Purcell limited system with excellent coherence times, making it a natural candidate for such experiments. The largest obstacle towards achieving single shot fluxonium readout is the severe signal-to-noise ratio degradation of the qubit readout by the microwave frequency amplification chain. This degradation can be minimized through the addition of a quantum-limited pre-amplifier to the chain. We have designed and constructed such an amplifier, the Josephson Parametric Converter (JPC), which achieves nearly quantum limited amplification with a bandwidth and dynamic range suitable for readout of our current fluxonium design, and are currently integrating the JPC and fluxonium. We will discuss experimental requirements of the combined JPC and fluxonium system and anticipated improvements in measurement fidelity and speed.

[1]Work supported by IARPA, ARO and NSF.

12:15PM B27.00006 Dispersive Readout of a Superconducting Flux Qubit Using a Microstrip SQUID Amplifier[1] , J.E. JOHNSON, UC Berkeley, E.M. HOSKINSON, C. MACKLIN, I. SIDDIQI, QNL, UC Berkeley, JOHN CLARKE, UC Berkeley — Dispersive techniques for the readout of superconducting qubits offer the possibility of high repetition-rate, quantum non-demolition measurement by avoiding dissipation close to the qubit. To achieve dispersive readout, we couple our three-junction aluminum flux qubit inductively to a 1-2 GHz non-linear oscillator formed by a capacitively shunted DC SQUID. The frequency of this resonator is modulated by the state of the qubit via the flux-dependent inductance of the SQUID. Readout is performed by probing the resonator in the linear (weak drive) regime with a microwave tone and monitoring the phase of the reflected signal. A microstrip SQUID amplifier (MSA) is used to increase the sensitivity of the measurement over that of a HEMT (high electron mobility transistor) amplifier. We report measurements of the performance of our amplification chain. Increased fidelity and reduced measurement backaction resulting from the implementation of the MSA will also be discussed.

[1]This work was funded in part by the U.S. Government and by BBN Technologies.

12:27PM B27.00007 SQUID-tunable microwave lumped-element oscillators and distributed resonators[1] , P. BHUPATHI, M.P. DEFEO, M. WARE, J.D. STRAND, B.L.T. PLOURDE, Syracuse University — We have fabricated lumped-element microwave oscillators and coplanar waveguide resonators consisting of a dc SQUID using submicron Al-AlOx-Al junctions with resonance frequencies in the range of several GHz. The SQUID oscillators consist of a dc SQUID shunted with a capacitor formed from superconducting layers. The CPW resonators are formed from Nb $\lambda/2$ coplanar transmission lines with a center conductor interrupted by an Al dc SQUID at the current anti-node of the fundamental mode. The resonance frequency can be varied by tuning the Josephson inductance of the SQUID with on-chip flux and bias-current lines. We discuss applications employing these devices, including a new readout scheme for superconducting flux qubits and for the detection of microwave cavity photons.

[1]Work supported by DARPA QuEST.

12:39PM B27.00008 Multiplexing Readout of a Qubit Array via a Single Transmission Line , MARKUS JERGER, STEFANO POLETTO, ALEXANDER LUKASHENKO, ALEXEY V. USTINOV, Physikalisches Institut, Karlsruhe Institute of Technology and DFG-Center for Functional Nanostructures (CFN), D-76128 Karlsruhe, Germany, PASCAL MACHA, UWE HÜBNER, EVGENI IL'ICHEV, Institute of Photonic Technology, PO Box 100239, D-07702 Jena, Germany — A resonant circuit coupled to a qubit displays a shift of its resonance frequency depending on the quantum state of the qubit. The qubit state can be thus measured by probing the resonator near its resonance frequency. By coupling every qubit to its individual resonator of distinct frequency, one can read out the state of an array of many qubits through a single microwave line coupled to all resonators. Moreover, this readout can be performed simultaneously by using a multi-tone microwave pulse with frequency-division multiplexing. We will present measurements on an ensemble of 7 superconducting flux qubits located on one chip and each coupled to an individual transmission-line resonator. We performed spectroscopy of all qubits and determined their parameters in a single measurement run. Our latest experiments on simultaneous preparation and readout of the 7-qubit array will be presented.

12:51PM B27.00009 Multiplexed dispersive readout of superconducting phase qubits[1] , YU CHEN, RAMI BARENDS, RADOSLAW BIALCZAK, JULIAN KELLY, MICHEAL LENANDER, ERIK LUCERO, MATTEO MARIANTONI, MATTHEW NEELEY, AARON O'CONNELL, PETER O'MALLEY, Department of Physics, Uinversity of California-Santa Barbara, DANIEL SANK, AMIT VAINSENCHER, HAOHUA WANG, MARTIN WEIDES, JAMES WENNER, THEODORE WHITE, YI YIN, JIAN ZHAO, ANDREW CLELAND, JOHN MARTINIS, Department of Physics, Uinversity of California-Santa Barbara — A dispersive readout scheme is being developed for superconducting phase qubits. By inductively coupling to a LC resonator, the measured state of the qubit (left or right side of the potential well) can be read out as a shift of the resonance frequency. Compared to our current SQUID readout, this method eliminates the generation of quasiparticles, increases the reliability by reducing the junction count per qubit from 4 to 1, and reduces the chip wire count since the readout can be frequency multiplexed.

[1]This work is supported by IARPA under ARO award W911NF-08-1-0336 and under ARO award W911NF-09-1-0375.

1:03PM B27.00010 Non-linear dispersive interaction in superconducting circuit QED , YI YIN, HAOHUA WANG, MATTEO MARIANTONI, RADOSLAW C. BIALCZAK, MIKE LENANDER, ERIC LUCERO, MATTHEW NEELEY, AARON O'CONNELL, DANIEL SANK, JIM WENNER, Physics Department, University of California, Santa Barbara, TSUYOSHI YAMAMOTO, NanoElectronics Research Laboratories, NEC Corporation, Japan, ANDREW CLELAND, JOHN MARTINIS, Physics Department, University of California, Santa Barbara — In circuit quantum electrodynamics, the strong coupling between superconducting qubits and a coplanar waveguide resonator (CPW) has been utilized to study the light-atom interaction. When the qubit is detuned far away from the resonator in frequency, linear dispersive interaction has been used for the readout of qubit states by measuring the pulling frequency of the resonator. Alternatively, we investigate dispersive interaction in a broader regime by measuring the accumulated dynamic phase with Wigner tomography. In the quasi-adiabatic process of tuning the qubit frequency, the dynamic phase measurement can be pushed to the case of zero detuning with up to the five-photon Fock state in the CPW resonator. The exotic non-linear behaviors of the qubit on resonator cat state and coherent state have been revealed, strongly depending on the strength of dispersive interaction. Our experimental data are consistent with the numerical calculation using the Jaynes-Cumming model.

1:15PM B27.00011 Circuit QED with a Nonlinear Resonator: ac-Stark Shift and Dephasing , FLORIAN R. ONG, CEA-Saclay and University of Waterloo, M. BOISSONNEAULT, F. MALLET, A. PALACIOS-LALOY, A. DEWES, A.C. DOHERTY, A. BLAIS, P. BERTET, D. VION, D. ESTEVE, CEA-SACLAY TEAM, U. DE SHERBROOKE TEAM, U. OF QUEENSLAND TEAM — Coupling a superconducting qubit to a superconducting resonator enables to investigate the interaction between light and matter with a unique flexibility of design, and allows to reach coupling regimes hardly accessible otherwise [Wallraff Nature 2004]. In this talk, we discuss the ac-Stark shift and the measurement induced dephasing of a qubit embedded in a *nonlinear* resonator, an architecture that has demonstrated high fidelity single-shot qubit state readout [Mallet Nat. Phys. 2009]. In our experiment, a transmon qubit [Koch PRA 2007] is capacitively coupled to a coplanar waveguide resonator incorporating a Josephson junction that provides a Kerr nonlinearity. We have measured the qubit spectrum while pumping the nonlinear resonator with a microwave tone. Measurements of the qubit frequency shift provide a sensitive probe of the intracavity field, yielding a precise characterization of the resonator nonlinearity. The qubit linewidth has a complex dependence on the pump frequency and amplitude, which is correlated with the gain of the nonlinear resonator operated as a small-signal amplifier. The corresponding dephasing rate is found to be close to the quantum limit for most pump parameters.

1:27PM B27.00012 Improved Superconducting Qubit Readout by Qubit-Induced Nonlinearities in the Straddling Regime , MAXIME BOISSONNEAULT, Universite de Sherbrooke, J.M. GAMBETTA, IQC and University of Waterloo, J. BOURASSA, A. BLAIS, Universite de Sherbrooke — In dispersive readout schemes, qubit-induced nonlinearities have typically limited the measurement fidelities by reducing the signal-to-noise ratio (SNR) when the measurement power is increased [1]. However, it has been recently shown that these nonlinearities, together with the many-level system (MLS) nature of superconducting qubits, can be used to improve qubit readout in some regimes [2]. Moreover, for the transmon qubit [3], it has been shown that when the resonator's frequency sits between two of the MLS' transition frequencies – the so-called straddling regime – contributions of higher levels add constructively to improve the SNR [4]. In this talk, we explore the advantages of using both the qubit-induced nonlinearties and the straddling regime for qubit readout.

[1] Boissonneault et al, PRA 77, 060305(R) (2007)
[2] Reed et al, PRL 105, 173601 (2010), Bishop et al, PRL 105, 100505 (2010), Boissonneault et al, PRL 105, 100504 (2010)
[3] Koch et al, PRA 76, 042319 (2007)
[4] Srinivasan et al, V26.00006, 2010 March Meeting.

1:39PM B27.00013 Purcell Protection and Cycling Transition Measurement with a Superconducting V-system , ANTHONY HOFFMAN, SRIKANTH SRINIVASAN, Princeton University, JAY GAMBETTA, Institute for Quantum Computing, ANDREW HOUCK, Princeton University — We perform time-domain experiments on a superconducting qubit with a V-level energy structure coupled to a superconducting, coplanar waveguide resonator. Quantum interference and the V-level energy scheme allow independent control of the qubit energy and dipole via two on-chip fast flux bias lines [1]. The tunable dipole is predicted to protect the qubit from cavity-induced spontaneous emission. We probe this "Purcell protection" by measuring the qubit lifetime at constant cavity-qubit detuning for a range of coupling strengths. We also show how the coupled cavity-qubit energy spectrum allows for a cycling-type measurement that is predicted to improve the signal to noise ratio of qubit state readout by as much as an order of magnitude.

[1] J.M. Gambetta et al., arXiv:1009.4470v1

1:51PM B27.00014 Quantum State Tomography of a Cooper-pair Box , SERGEY NOVIKOV, V. ZARETSKEY, B. SURI, Z. KIM, Dept. of Physics, Univ. of Maryland, B.S. PALMER, Lab. for Physical Sciences, F.C. WELLSTOOD, JQI, CNAM, Dept. of Physics, Univ. of Maryland — A 4-8 GHz microwave pulse shaping system with 3 ns Gaussian pulse rise time, arbitrary pulse envelope and phase control has been implemented. The system utilizes a two-channel 1 GSa/s DAC board[1] to supply control voltages to an IQ mixer. The signals to the mixer have been optimized to obtain an on-off ratio of > 85 dB and phase deviations $< 5\%$. The setup has been used to manipulate an $Al/AlO_x/Al$ Cooper-pair box (CPB) qubit coupled to a lumped-element microwave resonator ($f_0 = 5.446$ GHz). The CPB has a charging energy $E_C/h = 6.25$ GHz and a maximum $E_J/h = 19$ GHz which was decreased to an effective $E_J/h = 6.1$ GHz by an external magnetic field. By measuring the microwave transmission at f_0 in a pulsed-probe scheme, we perform a dispersive readout of the qubit. We present tomography data on the $|g\rangle$, $|e\rangle$, $(|g\rangle + |e\rangle)/\sqrt{2}$ and $(|g\rangle + i|e\rangle)/\sqrt{2}$ states. We find good agreement with theory, confirming that we have achieved the desired microwave pulse control.

[1]Designed by J. Martinis at UCSB and fabricated by HSCC.

2:03PM B27.00015 A phase qubit coupled to an RF-SQUID resonator , JED WHITTAKER, SHANE ALLMAN, University of Colorado at Boulder, KATARINA CICAK, FRANCOIS NGUYEN, NIST, ADAM SIROIS, University of Colorado at Boulder, JOHN TEUFEL, EVA ZAKKA-BAJJANI, RAYMOND SIMMONDS, NIST — We have coupled a tunable cavity (an RF-SQUID resonator) to a phase qubit. The resonator can be used both for state transfer experiments as well as a measurement/readout device for the qubit. Specifically, it can be used in three different ways to help interrogate the state of the qubit. First, changes in the resonator frequency can be monitored in order to read out the qubit state after a conventional fast measure pulse is applied to the qubit bias flux. Second, we can perform a linear dispersive measurement of the qubit state using the coupled interaction between the qubit and the resonator. Here, the resonator will have a qubit-state dependent frequency shift. Finally, we can exploit the nonlinearity of the resonator by driving it into the bifurcated regime and performing a single- shot measurement of the state of the qubit. I will discuss the design, fabrication, and operation of this system.

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B28 DMP: Focus Session: Carbon Nanotubes and Related Materials: Growth, Sorting and Properties C156

11:15AM B28.00001 Fundamentals and applications of monodisperse carbon-based nanomaterials , MARK HERSAM, Northwestern University — Carbon-based nanomaterials have attracted significant attention due to their potential to enable and/or improve applications such as transistors, transparent conductors, solar cells, batteries, water purification systems, infrastructure materials, drug delivery, and biosensors. This talk will delineate chemical strategies for tuning and enhancing the properties of these promising nanomaterials. For example, we have developed and commercialized a scalable technique for sorting single-walled carbon nanotubes (SWCNTs) by their physical and electronic structure using density gradient ultracentrifugation (DGU). The resulting monodisperse SWCNTs possess unprecedented uniformity in their electronic and optical properties, which enables the fabrication of high performance thin film field-effect transistors, optoelectronic devices, and transparent conductors. The DGU technique also enables multi-walled carbon nanotubes to be sorted by the number of walls, and solution phase graphene to be sorted by thickness, thus expanding the suite of monodisperse carbon-based nanomaterials. By recently extending our DGU efforts to SWCNTs and graphene dispersed in biocompatible polymers (e.g., DNA, poloxamers, etc.), new opportunities have emerged in biomedical applications. Ultimately, the ability to control structure and surface chemistry with sub-nanometer precision enables optimized properties for a diverse range of technologies that employ carbon-based nanomaterials.

11:51AM B28.00002 Electronic separation of dispersed carbon nanotubes in solution by Lorentz forces , CHARISHMA SUBBAIAH, JOSHUA WOOD, JOSEPH LYDING, University of Illinois at Urbana-Champaign — Use of single-walled carbon nanotubes (SWNTs) in industry compatible device applications requires top-down control of SWNT electronic type. Therefore, we develop a technique for SWNT electronic separation, increasing the relative distribution of metallic SWNTs in solution by a magnetically induced Lorentz force. We take solutions of SWNTs in n-methylpyrrolidone and sonicate them, making a disperse solution on which we apply a non-uniform voltage waveform. This waveform generates a magnetic field that couples more strongly with metallic SWNTs than semiconducting SWNTs, due to a higher metallic SWNT magnetic moment, separating the tubes by Lorentz force. By conducting SWNT spectrophotometric measurements in the UV-vis-IR region, we assess the separation effectiveness. From the extracted supernatant solution, we observe a multi-fold absorbance enhancement in the metallic SWNT transition regions [1]. Additionally, the small full-width at half maximum in the absorbance peaks suggests that we are selecting a small number of metallic chiralities in our separation.

[1] Ausman et al., J. Phys. Chem. B. 104, 8911 (2000).

12:03PM B28.00003 Horizontally Aligned Carbon Nanotube Growth: Defects and Film Density[1] , W.D. TENNYSON, D. SHI, E.S. SANCHEZ, J.C. KEAY, M.B. JOHNSON, D.E. RESASCO, University of Oklahoma — Horizontally-aligned single-walled carbon nanotubes (SWNTs) were grown on ST-cut quartz by chemical vapor deposition (CVD). The 0.2-0.3 nm thick thermally evaporated Fe catalyst was patterned using standard liftoff processes both parallel and perpendicular to the $< 2\bar{1}\bar{1}0 >$ quartz surface (the SWNT alignment axis). Enhanced SWNT film density and improved film uniformity were observed by atomic force microscopy (AFM) and scanning electron microscopy (SEM) when water was included with the carbon feed source (ethanol). For SWNT films without water, the SWNT linear density within 1 μm of the catalyst edge was 8 SWNT/μm and down to 2 SWNT/μm at 10 μm from the edge. However, films grown with water exhibited similar linear densities both near and far from the catalyst edge, 6 SWNT/μm. AFM observations suggest that tube-tube interactions during growth contribute to a reduced the linear SWNT density. Aligned SWNTs were observed to terminate when they intersected a non-aligned SWNT. Water-assisted growth reduced the concentration of unaligned SWNTs near the catalyst edge, resulting in a higher fraction of nanotubes extending from the catalyst.

[1] CaNTeC & SWeNT

12:15PM B28.00004 Utilizing real time transmission electron microscopy to understand the mechanisms of nanotube nucleation, growth and growth termination , ERIC A. STACH, Purdue University — In order for carbon nanotubes to find widespread application, we must have a deeper understanding of the mechanisms by which they nucleate, growth and cease growth, in an effort to fully control the resulting structures. Here we will describe how we can exploit the unique capabilities of in-situ environmental cell transmission electron microscopy to observe multiple aspects of these processes. With this approach we can directly visualize how the catalysts that mediate nanotube growth respond to various changes in the growth environment, and correlate these changes with the resulting nanotube structures. In the first part of the presentation, we will investigate how dynamic changes in the catalyst morphology are correlated with the termination of growth in vertically aligned SWNT arrays. In particular, we have investigate how the processes of catalyst coarsening, Ostwald ripening and diffusion into the catalyst support can lead to growth termination, and we will describe how changes in the growth feedstock - in particular the incorporation of controlled amounts of water vapor - can alter the catalyst evolution. In the second portion of the presentation, we will describe how altering other aspects of the growth feedstock - in this case the carrier gas, in combination with the water vapor content - can not only affect catalyst morphological evolution, but can also significantly bias the chiral distribution of the resulting nanotubes. We will correlate the changes in growth ambient with a faceting / defacting transition, as well as a resulting change in the rate of Ostwald ripening.

12:51PM B28.00005 In situ diagnostics of the pulsed growth of graphene and carbon nanotubes , DAVID GEOHEGAN, ALEX PURETZKY, JASON READLE, CHRISTOPHER ROULEAU, MURARI REGMI, GYULA ERES, GERD DUSCHER, MINA YOON, Oak Ridge National Laboratory, OAK RIDGE NATIONAL LABORATORY TEAM — Non-equilibrium, pulsed gas delivery and pulsed heating synthesis approaches are used to explore and compare the kinetics and mechanisms of carbon nanotube and graphene growth on metal thin-films. Time-resolved, in situ optical reflectivity of growing nanotubes and graphene reveal the growth kinetics resulting from well-controlled, pulsed fluxes of acetylene by chemical vapor deposition. Alternatively, pulsed laser heating of substrates is used to provide well-defined transient growth temperature profiles for growth by chemical vapor deposition. Pulsed gas fluxes are shown to control the density and diameter of nanotubes in vertically-aligned nanotube arrays with nanoparticles of different size repeatedly nucleating, growing, and terminating growth in accordance with an empirical growth model. The pulsed processing approach is used to grow vertically aligned nanotube arrays with variable density. Research sponsored by the Materials Science and Engineering Division, Basic Energy Sciences, U.S. Department of Energy. A portion of this research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Scientific User Facilities Division, U.S. Department of Energy.

1:03PM B28.00006 Growth of Ultra-High Density Vertically-Aligned Carbon Nanotube Forests , JOHN ROBERTSON, SANTIAGO ESCONJAUREGUI, MARTIN FOUQUET, BERNHARD BAYER, STEPHAN HOFMANN, Cambridge University — We present a general catalyst design method to synthesise ultra-high density, aligned forests of carbon nanotubes by cyclic deposition and annealing of catalyst thin-films. This leads to nanotube forests with an area density of at least 10^{13} cm^{-2}, over one order of magnitude higher than existing values (Hata 2004, Zhong 2006), and close to the limit of a fully dense forest. The technique consists of cycles of ultra-thin metal film deposition, annealing, and immobilisation. The nanotubes are then grown as normally by Chemical Vapor Deposition. These ultra-dense forests are needed to use carbon nanotubes as vias and interconnects in integrated circuits and as thermal interface materials. Further density increase to 10^{14} cm^{-2} by reducing nanotube diameter is possible.

1:15PM B28.00007 Carbon Nanotubes with Temperature Invariant Viscoelasticity from -196°C to 1000°C , MING XU, Technology Research Association for Single Wall Carbon Nanotubes (TASC); AIST, Japan — Viscoelasticity describes the ability of a material to possess both elasticity and viscosity. Viscoelastic materials, such as rubbers, possess a limited operational temperature range, (e.g., for silicone rubber: -55 to 300°C) above which the material breaks down and below which the material undergoes a glass transition and hardens. This is because molecular motion that is the origin of viscoelasticity is a thermally activated process. We created a viscoelastic material composed from a random network of long interconnected carbon nanotubes that exhibited an operational temperature range from -196°C to 1000°C [1]. The viscoelastic properties (storage modulus, loss modulus, and damping ratio) measured by DMA in N_2 ambient were nearly constant over an exceptionally wide temperature range (-140°C∼600°C). As exemplified by the vibration isolator demonstration, the CNT material showed viscoelasticity beyond the DMA limitation at -190°C (immersed in liquid nitrogen) and at >900°C (exposed to butane torch). And we implemented impact tests at -196°C, 25°C and 1000°C using a steel ball and analyzed the ball tracks. The ball tracks were identical for all cases as observed by SEM and 3-D mapping that suggested unvarying viscoelastic properties across this 1200°C temperature range. We interpret that the thermal stability stems from energy dissipation through the zipping and unzipping of carbon nanotubes at contacts. Quantitatively, the viscoelastic properties by DMA showed that the CNT material possessed similar stiffness (storage modulus 1MPa), higher dissipation ability (loss modulus (0.3MPa) and damping ratio (0.3) than silicone rubber at room temperature. Further DMA characterization from -140°C to 600°C demonstrated temperature invariant frequency stability (0.1-100Hz), the same level of reversible deformation (critical strain 5%) and fatigue resistance (1,000,000 cycles, 100Hz).

[1] Xu, M.; Futaba, D. N.; Yamada, T.; Yumura, M.; Hata, K. *Science* (Accepted)

1:51PM B28.00008 Understanding Chiral-Selective Growth of Carbon Nanotubes: In-Situ Raman Studies of Individual Single Walled Carbon Nanotube Growth , RAHUL RAO, DAVID LIPTAK, TONYA CHERUKURI, DAYLOND HOOPER, Air Force Research Laboratory, BORIS YAKOBSON, Rice University, BENJI MARUYAMA, Air Force Research Laboratory — In-situ Raman scattering has been used to obtain growth kinetics of individual single-walled carbon nanotubes (SWNTs) using a custom designed cold-wall chemical vapor deposition (CVD) chamber coupled to a Raman spectrometer. Raman spectra are collected during SWNT growth and plots of the G band area versus time are fitted to self-exhausting exponential curves, from which we obtain SWNT growth rates and catalyst lifetimes (time constant). Chiral index assignments are made for several individual SWNTs via analysis of the radial breathing modes. The growth rate of the SWNTs is shown to be proportional to the chiral angle. In addition we find a positive correlation between SWNT length (obtained from SEM analysis) and the growth rate. This confirms the model put forth by Ding *et al.* [1] which links SWNT growth rate to the chiral angle. A growth model based on our results illuminates an as-yet unexplained distribution in the chiral yield of typical CVD-grown nanotubes as being driven by chiral-selective growth kinetics. [1] Ding, F; Haturyunyan, A; Yakobson, B, I; Dislocation theory of chirality-controlled nanotube growth, Proc. Natl. Acad. Sci., 106, 2506, 2009

2:03PM B28.00009 Dislocation Dynamics in Multishell Carbon Nano-Onions[1] , TRAIAN DUMITRICA, EVGENIYA AKATYEVA, University of Minnesota, JIANYU HUANG, Sandia National Laboratories — Graphite has long served as a model material to understand dislocations. An early work on natural graphite provided factual evidence for the existence of screw dislocations. Recently, synthetic carbon nanostructures began to be explored in order to understand dislocations at the nanoscale. Here we study the 1/2<0001> edge dislocation in nested multishell carbon onions [1]. We report in situ electron microscopy observations of dislocation dissociation and annihilation processes in individual nanometer-sized carbon onions. Essential for these processes is the counterintuitive motion of the 1/2<0001> edge from the outer surface to the inner region, which cross-links or unlinks a large number of shells. The correlation with atomistic simulations and analysis of the energy, which separates the strain and edge components, indicates that this inward glide originates in the reduction of edge with each inwards glide step, an effect specific to the spherical topology.

[1] E. Akatyeva, J. Y. Huang and T. Dumitrica, Phys. Rev. Lett. 105, 106102 (2010).

[1]We thank NSF CAREER Grant No. CMMI-0747684, NSF Grant No. DMR-1006706, and NSF MRSEC Grants No. DMR-0212302 and No. DMR-0819885.

Monday, March 21, 2011 11:15AM - 2:15PM –
Session B29 GQI: Advances in Ion Trap Quantum Computation C148

11:15AM B29.00001 Trapped ion arrays for quantum simulation[1] , RICHART SLUSHER, Georgia Tech Research Institute — Trapped ions have been used to demonstrate a broad range of quantum information processes with high fidelity[2] and are an obvious choice for quantum simulations. Several quantum simulations have already been demonstrated with ions.[3,4] The present goal is to simulate quantum systems that cannot be achieved with classical computation using more than 20 ions. It is challenging to assemble more than 20 ions in suitable arrays for quantum simulation of arbitrary model systems. Present ion trap based quantum simulations with up to 20 ions are now in progress. This talk describes ion trap micro-fabrication techniques and designs that have the potential to increase the number of coupled ions to the range between 50 and 100 ions. High precision ion traps are fabricated using silicon VLSI techniques on silicon wafers with aluminum electrodes.[5] At the Georgia Tech Research Institute we are designing, fabricating and testing ion trap arrays that will contain and accurately control at least 50 ions in linear chains of equally spaced ions. Large numbers of equally spaced ions have recently been shown[6] to be stable in anharmonic trap potentials that are easily obtained in the micro-fabricated traps. The limits on quantum simulation accuracy due to errors in the ion trap parameters will be discussed.

[1]Supported by IARPA and DARPA.

[2]D. Leibfried, D. J. Wineland, R. B. Blakestad, J. J. Bollinger, J. Britton, J. Chiaverini, R. J. Epstein, W. M. Itano, J. D. Jost, E. Knill, C. Langer, R. Ozeri, R. Reichle, S. Seidelin, N. Shiga, and J. H. Wesenberg, Hyperfine Interactions **174**, 1 - 7 (2007). Proc. 4th Int. Conf. Trapped Charged Particles and Fundamental Physics (TCP 2006), Parksville, Canada 3-8 Sept. 2006.

[3]K. Kim, M.-S. Chang, S. Korenblit, R. Islam, E. E. Edwards, J. K. Freericks, G.-D. Lin, L.-M. Duan, and C. Monroe, *Nature* **465**, 590 (2010).

[4]E. E. Edwards, S. Korenblit, K. Kim, R. Islam, M.-S. Chang, J. K. Freericks, G.-D. Lin, L.-M. Duan, and C. Monroe, Phys. Rev. **B 82**, 060412 (2010).

[5]D.R. Leibrandt, J. Labaziewicz, R.J. Clark, I.L. Chuang, R.J. Epstein, C. Ospelkaus, J.H. Wesenberg, J.H. Bollinger, D. Leibfried, D. Wineland, D. Stick, J. Sterk, C. Monroe, C.-S. Pai, Y. Low, R. Frahm, and R.E. Slusher, Quant. Inf. Comp. **9**, 901 (2009)

[6]G.-D. Lin, S.-L. Zhu, R. Islam, K. Kim, M.-S. Chang, S. Korenblit, C. Monroe, and L.-M. Duan, Europhys. Lett. **86**, 60004 (2009).

11:51AM B29.00002 Laser-induced charging of microfabricated ion traps , GUANG HAO LOW, MIT, SHANNON X. WANG, sxwang@mit.edu, NATHAN LACHENMYER, YUFEI GE, PETER HERSKIND, ISAAC L. CHUANG, MIT — Microfabricated ion traps are promising candidates for realizing large-scale quantum computers, but small trap sizes leads to increased sensitivity of the trapped ions to surface effects, including localized charging of the trap electrodes. Laser-induced charging on microfabricated ion traps is studied by monitoring the ion micromotion over a period of up to 20 minutes that a laser is incident on the trap. The ion is trapped 100 μm above the metal surface and the trap is operated at 6K. The lasers used are at 405, 460, and 674 nm, which are relevant atomic transitions in Sr+ ions, and the typical intensity at the trap is 10^{35} photons/sec. The ion's micromotion signal is related to the number of charges created on the trap. A wavelength and material dependence of the charging behavior is observed: lasers at lower wavelengths cause more charging, and aluminum exhibits more charging than copper or gold. We describe the charging dynamic based on a rate equation approach.

12:03PM B29.00003 Superconducting microfabricated ion traps , SHANNON X. WANG, YUFEI GE, JAROSLAW LABAZIEWICZ, MIT, ERIC DAULER, MIT Lincoln Laboratory, KARL BERGGREN, ISAAC L. CHUANG, MIT — We fabricate superconducting ion traps with niobium and niobium nitride and trap single ^{88}Sr ions at cryogenic temperatures. The superconducting transition is verified and characterized by measuring the resistance and critical current using a 4-wire measurement on the trap structure, and observing change in the rf reflection. The lowest observed heating rate is 2.1(3) quanta/sec at 800 kHz at 6 K and shows no significant change across the superconducting transition, suggesting that anomalous heating is primarily caused by noise sources on the surface. This demonstration of superconducting ion traps opens up possibilities for integrating trapped ions and molecular ions with superconducting devices.

12:15PM B29.00004 Microfabricated surface trap for scalable ion-photon interfaces , PETER HERSKIND, SHANNON WANG, MOLU SHI, YUFEI GE, MARKO CETINA, ISAAC CHUANG, MIT — The combination of high-finesse optical mirrors and ion traps is attractive for quantum light-matter interfaces, which represents an enabling resource for large-scale quantum information processing. We report on a scalable approach to ion-photon interfaces based on a surface electrode ion trap microfabricated on top of a highly reflective mirror. An aperture in the central electrode, directly below the ion, allows the mirror to interact with the ion. The integration of such mirrors is scalable as several mirror apertures may be added with no additional overhead for fabrication. Furthermore, the design provides a path for reaching the strong coupling regime of Cavity QED, where an ion-cavity system can be realized by adding a small concave mirror above the trap mirror. The quality of the mirror is not significantly compromised in the course of fabrication and we have measured an increase in losses for light at 422 nm at the level of 100 ppm. The functionality of the mirror has also been verified by light collection from, and imaging of, the ion 169 ± 4 μm above the mirror. Despite its proximity, we find that the presence of the mirror does not perturb the trap. Trapping is stable with laser cooled ion lifetimes of several hours and we observe only minimal sensitivity to laser-induced charging. Furthermore, through operation of the trap in a cryostat at 15 K the heating rate of the ion is a the level of only 0.1 quanta/ms.

12:27PM B29.00005 Ion crystal transducer for strong coupling between single ions and single photons , LUCAS LAMATA, Max-Planck-Institut fuer Quantenoptik, DAVID LEIBRANDT, National Institute of Standards and Technology, ISAAC CHUANG, Center for Ultracold Atoms, Department of Physics, MIT, IGNACIO CIRAC, Max-Planck-Institut fuer Quantenoptik, MIKHAIL LUKIN, ITAMP, Harvard-Smithsonian Center for Astrophysics, and Department of Physics, Harvard University, VLADAN VULETIC, Center for Ultracold Atoms, Department of Physics, MIT, SUSANNE YELIN, ITAMP, Harvard-Smithsonian Center for Astrophysics, and Department of Physics, University of Connecticut — A quantum interface between single photons and single ions in an ion crystal is proposed. The coupling between single photon and single particle is collectively enhanced via a collective internal ion state and a phonon state. Applications for this scheme include single-photon generation, a memory for a quantum repeater, and a deterministic photon-photon or photon-ion entangler.

12:39PM B29.00006 Temperature driven structural phase transition for trapped ions , ZHE-XUAN GONG, GUIN-DAR LIN, LU-MING DUAN — A Wigner crystal formed with trapped ion can undergo structural phase transition, which is determined only by the mechanical conditions on a classical level. Instead of this classical result, we show that through consideration of quantum and thermal fluctuation, a structural phase transition can be solely driven by change of the system's temperature. We determine a finite-temperature phase diagram for trapped ions using the renormalization group method and the path integral formalism, and propose an experimental scheme to observe the predicted temperature-driven structural phase transition, which is well within the reach of the current ion trap technology.

12:51PM B29.00007 Differential Stark shift measurement of clock states of Yb+ using an optical frequency comb , QUDSIA QURAISHI*, DAVID HAYES, DAVID HUCUL, DZMITRY MATSUKEVICH, SHANTANU DEBNATH, SUSAN CLARK, CHRIS MONROE, JQI, Univ of Maryland Dept of Physics and NIST — Quantum information processing with trapped ions has traditionally involved state preparation, manipulation (eg. quantum gates) and detection using CW lasers. Quantum gates implemented with ions typically involve optical Raman transitions between two atomic levels. An optical frequency comb, emitted by a pulsed laser, is an excellent tool for bridging atomic frequency differences. Previously, we demonstrated quantum gates and separately, ultrafast spin manipulation, using pulsed lasers [1,2]. Unlike the CW case, employing pulsed lasers has the marked advantage of both low spontaneous emission and low AC Stark shifts, because the high powers available from pulsed lasers allow for larger detunings from optical resonance. Here, we show both experimentally and theoretically the scaling of the differential Stark shift with detuning (6 THz to 20 THz) of the Raman fields, achieving values of 10^{-3} of the Rabi frequency. [1] D. Hayes, et al., Phys. Rev. Lett. 104, 140501 (2010) [2] W. C. Campbell, et al., Phys. Rev. Lett. 105, 090502 (2010). *Currently NRC postdoc with SEDD, ARL, Adelphi, MD. Support: DARPA OLE under ARO contract, IARPA under ARO contract, NSF PIF Program, NSF PFC at JQI and *IC Postdoc administered by the NGA.

1:03PM B29.00008 "Tack" ion trap for efficient photon collection.[1] , CHEN-KUAN CHOU, GANG SHU, NATHAN KURZ, THOMAS NOEL, JOHN WRIGHT, BORIS BLINOV, University of Washington — Trapped, laser-cooled atoms and ions produce intense fluorescence of the order 10^7 – 10^8 photons per second. Detection of this fluorescence enables the efficient measurement of the quantum state of qubit based on the trapped atoms. Thus, it is desirable to collect a large fraction of the (isotropically emitted) photons to make the detection faster and more reliable. Additionally, efficient fluorescence collection can improve the speed and fidelity of remote ion entanglement and quantum gates. Refractive and reflective optics, as well as optical cavities, and, recently, bare multimode optical fibers have all been used to collect the trapped ion fluorescence with up to 10% efficiency. Here we show a novel ion trap design that incorporates a high numerical aperture metallic spherical mirror as the integral part of the trap itself (the RF electrode) which enables up to 35% solid angle collection of trapped ion fluorescence. The movable central needle-shaped electrode of this "tack" trap allows precise placement of the ion at the focus of the spherical mirror. We also study the properties of the images formed by the spherical mirror and comment on possible methods for aberration correction. Owning to the simplicity of its design, this trap structure can be adapted for mircofabrication and integration into more complex trap architectures.

[1]Supported by National Science Foundation and IARPA

1:15PM B29.00009 Towards laser cooling of a LC-resonator via trapped ions , SOENKE MOELLER, NIKOS DANIILIDIS, UC Berkeley, BOYAN TABAKOV, University of New Mexico, AARON BRADLEY, HARTMUT HAEFFNER, UC Berkeley — We will discuss our experimental progress towards coupling strings of trapped ions to an LC-resonator. The goal of our experiments is to cool the resonant mode of a superconducting high-quality resonant circuit to ultra-low temperatures. By continuously laser cooling a crystal of ions coupled to the circuit, energy is removed from the resonator. For quality factors on the order of 10^5, the time-scale of the environment-to-mode coupling, i.e. the time for the resonant mode of the LC-resonator to thermally equilibrate, can be on the order of a second. Thus, engineering an ion-resonator coupling of 10$\sim$kHz results in a reduction of the electronic temperature by four orders of magnitude as compared to the ambient temperature of the resonator. The expected temperatures below 1mK are extremely low approaching even the vibrational ground state of the oscillator mode, enabling novel quantum electronics applications in the solid state.

1:27PM B29.00010 Micro-Fabricated Surface Electrode Y-Junction Ion Traps , DAVID MOEHRING, MATTHEW BLAIN, ROBERT COOK, KEVIN FORTIER, RAYMOND HALTLI, CLARK HIGHSTRETE, DANIEL STICK, CHRIS TIGGES, Sandia National Laboratories — We will present results of the design, operation, and performance of two different Y-Junction surface ion micro-traps fabricated at Sandia. Recent progress in the testing of the micro-traps will be highlighted, including the successful shuttling of single and multiple ions, ion-chain splitting and recombination, and the validation of simulations with experiments. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

1:39PM B29.00011 Emergent effective spin models in ion-trap-based quantum simulators[1] , CHENG-CHING JOSEPH WANG, Georgetown University, UMD AND JQI COLLABORATION — We show how effective spin models emerge from the interaction of laser light with the ions in a linear Paul trap. It has been shown that quantum Ising models can be studied by adiabatic state evolution in a transverse magnetic field which is ramped from large to small values. The standard proof involves and adiabatic elimination of the phonons in the Lamb-Dicke regime. We discuss here that such an elimination can be problematic due to the inherent entanglement between the spins and the phonons. If the magnetic field is ramped sufficiently fast, one can show that all quantum state probabilities measured along the Ising field axis are independent of the phonons. But if the field is ramped more slowly, then the phonons and spins become entangled. Nevertheless, the main effects are to change the spin entanglement of the quantum states rather than the probabilities of the different states in the wavefunction. We present numerical evidence to illustrate these points.

[1]This work was supported under ARO grant number W911NF0710576 with funds from the DARPA OLE Program.

1:51PM B29.00012 Individual addressing of trapped ions using a MEMS beam steering system , TAEHYUN KIM, CALEB KNOERNSCHILD, EMILY MOUNT, STEPHEN CRAIN, RACHEL NOEK, DANIEL GAULTNEY, PETER MAUNZ, JUNGSANG KIM, Duke University — Implementation of single-qubit and two-qubit quantum gates in a long linear chain of trapped ions generally requires the manipulation of qubits stored in individual ions using a set of laser beams. Individual addressing has been demonstrated with acousto-optic and electro-optic deflectors, by using the Zeeman shift due to a magnetic field gradient, and by separating the ions. Microelectromechanical system (MEMS) technology offers an alternative approach using micromirrors to focus laser beams on individual ions. Advantages of this approach are its broadband optical performance and scalability to more beams and multiple dimensions. We report progress towards integrating a MEMS beam steering system with an Yb ion trap experiment. The MEMS system will direct an ultraviolet beam with waist of $\sim$1.5μm at the ions across a 20μm range. For a designed ion separation of 4um this allows addressing up to 5 ions. The far-detuned laser will induce an AC Stark shift on a single ion in the chain, and the induced phase shift can be measured by Ramsey spectroscopy.

2:03PM B29.00013 Scalable micro-scale optics for planar ion traps , TRUE MERRILL, Georgia Institute of Technology, HARLEY HAYDEN, CHIEN-SHING PAI, Georgia Tech Research Institute, RACHEL NOEK, JUNGSANG KIM, Duke University, CURTIS VOLIN, Georgia Tech Research Institute — Efficient collection of fluorescence from atomic ions is required for fast high-fidelity measurement in ion trap quantum information processing. Conventional multi-element lens stacks can achieve photon collection efficiencies as high as 5%, however these systems typically have restricted field-of-view and are not generally scalable to image large arrays of ions. We report the development and fabrication of planar traps with integrated micro-scale spherical mirrors with an expected 15% collection efficiency. The mirror shape is controlled with a combination of silicon wet-processing and polishing techniques while maintaining a surface roughness below $\sigma_{RMS} < 10$ nm. The design allows for multiple integrated mirrors in a single chip allowing for the simultaneous measurement of many ions over a 10 mm object space.

Monday, March 21, 2011 11:15AM - 2:15PM –
Session B30 DCMP: Graphene: Transport and Correlations C147/154

11:15AM B30.00001 Magnetoconductance Oscillations in High-Mobility Suspended Bilayer and Trilayer Graphene , WENZHONG BAO, ZENG ZHAO, HANG ZHANG, GANG LIU, PHILIP KRATZ, LEI JING, JAIRO VELASC, DMITRY SMIRNOV, CHUN NING LAU, DEPARTMENT OF PHYSICS, UNIVERSITY OF CALIFORNIA, RIVERSIDE, RIVERSIDE, CA 92521 TEAM, NATIONAL HIGH MAGNETIC FIELD LABORATORY, TALLAHASSEE, FL 32310 COLLABORATION — We observed pronounced magnetoconductance oscillations on suspended bilayer and trilayer graphene devices with mobilities up to 270,000 cm^2/Vs. For bilayer devices, we observe conductance minima at all integer filling factors n between 0 and -8, as well as a small plateau at n=1/3. For trilayer devices, we observe features at n=-1, -2, -3 and -4, and at n$\sim$0.5 that persist to 4.5K at B=8T. All of these features persist for all accessible values of Vg and B, and could suggest the onset of symmetry breaking of the first few Landau (LL) levels and fractional quantum Hall states.

11:27AM B30.00002 Novel Excitonic Effects in Graphene and Bilayer Graphene[1] , LI YANG, Department of Physics, Washington University in St. Louis — Through first-principles calculations with many-body effects included, we have revealed unique excitonic effects in the high-frequency regime (10 $\sim$ 20 eV) of optical spectra of graphene and bilayer graphene (BLG). Despite their different symmetries, the parallel σ and π* bands result in enhanced excitonic effects in such two-dimensional semimetals; one narrow resonant exciton is discovered to form an isolated peak below the prominent absorption continuum with a surprisingly large binding energy, 270 meV in graphene and 80 meV in BLG. Moreover, because of its extremely weak resonant character, this exciton exhibits a bound electron-hole wave function.

[1]Computational resources are provided by Lonestar of Teragrid at the Texas Advanced Computing Center.

11:39AM B30.00003 Metal-insulator transitions in graphene , MARIO AMADO, Universidad Complutense de Madrid, Spain, ENRIQUE DIEZ, Universidad de Salamanca, Spain, FRANCESCO ROSSELLA, VITTORIO BELLANI, Universita degli Studi de Pavia, Italy, DAVID LOPEZ-ROMERO, CT-ISOM Universidad Poletcnica de Madrid, Spain, DUNCAN MAUDE, Laboratoire national des champs magnetiques intenses, Grenoble, France — We investigate the metal-insulator quantum phase transitions that appear in the quantum Hall effect, namely the plateau-insulator and plateau-plateau transitions We have performed magnetotransport experiments with the magnetic field as the driving parameter in the temperature range from 4K up to 230K and magnetic fields up to 28T. The analysis of the temperature dependence of the Hall and longitudinal resistivity reveals the non-universality of the critical exponent for the metal-insulator transition when varying the density of carriers. We also find relevant discrepancies with recent works concerning the value of the critical exponent of the plateau-plateau transition.

11:51AM B30.00004 Conductivity of Coulomb interacting massless Dirac particles in graphene[1]

, VLADIMIR JURICIC, Lorentz-Instituut for Theoretical Physics, Universiteit Leiden, The Netherlands, OSKAR VAFEK, National High Magnetic Field Laboratory and Department of Physics, Florida State University, USA, IGOR HERBUT, Department of Physics, Simon Fraser University, Canada — The ac conductivity of the Coulomb interacting Dirac fermions in graphene is considered in the collisionless regime using a variant of the dimensional regularization with the spatial dimension $D = 2 - \epsilon$ for $\epsilon > 0$. We show that this regularization procedure preserves the Ward-Takahashi identity associated with the charge conservation [1], and as such it can serve as a consistent regularization of the entire interacting field theory. As a consequence of the explicitly preserved $U(1)$ gauge symmetry, the dimensional regularization yields the same result for the Coulomb correction to the conductivity when calculated using the current-current and the density-density correlators, which is, nevertheless, different than the ones previously reported in the literature. References: [1] V. Juricic, O. Vafek, and I. F. Herbut, ArXiv:1009.3269 (Phys. Rev. B, in press).

[1]V. J. acknowledges the support of the Netherlands Organization for Scientific Research.

12:03PM B30.00005 Plasma Excitations of Dressed Dirac Electrons in Graphene[1]

, OLEKSIY ROSLYAK, Hunter College, CUNY, DANHONG HUANG, AFRL, Kirkland Airforce Base, ANDRII IUROV, GODFREY GUMBS, Hunter College, CUNY — The dispersion relation for the collective plasma excitations of optically dressed Dirac electrons in single and double graphene layers is calculated in the random-phase approximation. The presence of circularly polarized light gives rise to an energy gap ϵ_g between the conductance and valence bands. The value of ϵ_g may be adjusted by varying the frequency and intensity of the light which could be sizable compared to that which is generated by spin-orbit coupling or sub-lattice symmetry breaking. We present numerical results for the dispersion relation for plasma excitations for various energy gaps and separation between graphene layers. The induced ϵ_g opens up a gap in the particle-hole continuum thus allowing plasmon excitations of short wave-length. An optical and acoustic phonon-like modes are obtained in the double layer configuration. Those are very sensative to the induced energy gap and symmtry breaking between the layers.

[1]This work was supported by contract # FA 9453-07-C-0207 of AFRL and the Air Force Office of Scientific Research (AFOSR).

12:15PM B30.00006 Variational approach to the excitonic phase transition in graphene[1]

, FERNANDO SOLS, Universidad Complutense de Madrid, JAVIER SABIO, FRANCISCO GUINEA, ICMM-CSIC (Madrid) — We analyze the Coulomb interacting problem in undoped graphene layers by using an excitonic variational ansatz. By minimizing the energy, we derive a gap equation which reproduces and extends known results. We show that a full treatment of the exchange term, which includes the renormalization of the Fermi velocity, tends to suppress the phase transition by increasing the critical coupling at which the excitonic instability takes place.

[1]Supported by MICINN (Spain), FIS2008-00124 and FIS2010-21372.

12:27PM B30.00007 First-principles study of polarization in graphene

, PRIYAMVADA JADAUN, YUGUI YAO, LEONARD F. REGISTER, QIAN NIU, SANJAY BANERJEE, The University of Texas at Austin — The emergence of polarization in monolayer graphene is investigated using first-principles calculations. We try to understand electronic polarization calculated using Berry phase technique as well as ionic polarization when in-plane symmetry is broken within the graphene lattice. The effect of underlying substrate as well as stress on this symmetry breaking is also explored.

12:39PM B30.00008 Graphene K and K' States at the Dirac Point

, LAWRENCE SNYDER, CHRISTOPHER WELLS, The University at Albany - SUNY, Chemistry Department — The graphene band structure states at the K and K' points and the Fermi level, the Dirac point, computed when a (1x1) unit cell is employed, fall at the gamma point when a (3x3) unit cell is employed. These states at the gamma point of the Brillouin zone for the (3x3) unit cell have a zero phase factor and are conveniently represented as molecular orbitals of pi electrons. These states are illustrated and discussed.

12:51PM B30.00009 Edges states and anomalous Aharonov-Bohm-type oscillation in anti-dot lattice graphenes formed by nanoporous alumina template mask

, J. HARUYAMA, T. SHIMIZU, J. NAKAMURA, Aoyama Gakuin University, T. MATSUI, H. FUKUYAMA, Tokyo University — Edge states of graphene with a zigzag structure theoretically have extremely high electronic density of states (EDOS), electron localization, and polarized spin transport as well [1]. However, few studies have reported on the experimental observation of edge states and related quantum phenomena. Here, we report on the nonlithographic and low-damage fabrication of honeycomb-like nanopore arrays (anti-dot lattice) on thin multilayered graphenes utilizing nanoporous alumina template masks [2]. We confirm the presence of high EDOS at the edges of the nanopores using STM observation. We find periodic magnetoresistance oscillations with two different periods over a wide magnetic field range (anomalous Aharonov-Bohm-type effect [3]) (e.g., high fields at where the diameter of cyclotron-motion electrons is smaller than diameter of the nanopore). These findings clearly suggest the presence of localized electrons and edge states at the nanopore edges of graphene.

[1] K. Nakada, G. Dresselhaus, M. S. Dresselhaus et al., Phys. Rev. B 54, 17954 (1996).
[2]T. Shimizu, J. Haruyama et al., To be published on Phys. Rev. Lett.
[3] D. Weiss, K.von Klitzing et al., Phys. Rev. Lett. 70, 4118 (1993).

1:03PM B30.00010 Snake orbits in graphene underneath an array of $Ni_{0.80}Fe_{0.20}$ nano-dots

, ADAM NEAL, JIANGJIANG GU, TONY LOW, PEIDE YE, Purdue University — The existence of snake orbits in 2DEG formed at AlGaAs/GaAs heterojunction is theoretically predicted and experimentally demonstrated by creating a spatially inhomogeous magnetic field [1]. Due to its ambipolar nature, graphene opens up new possibilities to investigate snake orbits and other exotic phenomena by simply creating a p-n junction in a homogenous magnetic field. We have fabricated periodic arrays of $Ni_{0.80}Fe_{0.20}$ nano-dots on graphene with the dot diameter of 80 nm or 150 nm and the period of 160 nm or 300 nm, respectively. A quasi-periodic magneto-resistance oscillation is observed in the low-temperature magneto-transport measurement. We ascribe it to Aharonov-Bohm oscillations induced by snake orbits of carriers underneath the nano-dots. Due to the high work-function of $Ni_{0.80}Fe_{0.20}$, it is possible to generate local circular n-p and p–p junctions underneath the nanodots, which form the snake orbits of carriers in an external applied magnetic field. Dependence of these oscillations on temperature and carrier density and simulation work on snake orbits will be presented.

[1] J.E. Muller, Phys. Rev. Lett. 68, 385 (1992); P.D. Ye et al., Phys. Rev. Lett. 74, 3013 (1995).

1:15PM B30.00011 Metal Electrode Effect on Electronic Transport through Graphene

, CHENG GONG, WEICHAO WANG, GEUNSIK LEE, BIN SHAN, KYEONGJAE CHO, Department of Materials Science and Engineering, The University of Texas at Dallas — Metal-graphene contact is one of key issues in graphene-based device applications. In this work, electronic transport through metal/graphene/metal end-contact structures with zigzag interface is investigated by first-principles non-equilibrium Green's function method. Double-dips transmission characteristics in Palladium/Graphene/Palladium are observed with a common positive dip and varied negative dips for graphene of different lengths. Transmission through the structure is suppressed by mode mismatch among different carbon localities perturbed by interface hybridization, yet intensities of the suppression at two dips are featured by distinctive channel potential profiles. Finite transmissions at Fermi level are attributed to both evanescent and propagating modes. This study benefits the understanding of the origins of contact resistance at metal/graphene interfaces.

1:27PM B30.00012 Casimir Interaction Between Graphene and Planar Systems[1] , DAVID DROSDOFF, LILIA WOODS, University of South Florida — Casimir forces become increasingly important as systems become miniaturized. Such fluctuation forces are studied between graphene, a potential future substitute for silicon based electronics, and other materials. Because graphene is one atomic layer thick, the Casimir force is relatively weak. Yet its singular electronic properties give rise to an attraction between graphene layers in the order of a factor of $\alpha \approx 1/137$ times smaller than the interaction between two ideal metal plates. For the case of the interaction between graphene and metamaterials, a strong reduction in the Casimir attraction or even repulsion may be found if the metamaterial is mostly magnetic in nature. Metamaterials with strong magnetic responses in the optical range may soon be possible as the rapid development of metamaterials continue. Other graphene configurations with metals and metamaterials are also studied.

[1]Financial support from the Department of Energy under contract DE-FG02-06ER46297 is acknowledged.

1:39PM B30.00013 Hot electron dynamics and Schwinger mechanism in graphene[1] , MENG-CHIEH LING, JÖRG SCHMALIAN, Ames Laboratory and Iowa State University — We investigate the nonlinear dc conductivity of graphene by explicitly solving the Boltzmann equation with relaxation and particle-hole pair production contributions and obtain the non- equilibrium electronic distribution function. First, by considering isotropic elastic electron-phonon scattering, we show that, in the limit of weak external electric field one recovers Ohm's law, while above a threshold field $E = (k_B T)/(ev_F\tau)$ the dc conductivity varies as the inverse of the external electric field. In particular, we obtain an explicit form for the scaling of the conductivity with respect to E/T. We then investigate how this result is affected by the Schwinger mechanism, which leads to particle-hole creation and, consequently, to interband transitions.

[1]Research supported by the U.S. DOE, Office of BES, Materials Science and Engineering Division

1:51PM B30.00014 Band structures of bilayer graphene superlattices , SI WU, MATTHEW KILLI, ARUN PARAMEKANTI, University of Toronto — We have studied the electronic band structures of bilayer graphene (BLG) superlattices. In BLG, there are two distinct types of superlattice modulations - chemical potential modulations and electric field induced gap modulations. We have solved energy bands for one- and two-dimensional superlattices for both kinds of modulations. We found, in particular, for a 2D superlattice with gap modulation, that the energy gap is one order smaller than that in a uniform electric field. The problem of a single charged impurity in gated BLG is also studied. Implications of our results on transport experiments are discussed.

2:03PM B30.00015 Giant inelastic tunneling in epitaxial grapheme mediated by localized states , KEES FLIPSE, KEVIN RUIT VAN DE, Eindhoven University of technology, JIRI CERVENKA, Academy of Sciences of the Czech Republic — Local electronic structures of nanometer-sized patches of epitaxial grapheme and its interface layer with SiC(0001) have been studied by atomically resolved scanning tunneling microscopy and spectroscopy. Localized states belonging to the interface layer of the graphene/SiC system show to have essential influence on the electronic structure of grapheme. Giant enhancement of inelastic tunneling, reaching 50% of the total tunneling current, has been observed at the localized states on a nanometer-sized graphene monolayer surrounded by defects.

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B31 DMP: Focus Session: van der Waals Bonding in Advanced Materials: Applications to Systems and Behaviors C145

11:15AM B31.00001 Physisorbed molecules: How their frictional and diffusive properties impact lubricity[1] , JACQUELINE KRIM, North Carolina State University — Friction and its consequences are of great concern from both a national security and quality-of-life point of view, and the economic impact of energy efficiency, wear, and manufacturing cannot be underestimated [1]. Lubrication schemes for many macroscopic applications have been solved, but an era of science and engineering is emerging where control of mechanical and electrical systems at the atomic level will be required [2]. A fundamental understanding of the dissipative and frictional properties of weakly adsorbed films, which are ubiquitous in these systems, is key to a vast range of emerging applications. This talk will begin with a discussion of how diffusive and frictional properties of adsorbed atoms and molecules governed by van der Waals interactions can be measured experimentally [3]. Selected example of how atomic scale mobility in physisorbed materials, even at very low coverage, can directly impact friction, tribological performance and/or device viability will then be presented, for systems spanning Micro- and Nano- ElectroMechanical Systems to avalanches in granular materials [4,5].

[1] "Surface science and the atomic-scale origins of friction: what once was old is new again", J. Krim, Surface Science **500** (1-3): 741-758, (2002)
[2] "QCM tribology studies of thin adsorbed films", J. Krim, Nano Today 2 (5): 38-43, (2007)
[3] "Sliding friction measurements of molecularly thin ethanol and pentanol films: How friction and spreading impact lubricity", B.P. Miller and J. Krim, J. Low. Temp. Phys., **157,** Special issue on Wetting, Spreading, and Filling, p 252 (2009)
[4] "Friction, Force Chains and Falling Fruit ", J. Krim and R.P. Behringer, Physics Today, **62,** pp. 66-67 (Sept. 2009)
[5] "Atomic-scale lubrication at ultra-low vapor coverages", D.A. Hook, B.P. Miller, B.M. Vlastakis, M.T. Dugger and J. Krim, submitted

[1]Work supported by NSF and AFOSR.

11:51AM B31.00002 Edge-dependent Static Friction of Adsorbed van der Waals Islands[1] , NICOLA VARINI, Udine Univ., Int. School Adv. Stud. (SISSA), CNR-IOM DEMOCRITOS, FURIO ERCOLESSI, Udine Univ., UGO TARTAGLINO, ANDREA VANOSSI, Int. School Adv. Stud. (SISSA), CNR-IOM DEMOCRITOS, ERIO TOSATTI, Int. School Adv. Stud. (SISSA), CNR-IOM DEMOCRITOS, ICTP — Rare gas islands adsorbed through van der Waals forces on metal surfaces do not slide freely, but exhibit static friction in QCM experiments. Static friction appears, unexpectedly, even for incommensurate and defect-free crystal surfaces, where sliding should be frictionless. Via atomistic simulations of Kr islands on Au(111), we show that the island edges may be the ultimate culprits. Adsorbate sliding requires the flow of solitons - tiny density and corrugation modulations with the beat periodicity between the two periodicities. For an island, we find an edge-originated energy barrier that blocks the soliton flow, keeping the island pinned. As the static friction force is reached, the barrier vanishes at one point on the edge, and new solitons enter the island, which becomes depinned. Unsurprisingly, we find that low surface corrugation and high temperature facilitate this edge depinning. However, the island's thermal expansion is large and leads to changeable commensurability upon heating, which gives rise to the possibility of re-entrant static friction.

[1]Supported by ESF FANAS/AFRI sponsored by the Italian CNR

12:03PM B31.00003 Why viscosities of Ne and Kr monolayers are so different on the Pb(111) surface[1] , RUQIAN WU, YANNING ZHANG, University of California, Irvine, V. BORTOLANI, Università di Modena e Reggio Emilia, Italy — Adsorption and segregation of Ne and Kr monolayers on the Pb(111) surface are examined through density functional calculations to understand the puzzling experimental observations of different tribological properties of these two rare gases. Theoretical results reveal weak but non-negligible interaction between rare gas and Pb(111), manifested as charge polarization and orbital intermixing. Because of its large atomic size, orbital polarizability and wave function extension, Kr binds with Pb(111) more strongly than does Ne. The activation energy of Kr segregation from the ground state hcp site to the metastable fcc site is 3.8 meV, substantially larger than that of Ne, 2.1 meV. This explains the drastic difference between the viscosities of Ne and Kr over Pb(111), observed at low temperatures using a quartz-crystal microbalance technique.

[1]Work was supported by DOE, Basic Energy Science, and NERSC.

12:15PM B31.00004 Tribological Characterization of Nanoclustered Lead Films , KEELEY M. STEVENS, JACQUELINE KRIM, North Carolina State University — For thin films of Pb on Ti, a system which does not wet, it is known that when studying coverages below the percolation transition measurement of surface friction via a sliding gas monolayer is an effective probe of electronic structure for the isolated lead nanoclusters.[1] This technique is capable of studying superconductors as they pass through the transition temperature. Motivated by on-going reports of quantum size effects in thin lead films grown on Si(111)[2] and Cu(001),[3] we examine the issue of nitrogen adsorption[4] onto such nanostructured films. Funding provided by NSF DMR.

[1]Highland, M. et al. in preparation.
[2]Ozer, M. et al. *J. Low Temp Phys.* **2009**, 157: 221-251.
[3]Li, W. et al. *Phys.Rev.B* **1993**, 48, 11: 8336-8344.
[4]Krim, J.and Widom, A. *Phys. Rev. B* **1988**, 38: 12184-12189.

12:27PM B31.00005 van der Waals bonded materials: vanadium pentoxide bulk structure , ELISA LONDERO, ELSEBETH SCHROEDER, Chalmers University of Technology — In this work we present a computational study of the layered oxide structure of vanadium pentoxide (V_2O_5) using the vdW-DF functional (M. Dion et al., Phys.Rev.Lett. **92**, 246401 (2004); T. Thonhauser et al., Phys. Rev. B **76**, 125112 (2007); K. Lee et al., Phys. Rev. B **82**, 081101 (2010)) which has proven to be able to capture the essential van der Waals interactions across matter separated by charge voids. We show that these forces play a substantial role for the description of the lattice constants and cohesion of this compound. In addition we document and handle a sensitivity to numerical noise in the evaluation of some exchange versions used with nonlocal correlation.

12:39PM B31.00006 Stacking and Registry Effects in Layered Materials: The Case of Hexagonal Boron Nitride , LEEOR KRONIK, NOA MAROM, Weizmann Institute of Science, JONATHAN BERNSTEIN, Tel Aviv University, JONATHAN GAREL, Weizmann Institute of Science, ALEXANDRE TKATCHENKO, Fritz Haber Institut, ERNESTO JOSELEVICH, Weizmann Institute of Science, ODED HOD, Tel Aviv University — The interlayer sliding energy landscape of hexagonal boron nitride (h-BN) is investigated via a van der Waals corrected density functional theory approach. It is found that the main role of the van der Waals forces is to anchor the layers at a fixed distance, whereas the electrostatic forces dictate the optimal stacking mode and the interlayer sliding energy. A nearly free-sliding path is identified, along which band gap modulations of 0.6 eV are obtained. We propose a simple geometric model that quantifies the registry matching between the layers and captures the essence of the corrugated h-BN interlayer energy landscape. The simplicity of this phenomenological model opens the way to the modeling of complex layered structures, such as carbon and boron nitride nanotubes. Reference: Marom et al., Phys. Rev. Lett. 105, 046801 (2010).

12:51PM B31.00007 van der Waals binding and band structure effects in graphene overlayers and graphane multilayers[1] , PER HYLDGAARD, JOCHEN ROHRER, Chalmers University of Technology — We study graphene formation (by selective Si evaporation) and adhesion on SiC surfaces as well as stacking and binding of graphane multilayers [1] using a number of versions of the van der Waals Density Functional (vdW-DF) method [2] and plane-wave density functional theory calculations. For the graphene/SiC systems and for the graphane multilayers we document that the bonding is entirely dominated by van der Waals (vdW) forces. At the same time we find that dispersive forces acting on the layers produce significant modifications in the graphene and graphane band structure. We interpret the changes and discuss a competition between wave function hybridization and interaction with the charge enhancement (between the layers) that results from density overlap.

[1] J. Rohrer and P. Hyldgaard, http://arxiv.org/abs/1010.2925
[2] Dion et al, PRL 92, 246401 (2004); V.R.Cooper, PRB 81, 161104(R) (2010), K. Lee et al PRB 82, 081101(R) (2010).

[1]Supported by Svenska Vetenskapsrådet VR #621-2008-4346.

1:03PM B31.00008 Noble gas adsorption on carbon nanotubes: insight from a van der Waals density functional study , DE-LI CHEN, WISSAM AL-SAIDI, KARL JOHNSON, University of Pittsburgh — Adsorption of nobel gases (Ar, Kr, Xe) on metallic and semiconducting carbon nanotubes (CNTs) is investigated using the van der Waals density functional (vdW-DF) developed by the Lundqvist and Langreth groups. Standard local and semi-local density functional methods do not describe nonlocal dispersive forces and fail in these systems. We found that the noble gases are underbound or even unbound with the generalized gradient approximation, while the bonding distance is underestimated at the local density approximation level of theory. In contrast, the vdW-DF approach gives considerable improvement in the description of the adsorption energies. We found no difference in the adsorption between the metallic and semiconducting nanotubes, indicating that the adsorption energies for rare gases on carbon nanotube are not strongly influenced by differences in the electronic structure of the nanotubes. The adsorption energies predicted from classical potentials are smaller than those from vdW-DF calculations by about 10-35%.

1:15PM B31.00009 Water droplet distributions in pure and functionalized single walled carbon nanotubes , CALLEN JOHNSON, The University of Tulsa, SUPRIYO GHOSH, XENIA TOMBOKAN, Bruker Corporation, PARAMESWAR HARI, The University of Tulsa, BRUKER CORPORATION TEAM, UNIVERSITY OF TULSA TEAM — In this study we investigated water droplet distribution in (1-2 nm diameter and 30 μs long) single walled carbon nanotubes (SWCNT) using time domain nuclear magnetic resonance (NMR). Annealing SWCNTs at 400°C resulted in a carbon nanotube with closed ends. We attached various amounts of water on the annealed SWCNT samples and measured the NMR spin-spin relaxation (T_2) distribution profile. The T_2 distributions were analyzed using the inverse Laplace transform to estimate the amount of water attached to the SWCNT. We performed NMR measurements on water distributions in pure CNT and functionalized CNT with OH and COOH radicals. The T_2 distribution curves for pure and functionalized SWCNTs show significant difference in water attachment. We also studied water distribution profile with the SWCNTs annealed at 800°C. Annealing at 800°C opens the ends of the SWCNTs. T_2 distribution curves at 400°C and 800°C will be compared to obtain the amount of free water attached on the outer and inner surface of pure and functionalized SWCNTs.

1:27PM B31.00010 How do hybrid functionals, dispersion interactions and quantum nuclei affect the structure of liquid water? , ZHAOFENG LI, ROBERT A. DISTASIO JR., ROBERTO CAR, Princeton University, XIFAN WU, Temple University — We report *ab-initio* molecular dynamics simulations of liquid water at STP and at the volume corresponding to experimental equilibrium density. These simulations are based on the hybrid functional PBE0 for the electrons and include approximate dispersion interactions according to Ref [1]. Nuclear quantum corrections were included as estimated by Ref [2]. We find that all of these components are important to significantly improve the agreement of the simulated structure with recent experimental analyses based on neutron and X-ray diffraction[3] and on NMR experiments. [4]

[1]A. Tkatchenko and M. Scheffler, Phys. Rev. Lett. **102**, 073005 (2009).
[2]J. Morrone and R. Car, Phys. Rev. Lett. **101** , 017801 (2008).
[3] A. Soper and C. Benmore, Phys. Rev. Lett. **101** , 065502(2008).
[4]K. Modig, B. Pfrommer, B Halle, Phys. Rev. Lett. **90** , 075502 (2003).

1:39PM B31.00011 Density, structure and dynamics of water: the effect of Van der Waals interactions[1] , MARIVI FERNANDEZ-SERRA, JUE WANG, Stony Brook University, GUILLERMO ROMAN, Universidad Autonoma de Madrid, EMILIO ARTACHO, University of Cambridge, JOSE SOLER, Universidad Autonoma de Madrid — We present a DFT AIMD study of liquid water using several GGA functionals as well as the van der Waals density functional (vdW-DF) of Dion et al. [PRL 92, 246401(2004)]. As expected, we find that the density of water is grossly underestimated by GGA functionals. When a vdW-DF is used, the density improves drastically and the experimental diffusivity is reproduced without the need of thermal corrections. We analyze the origin of the density differences between all the functionals. We show that the vdW-DF increases the population of non-H-bonded interstitial sites, at distances between the first and second coordination shells. However, it excessively weakens the H-bond network, collapsing the second coordination shell. This structural problem is partially associated to the choice of GGA exchange in the vdW-DF. We show that a different choice for the exchange functional is enough to achieve an overall improvement both in structure and diffusivity. Jue Wang et al. J. Chem. Phys, 133, (2010).

[1]1This work is supported by DOE award numbers DE-FG02-08ER46550 and DE-SC0003871.

1:51PM B31.00012 Van der Waals Density Functional Simulations of Liquid Water[1] , JUN WU, CUI ZHANG, GIULIA GALLI, FRANCOIS GYGI, University of California Davis, Davis, CA95616 — We compare two versions of van der Waals density functionals (DRSLL [1], LMKLL [2]) in electronic structure computations of weakly bonded systems. The functionals are implemented in the Qbox code [3] and are verified by reproducing published binding energies and equilibrium separations of several weakly bonded dimers. Vibrational frequencies of the water monomer and dimer computed using the above van der Waals functionals are not improved compared to PBE results. We present results of molecular dynamics simulations of liquid water using the DRSLL and LMKLL functionals and compare radial distribution functions with corresponding results obtained with GGA functionals.

[1] M. Dion et al. Phys. Rev. Lett. 92, 246401 (2004).
[2] K. Lee et al. Phys. Rev. B 82, 081101 (2010).
[3] http://eslab.ucdavis.edu/software/qbox

[1]Supported by NSF-OCI 0749217.

2:03PM B31.00013 Ice under pressure: the role of van der Waals forces in hydrogen bonding[1] , EAMONN MURRAY, GIULIA GALLI, UC Davis — We will discuss the evolution of the role of van der Waals interactions in hydrogen bonding in high pressure phases of ice. Here, we compare first principles results of the structural and electronic properties of ice using several different approaches to the calculation of exchange and correlation energies. These include the non-local vdW density functional of Dion *et al*[2], the revised vdW density functional of Lee *et al*[3] and the EXX/RPA approach based on an eigenvalue representation of the dielectric matrix[4] along with the semilocal functional PBE and hybrid functional PBE0.

[1]Work supported by grant SciDAC-e DE-FC02-06ER25777
[2]M. Dion, H. Rydberg, E. Schröder and D. Langreth, Phys. Rev. Lett. **92**, 246401 (2004)
[3]K. Lee, É. D. Murray, L. Kong, B. I. Lundqvist and D. C. Langreth, Phys. Rev. B **82**, 081101 (2010)
[4]D. Lu, Y. Li, D. Rocca and G. Galli, Phys. Rev. Lett. **102**, 206411 (2009)

Monday, March 21, 2011 11:15AM - 2:03PM –

Session B32 DMP: Focus Session: Optical Properties of Nanostructures and Metamaterials II

C144

11:15AM B32.00001 ABSTRACT WITHDRAWN –

11:27AM B32.00002 Optical Properties of Metal-Dielectric-Metal (MDM) Nanoantennas , BHUWAN JOSHI, Kent State University, XUEJIN WEN, Ohio State University, KAI SUN, University Of Michigan, WU LU, Ohio State University, QI-HUO WEI, Kent State University — We present a new design of plasmonic nanoantennas and study their optical properties. The nanoantennas consist of two metal blocks (cuboids or cylinders) stacked vertically with a dielectric spacer. The results from numerical simulations show that such plasmonic nanoantennas exhibit various cavity resonance modes which produce sharp peaks in the near field spectra and leave dips in the far field scattering spectra. Nanofabrication and characterization of these nanoantennas will also be presented in the talk.

11:39AM B32.00003 Designing broadband plasmonic nanoantennas for ultrasensing , ZHENHUAN YI, KAI WANG, DMITRI V. VORONINE, ANDREW TRAVERSO, ALEXEI SOKOLOV, Institute for Quantum Science and Engineering, Texas A&M University, College Station, TX 77843 — Various designs of broadband plasmonic nanoantennas made of gold and silver nanospheres are considered and optimized for ultrasensitive spectroscopic applications. The simulated nanostructures show a broadband optical response which may be tuned by varying the size, position and composition of nanospheres. Near-field enhancement in nanoantenna hot spots is analyzed and compared with previous literature results in the case of a fractal plasmonic nanolens. Broadband plasmonic nanoantennas may allow detecting ultrasmall concentrations of toxic materials and may be used for decoding DNA and for ultrafast nanophotonics applications.

11:51AM B32.00004 Optical nanoantennas: controlled emission of single photon sources , NIEK VAN HULST, ICFO - the Institute of Photonics Sciences (Barcelona) — Nanoscale quantum emitters are key elements in quantum optics and sensing. However, efficient optical excitation and detection of such emitters involves large solid angles, due to their omnidirectional interaction with freely propagating light and due to limits of diffraction. Optical nanoantennas offer both nanoscale localization and efficient interaction. Here we focus on the control of the interaction of single photon emitters (molecules, quantum dots) with radiation through metal nanorod antennas. First a novel analytical model is presented, which shows the continuous evolution of the properties of optical antennas as they become increasingly bound, i.e. plasmonic. The model accurately describes the complete emission process, the radiative decay rate, quantum efficiency, and angular emission, moreover gives a quantitative description of the gradual emergence of sub-radiant, super-radiant, and dark modes. Next we investigate experimentally the coupling of a single quantum dot to a nanorod of increasing length. The angular luminescence of the quantum dot is detected through increasingly higher order antenna modes. Simultaneously the emission is strongly polarized and enhanced. Direct confrontation with theory allows to determine the coupling efficiency of the quantum dot to the antenna. Finally, we present unidirectional emission of a single emitter by coupling to a nanofabricated Yagi-Uda antenna. A quantum dot is placed in the near field of the antenna so that it drives the resonant feed element of the antenna. The resulting quantum-dot luminescence is strongly polarized and highly directed into a narrow forward angular cone. The directionality of the quantum dot can be controlled by tuning the antenna dimensions. Thus our results show the potential of optical antennas to communicate energy to, from, and between nano-emitters.

A.G.Curto et al., Science 329, 930 (2010)

12:27PM B32.00005 Plasmon-mediated polarization-tuneable enhancement of optical absorption in a polymer film[1] , EDWARD J. OSLEY, PAUL G. THOMPSON, CLAUDIU G. BIRIS, NICOLAE C. PANOIU, PAUL A. WARBURTON, University College London — We have fabricated and characterized arrays of nanoscale apertures displaying polarization-tuneable localized surface plasmon (LSP) resonances in the infrared. Arrays of asymmetric cruciform apertures were milled in a gold film using a focused ion beam and subsequently coated with Poly(methyl methacrylate) (PMMA). The aperture geometry is designed so that for a certain polarization state of the incident wave the LSP resonance occurs at the same wavelength as the C=O bond absorption peak in PMMA. The nanostructured film results in an order of magnitude increase in the absorption in PMMA by comparison with a continuous film. By changing the in-plane electric-field polarization of the incident light the LSP resonance shifts away from the PMMA absorption peak, allowing us to quantify the role of plasmonic field-focussing on infrared optical absorption in the polymer film. Numerical simulations show that the increased optical absorption is due to the field enhancement both inside the apertures as well as in their close proximity. We will discuss how this technique may be applied to studies of plasmon-mediated field focussing in other materials including photovoltaic materials.

[1]Work supported by EPSRC

12:39PM B32.00006 Plasmonic-molecular resonance coupling , JIANFANG WANG, The Chinese University of Hong Kong — Localized plamsons have been widely used to enhance optical signals. The plasmon enhancement requires optically active species to be close to the metal surface. The presence of active species can affect the plasmon resonances. Understanding the plasmon-molecule interactions is of importance for both enhancing optical signals and developing plasmon shift-based sensors. We have studied the resonance coupling between Au nanocrystals (NCs) and dyes. The coupling strength can be tuned by varying NC plasmon wavelength. The maximum plasmon shift reaches above 120 nm, which is about 10 times larger than that caused by the local index increase. The plasmon shift decays rapidly as the dye-NC spacing is increased. In addition, the coupling strength is strongly dependent on the molecular properties but independent on the NC shape and size. We have further measured the resonance coupling on single Au NCs. The resonance coupling reveals a unique three-band structure. These single-particle studies will greatly help in understanding the fundamental aspects of the resonance hybridization and designing various plasmon-enhanced spectroscopies.

12:51PM B32.00007 ABSTRACT WITHDRAWN –

1:03PM B32.00008 Advanced Material Models for Nano-Plasmonic Systems via Discontinuous Galerkin Methods , KURT BUSCH, Karlsruhe Institute of Technolgy, Karlsruhe, Germany — Nano-Plasmonic systems offer a tremendous potential for the controlled delivery and extraction of electromagnetic energy to and from tiny objects such as molecules and quantum dots in their immediate vicinity. In view of the increasing sophistication of fabrication and spectroscopic characterization, quantitative computational approaches face challenges that go well beyond the usual description of metals as linear dispersive materials. These challenges include the development of material models that describe the (potentially) strongly nonlocal and nonlinear optical response of such metallic nano-structures themselves as well as the strongly modified light-matter interaction that is mediated by them. This talk reports on the progress of applying the Discontinuous-Galerkin Time-Domain (DGTD) method to the quantitative analysis of nano-plasmonic systems using advanced material models. This includes the efficient modeling of complex geometric features via curvilinear elements, the improvement of the time-stepping scheme via tailored low-storage Runge-Kutta schemes, and the incorporation of optically anisotropic media. In addition, this talk reports on recent results regarding the development and application of advanced material models that are based on a hydrodynamic description of the metal's conduction electrons. By coupling the Maxwell equations to this treatment of the free electrons as a plasma in a confined geometry one is able to capture nonlocal and nonlinear effects and to analyze their consequences.

1:39PM B32.00009 Suppression of Landau Damping in Metal Nanostructures via Quantum Size Effect[1] , XIAOGUANG LI, University of Tennessee-Knoxville, DI XIAO, Oak Ridge National Laboratory, ZHENYU ZHANG, Oak Ridge National Laboratory, University of Tennessee-Knoxville, University of Science and Technology of China — Using the matrix random phase approximation, we study the tunability of localized surface plasmon resonance in small metal nanostructures, where the Landau damping is the dominant dissipation channel and the intrinsic limit to plasmonics technique. We find that the linewidth of plasmon can be effectively suppressed due to the quantization of electron-hole pair energy in various highly confined geometries, where the strength of Landau damping oscillates as the scale of system. Moreover, beyond a classical surface scattering picture, the oscillatory effect can be illustrated with an electron-hole pair description, which can be used to understand many other properties of plasmon. Our results show the possibility to control the Landau damping and therefore should be able to stimulate more efforts on future plasmonics of small nanostructures.

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

1:51PM B32.00010 Excitation of electromagnetic modes in spheres[1] , RAUL GARCÍA-LLAMAS, Universidad de Sonora, LUIS RAMIREZ-RODRIGUEZ, Posgrado en Física, Universidad de Sonora — A study of the excitation of whispering gallery modes (WGM) in non-dispersive dielectric micro sphere is presented. The Near-Field intensity behavior of the nano-jets, sub-wavelength volume regions, is presented as a function of the radii of the sphere in resonant and off-resonant conditions. A similar study is presented for nano metallic sphere.

[1]CONACYT

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B33 DMP DCOMP: Focus Session: Dielectric, Ferroelectric, and Piezoelectric Oxides: Electronic Conduction and Defects C143/149

11:15AM B33.00001 Conduction at different ferroelectric domain walls in $BiFeO_3$, SAEEDEH FAROKHIPOOR, CHRISTOPHE DAUMONT[1], BEATRIZ NOHEDA, Zernike Institute for Advanced Materials, University of Groningen — $BiFeO_3$ (BFO) is, at room temperature, a rhombohedrally distorted, ferroelectric perovskite. There are eight possible polarization directions (or domains) and three different types of domain walls, namely, 180° (ferroelectric) and 109° and 71° (ferroelectric and ferroelastic) domain walls. Recent works have shown that the domain walls of BFO can display functionalities different from those of the domains, generating photocurrents [1], inducing exchange bias [2] and displaying conductivity at room temperature [3]. Conduction has been reported at 180° and 109° domain walls[3] and it was proposed that the reduction of the band gap, associated with the suppression of ferroelectric distortions, at domain walls was responsible for the observed conduction[3]. It is, however, not yet clear if and how other (extrinsic) mechanisms affect the conductivity at the walls. In order to help clarifying the origin of domain wall conductivity, we have performed temperature, thickness and orientation dependent local conductivity measurements in BFO thin films. The results will be discussed in this presentation.

[1] S.Y. Yang, Nature Nanotech. 5, 143 (2010); [2] L.W. Martin et al. Nano Letters 8, 2050 (2008);[3] J. Seidel et al., Nature Mat. 8, 229 (2009).

[1]Present address: THALES-CNRS (France)

11:27AM B33.00002 Electronic Transport properties of ultra-thin $BiFeO_3$, DIPANJAN MAZUMDAR, Center for Materials for Information Technology, University of Alabama, Tuscaloosa, AL 35487, OLEG MRYASOV, VILAS SHELKE, Center for Materials for Information Technology, University of Alabama, Tuscaloosa AL 35487, STEPHEN JESSE, ARTHUR BADDORF, SERGEI KALININ, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge Tennessee., ARUNAVA GUPTA, Center for Materials for Information Technology, University of Alabama, Tuscaloosa AL 35487 — We have investigated the electronic transport properties of rhombohedral (R) and the nearly-tetragonal (T) phase of $BiFeO_3$ using beyond density functional techniques, and combined with nanoscale I-V transport measurements. Using Quasi-particle GW approximation, we show the R and T phase to have significantly different electronic structures. We find that the T phase has significantly lower effective mass at the conduction band edge compared to the R phase leading to a lower effective barrier height for tunnel electrons (0.38 eV vs 3.6 eV). We therefore anticipate that tunnel devices with T phase BFO to have significantly lower resistances. Local transport measurements performed on ultra-thin BFO R phase are consistent with this inference. Tunneling measurements on the tetragonal phase films are also presented.

11:39AM B33.00003 Oxygen vacancies in lanthanum aluminate ($LaAlO_3$) , JOSHUA SAYRE, NICOLA SPALDIN, University of California, Santa Barbara — Oxygen vacancies can affect the properties of an oxide in various manners such as increasing its ion or electronic conductivity, changing its lattice constant or causing dielectric breakdown. The aim of this research is to investigate structural changes and consequent changes in properties caused by oxygen vacancies in a model complex oxide, lanthanum aluminate, $LaAlO_3$. We use density functional theory with the generalized gradiant approximation (GGA) and within the VASP package to calculate the structure and properties of representative oxygen vacancy profiles. We find that the presence of oxygen vacancies modifies the pattern of rotations of the oxygen octahedra. We discuss the implications of our results for understanding the correlation between epitaxial strain in oxide thin films and intrinsic defect profiles.

11:51AM B33.00004 Defect-Induced Electronic Structures and Formation Energies of Vacancy Complexes in $SrTiO_3$, JIYEON KIM, CHOONG H. KIM, ROKYEON KIM, JAEJUN YU, Center for Strongly Correlated Materials Research, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea — Recently defect induced ferroelectricity in $SrTiO_3$ has been reported at room temperature. Strontium-oxygen vacancies were suggested as a possible source of electric polarization regarding to the existence of mid-gap states. To understand the detailed electronic structures induced by defects and their formation energies, we carried out density-functional-theory calculations for various defects such as Sr, Ti, O, Sr-O, Sr-O- O vacancies. We employed the LDA+U method as implemented in the VASP code to describe the d-orbital occupation at the Ti- site due to the presence of oxygen vacancy. A complex of Sr-O-O vacancies is found to contribute to the localized electronic states in the band gap and its formation energy is small enough to form easily under the poor oxygen limit. We conclude that the vacancy-complex defects play a crucial role in determination of the physical properties of $SrTiO_3$ thin films.

12:03PM B33.00005 Quasiparticle electronic structure calculations of F centers in $SrTiO_3$ perovskite , CHANDRIMA MITRA, ALEX DEMKOV, University of Texas at Austin — Among the broad class of oxides, ABO_3 perovskites have attracted a lot of attention in the recent past due to its beneficial material properties. $SrTiO_3$ is one such example of this class of compounds. It shows a wide range of properties from being ferroelectric to exhibiting superconducting properties in doped $SrTiO_3$. The anomalous dielectric properties in this material make it a potential candidate for technological applications. However, being a semicovalent oxide, the complexities in its electronic structure have hindered a proper characterization of the system. For instance, the intrinsic excitonic luminescence, in this system, is not well understood and there is no general agreement as to whether it is caused by defects or due to self trapped excitons. This calls for an accurate theoretical description of the electronic levels as well as the various defect states in this material. In this work we present results for quasiparticle GW calculations of pure as well as *defective* $SrTiO_3$ containing oxygen vacancies which form F centers in these compounds. From a quasiparticle description of the system excitonic properties of $SrTiO_3$ will be examined.

12:15PM B33.00006 Charge transition levels of oxygen vacancies in monoclinic hafnia[1] , MANISH JAIN, University of California at Berkeley and Lawrence Berkeley National Laboratory, JAMES R. CHELIKOWSKY, University of Texas at Austin, STEVEN G. LOUIE, University of California at Berkeley and Lawrence Berkeley National Laboratory — We perform electronic structure calculations on oxygen vacancies in hafnia using a combined density functional theory (DFT) and GW formalism. This formalism corrects for the error in calculating formation energy and charge transition levels using standard DFT. While the formalism is, in principle, exact; in previous calculations of this kind, one makes several approximations to make the calculation tractable. We assess the impact of these approximations on the charge transition levels of the oxygen vacancy in hafnia. In particular, we examine the assumption that the quasiparticle wavefunctions are the same as DFT wavefunctions for the defect states. We show that this assumption can lead to erroneous results in this system and present the charge transition levels without making use of this assumption. We also explore the possibility that these defects are negative U centers.

[1]This work was supported by National Science Foundation Grant No. DMR10-1006184, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231 and DE-SC0001878. Computational resources have been provided by NSF through TeraGrid resources at NICS

12:27PM B33.00007 ABSTRACT WITHDRAWN –

12:39PM B33.00008 Disproportionation and comproportionation reactions of resistive switching in polycrystalline NiOx films , FOREST S.-S. CHIEN, YI-TA WU, GUAN-LONG LAI, Department of Physics, Tunghai University, Y.H. LAI, Department of Chemistry, Tunghai University — The NiO_x thin film exhibit excellent bistable unipolar resistive switching, which has strong potential in nanoscale nonvolatile-memory applications. The underlying mechanism of NiOx resistive switching is still in debate. We studied the chemical bonding states of Ni 2p and O 1s at high/low resistance spots by focused X-ray photoemission spectroscopy. The disproportionation and comproportionation reactions of $3NiO \leftrightarrow Ni + Ni_2O_3$, accounts for the resistive switching of NiO_x. The calculated Gibbs energy of the reaction indicates the reversibility of the reaction thermochemically. The dynamic breathing of the filaments with switching was observed by conducting atomic force microscopy.

12:51PM B33.00009 The effect of oxygen migration for random resistance access memory in oxide-based devices[1] , ZHAOLIANG LIAO, Louisiana State University & Institute of Physics, Chinese Academy of Sciences, PENG GAO, YANG MENG, HONGWU ZHAO, XUEDONG BAI, DONGMIN CHEN, Institute of Physics, Chinese Academy of Sciences — The observed electric field induced resistance switching in metal oxide thin films is generally thought to arise from the creation or annihilation of oxygen defects. By depositing different kinds of metal electrodes on $Pr_{0.7}Ca_{0.3}MnO_3$ and CeO_2 thin films to construct sandwiched devices, we found that the devices can be categorized into two groups with different switching behaviors, depending on the Gibbs free energy of oxidation of the top electrodes with respect to that of underneath metal oxide. *In-situ* TEM measurements show a structure change with an applied electric field. Our analysis indicates that the structure change is related to the oxygen migration driven by external electric field. Therefore, it suggests that not only the oxygen defects but also their migration play important roles in the functionality of oxide-based devices

[1]This work is supported by NSFC, China and Z.L Liao acknowledges finacial support from DOE through grant #DE-SC0002136.

1:03PM B33.00010 Conduction and Loss Mechanisms in Flexible Oxide-Based Memristors , J.L. TEDESCO, N. GERGEL-HACKETT, L. STEPHEY, A.A. HERZING, M. HERNANDEZ-MORA, C.A. HACKER, J. OBRZUT, L.J. RICHTER, C.A. RICHTER, National Institute of Standards & Technology — In order to study the conduction and loss mechanisms behind their operation, flexible sol-gel based memristors were fabricated with differing oxide film thicknesses and device sizes. XPS, TEM, EELS, and VASE measurements indicated the oxide was amorphous TiO_2, with a significant fraction of organic material. Analysis of the bias and sweep rate dependence of the devices suggested the switching mechanism was induced by charge flow in the memristor and not by the electric field. Further analysis of the I-V curves indicated that once the memristors were switched into the high-current "ON" state, conduction through them generally became ohmic. Once such memristors were cut to yield two smaller devices, there was typically only one device that remained ohmic, indicating that localized conduction pathways caused switching in the flexible memristors. There was a shift in the capacitance-frequency and conductance-frequency measurements following switches between the "ON" and "OFF" states of the devices, indicating that an additional dielectric loss mechanism was present in these films that was not present in ordinary TiO_2 films. This loss mechanism is attributed to dipoles in the organic constituents of the films that are by-products of the sol-gel process.

1:15PM B33.00011 Capacitive network near the metal insulator transition in Vanadium Dioxide , J.G. RAMIREZ, E.J. PATINO, Universidad de los Andes, R. SCHMIDT, Universidad Complutense de Madrid, A. SHARONI, Bar-Ilan University, M.E. GOMEZ, Universidad del Valle, I.K. SCHULLER, University of California-San Diego — Recent infrared spectroscopy and transport measurements in nano-scaled junction of VO2 have revealed the existence of phase separation into metallic and insulating phases. Here we present Impedance spectroscopy measurements performed in high quality Vanadium dioxide (VO_2) thin films for the first time. This technique allows distinguishing between the resistive and capacitive response of the VO_2 films and provides the dielectric properties across the metal-insulator transition (MIT). The film capacitance exhibits an unusual increase close to the MIT which implies the formation of a capacitor network produced by the nanoscale phase separation of metallic and insulating phases. This work has been supported by AFOSR, COLCIENCIAS, CENM and Ramon y Cajal Fellowship.

1:27PM B33.00012 Substitution site for Zn in $LiNbO_3$ from detailed EXAFS analysis[1] , FRANK BRIDGES, BRAD CAR, UCSC, JAIME CASTILLO, Universidad Tecnologica d la Mixteca, MICHAEL KOZINA, SCOTT MEDLING, UCSC — We report detailed EXAFS studies of Zn doped $LiNbO_3$, at the Zn and Nb K-edges, as a function of dopant and as a function of temperature. For this material there exist several models concerning the substition site(s) for Zn. Our data are only consistent with Zn substitution on the Li site. Any substitution on the Nb site is very small. Further as the Zn concentration changes from 5-9% the EXAFS r-space function for the Zn K-edge changes very little, a slight amplitude reduction consistent with increased local disorder for increasing Zn concentration. Our detailed analysis shows that the nearest O neighbors to Zn are slightly pulled inward while the nearst metal atoms - Nb - are pushed away. We cannot tell if there are vacancies on the Li sites because Li is a very weak backscatterer, and the amplitude of the rather long Zn-Li peak is very low. We discuss and compare our results with previous proposed models and with recent calculations for other defects that suggest that many +2 dopants substitute at the Li site.

[1]Support: UCMEXUS grant SC-10-19

1:39PM B33.00013 Structure and Magnetic Properties of Electron Doped $YMnO_3$, TIAN YU, PENG GAO, TREVOR TYSON, New Jersey Institute of Technology — Combined local and long range structural measurements were conducted on the electron doped ferroelectric $Y_{1-x}Zr_xMnO_3$ system. Doping by Zr is found to maintain the hexagonal structure for a large range of x-values. The location of Zr in the lattice is identified and changes in structure with doping are followed. These details of the local structure are examined by x-ray diffraction and x-ray absorption spectroscopy and compared with detailed magnetic studies to correlate the impact of electron doping and atomic structure on the magnetic order in these systems. This work is supported by DOE Grant DE-FG02-07ER46402.

1:51PM B33.00014 First-principles calculations of Ti and O NMR chemical shift tensors in ferroelectric perovskites[1] , DANIEL PECHKIS, ERIC WALTER, HENRY KRAKAUER, College of William and Mary — Complementary chemical shift calculations were carried out with embedded clusters, using quantum chemistry methods, and with periodic boundary conditions, using the GIPAW approach[2] within the Quantum Espresso package.[3] Compared to oxygen chemical shifts, $\hat{\delta}$(O),[4] cluster calculations for $\hat{\delta}$(Ti) were found to be more sensitive to size effects, termination, and choice of gaussian-type atomic basis set, while GIPAW results were found to be more sensitive to the pseudopotential construction. The two approaches complemented each other in optimizing these factors. We show that the two approaches yield comparable chemical shifts for suitably converged simulations, and results are compared with available experimental measurements.

[1]Supported by ONR
[2]C. J. Pickard and F. Mauri Phys. Rev. B **63**, 245101 (2001)
[3]P. Giannozzi et al., Journal of Physics: Condensed Matter **21**, 395502 (2009)
[4]D. L. Pechkis, E. J. Walter, and H. Krakauer. J. Chem. Phys. **131**, 184511 (2009)

2:03PM B33.00015 Electrical Breakdown in Lightning Arrestor Connector (LAC) Devices , HAROLD P. HJALMARSON, KENNETH KAMBOUR, Sandia National Laboratories, ANDREW C. PINEDA, U.S. Air Force Research Laboratory — Lightning arrestor connector (LAC) devices protect electronic devices by providing a conductive path to ground for electrical power surges caused by lightning. Such devices consist of an insulating material between electrodes. This insulation region is composed of an air gap and a high permittivity dielectric. In this presentation, the physics of the phenomena active in the early stages of the flow of transient electrical current will be described. The conditions that lead to thermal breakdown of the dielectric will also be discussed.–Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B34 DMP GMAG: Focus Session: Interfaces in Complex Oxides - Spectroscopy and Growth C141

11:15AM B34.00001 Strain-modulated asymmetric orbital–lattice interactions in correlated oxide heterostructures[1] , J. CHAKHALIAN, Univeristy of Arkansas, J. RONDINELLI , JIAN LIU, B. GRAY, M. KAREEV, E.J. MOON, J. COHN, M. VARELA, S.G. ALTENDORF, F. STRIGARI, B. DABROWSKI, L.H. TJENG, P.J. RYAN, J.W. FREELAND — Artificial structuring of quasi-two dimensional correlated electron thin films and heterointerfaces offers an arena to discover innovative functionalities by harnessing electronic and orbital degrees of freedom. To harness this potential understanding of how structurally linked correlated electronic responses are modified through epitaxial constraints at the substrate–film hetero-interface is clearly required. We use a suite of advanced experimental probes along with ab-initio calculations to show how compressive and tensile bi-axial strain lead to unusual asymmetrical orbital responses. Microscopic studies based on resonant X-ray spectroscopies reveal that the asymmetry leads to a new ground state with a ligand hole density and chemical bond covalency that is modulated by the sign of the epitaxial constraint at the interface.

[1]J.C. was supported by DOD-ARO under the Contract No. 0402-17291 and NSF Contract No. DMR-0747808.

11:27AM B34.00002 Structural effects on the electronic properties of epitaxially strained $RNiO_3$ thin films , I.C. TUNG[1], Department of Materials Science and Engineering, Northwestern University, JIAN LIU, B. GRAY, J. CHAKHALIAN, Department of Physics, University of Arkansas, J. RONDINELLI, P. RYAN, J.W. KIM, Advanced Photon Source, Argonne National Laboratory, M.J. BEDZYK, Department of Materials Science and Engineering, Northwestern University, J.W. FREELAND, Advanced Photon Source, Argonne National Laboratory — Since the metal–insulator (MI) transition is a hallmark of strongly correlated materials, understanding the behavior of the MI transition of $RNiO_3$ (R=rare earth) thin films subjected to confinement, lattice misfit and broken symmetry at the interface in the ultra-thin limit is fundamentally and technologically important [1]. Here we present a study of the effect of the lattice symmetry with epitaxial strain in thin films of $LaNiO_3$ and $NdNiO_3$ grown on $SrTiO_3$(001) substrates by pulsed laser deposition. A combination of x-ray diffraction, soft x-ray absorption spectroscopy, and temperature-dependent resistivity has been applied to elucidate structural and electronic properties of the samples. Work at the Advanced Photon Source, Argonne is supported by the U.S. Department of Energy, Office of Science under Contract No. DE-AC02-06CH11357.

[1] Jian. Liu et al., Appl. Phys. Lett. 96, 233110 (2010).

[1]Advanced Photon Source, Argonne National Laboratory

11:39AM B34.00003 Orbital engineering near La_2NiO_4-La_2CuO_4 superlattice interfaces[1] , S. SMADICI, J.C.T. LEE, J. MORALES, P. ABBAMONTE, University of Illinois at Urbana-Champaign, IL 61801, G. LOGVENOV, A. GOZAR, I. BOZOVIC, Brookhaven National Laboratory, NY 11973 — Orbital states of transition metal oxides present the opportunity of adjusting material properties to a specific purpose (orbital engineering). A comparison of the resonant soft x-ray reflectivity of La_2NiO_4-La_2CuO_4 superlattices at Ni L and Cu L edges shows different spatial distributions of the occupation of Ni $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ orbitals in the LNO layers. This modulation of the Ni valence is possible through a pronounced modulation of the density of oxygen interstitial dopants within the structure which does not follow exactly the structure itself. This is the first observation of orbital engineering in a 214 oxide.

[1]This work was supported by Grants DE-FG02-06ER46285, DE-AC02-98CH10886, MA-509-MACA, DE-FG02-07ER46453 and DE-FG02-07ER46471.

11:51AM B34.00004 Orbital Control in single unit cell LaNiO3/LaAlO3 superlattices , J.W. FREELAND, Argonne National Laboratory, J. LIU, B. GRAY, M. KAREEV, University of Arkansas, J.W. KIM, P.J. RYAN, Argonne National Laboratory, R. PENTCHEVA, University of Munich, J. CHAKHALIAN, University of Arkansas — Oxide heterostructures built from strongly correlated electron materials offers unique opportunity to generate new ground-states by altering the balance of competing energies in the system. In pursuit of rational control of orbital polarization, we present a combined experimental and theoretical study of single unit cell $LaNiO_3/LaAlO_3$ superlattices[1]. Polarized x-ray absorption spectra show a distinct asymmetry in the orbital response under tensile vs. compressive strain. A splitting of orbital energies $\sim$100 meV with octahedral distortions is found for the case of compressive strain which is much smaller than the $3d$ bandwidth. In sharp contrast, for tensile strain, no splitting is found although a strong orbital polarization is still present. Density functional theory calculations of the electronic properties reveal that the asymmetry results from a combination of strain effects and altered covalency in the bonding across the interfacial apical oxygen to the Al site, leading to the opening of a pseudogap in the heterostructure for tensile strain. Work at Argonne, including the Advanced Photon, is supported by the U.S. Department of Energy, Office of Science, and Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357. [1] J.W. Freeland et. al. arXiv:1008.5618

12:03PM B34.00005 Realistic DMFT calculations for nickelate superlattices , M.J. HAN, Columbia University, XIN WANG, University of Maryland, CHRIS A. MARIANETTI, ANDREW J. MILLIS, Columbia University — We present phase diagram, photo-emission and RIXS (resonant inelastic X-ray scattering) spectra, orbital polarization, and Fermi surface plots for LaNiO3/LaXO3 superlattice (X=Al, Ga,...) obtained from DMFT (dynamical mean-field theory) calculation based on a realistic multi-band tight-binding model derived from DFT (density functional theory) calculations and in particular including oxygen orbitals. Our results indicate that heterostructuring is unlikely to produce one band model physics and point toward a new view of metal-insulator transition of this system. This work is supported by ARO via grant No. W911NF0910345-56032PH.

12:15PM B34.00006 Conductivity enhancement of ultrathin $LaNiO_3$ films in superlattices

JUNWOO SON, JAMES M. LEBEAU, S. JAMES ALLEN, SUSANNE STEMMER, University of California, Santa Barbara — The transport properties of heterostructures with Mott materials, such as $LaNiO_3$, have been predicted to exhibit unusual phenomena not present in the bulk. Prior studies have shown that ultrathin $LaNiO_3$ films exhibit strongly localized behavior, whereas thicker films remain metallic. Here, we report on epitaxial $[SrTiO_3(3\text{ u.c.})/LaNiO_3(4\text{ u.c.})]_n$ superlattices on (001) $(LaAlO_3)_{0.3}(Sr_2AlTaO_6)_{0.7}$ (LSAT) substrates (u.c. = unit cell). X-ray diffraction and Z-contrast imaging confirm sharp interfaces. The sheet resistance of the superlattices is explored as a function of temperature and number of bilayers. All superlattices with more than 2 layers were metallic whereas 4 u.c. $LaNiO_3$ films and a single 4 u.c. $LaNiO_3$/3 u.c. $SrTiO_3$ bilayer were both insulating. The sheet resistance of superlattices decreases with n. Possible models for the electrical characteristics will be discussed. The first model attempts to describe the sheet resistance with conduction through parallel-connected $LaNiO_3$ layers and conductive interfacial layers. The second model is based on coupling of layers, each of which is near the percolation threshold for a metal-insulator transition, and explains the difference in conductivity of single layers and superlattices without invoking interfacial layers.

12:27PM B34.00007 Electric-Field Control of the Metal-Insulator Transition in Nickelate Thin Films

RAOUL SCHERWITZL, PAVLO ZUBKO, University of Geneva, IGNACIO GUTIERREZ-LEZAMA, SHIMPEI ONO, ALBERTO MORPURGO, University of Geneva, GUSTAU CATALAN, CIN2, JEAN-MARC TRISCONE, University of Geneva — The rare-earth perovskite nickelates ($RNiO_3$) are a fascinating family of compounds displaying a sharp temperature-driven metal-insulator (MI) transition with resistance changes of several orders of magnitude. From a fundamental point of view, these materials present an ideal system to study MI transitions since, in contrast to most oxides, a complete evolution from itinerant to localized behavior can be achieved without doping. From a technological point of view, the nickelates are just as exciting, as the large changes and thermal hysteresis in resistance may find uses in various electronic applications, particularly if the MI transition could be tuned using an electric field. We discuss the electric field control of the MI transition in $NdNiO_3$. The electric double layer technique was used in order to obtain very large charge carrier density modulations (exceeding 10^{15} cm^{-2}), enabling us to reversibly tune the transition temperature by more than 50 K and to achieve electro-conductivities as high as 60000% [1].

[1] R. Scherwitzl *et al.*, Adv. Mater., doi: 10.1002/adma.201003241 (2010)

12:39PM B34.00008 Interface Structures in Ferromagnetic $LaMnO_3$-$SrMnO_3$ Superlattices

AMISH SHAH, Arizona State University, QUENTIN RAMASSE, SuperSTEM Laboratory, UK, STEVEN MAY, ANAND BHATTACHARYA, Argonne National Laboratory, XIAOFANG ZHAI, JAMES ECKSTEIN, JIAN-MIN ZUO, University of Illinois at Urbana-Champaign, JOHN SPENCE, Arizona State University — We have investigated the interfaces of $LaMnO3_{2n}$-$SrMnO3_n$ (LMO/SMO) superlattices. Charge density calculations have predicted a leakage of Mn e_g electrons from LMO into SMO.[1] For n=1, these electrons are expected to be distributed throughout all films in the superlattice, while for $n > 3$, the electrons are expected to be localized within a few layers near the interfaces. Using aberration corrected STEM coupled with EELS, we probed a $LMO_{11.8}$-$SMO_{4.4}$ superlattice at high spatial resolution to examine interfacial states. We find that the LMO on SMO interface is structurally sharper than SMO on LMO interfaces. Extra interfacial states above the Fermi level are localized to 1 unit cell of the sharp LMO/SMO interface while the states are weak or absent at the rougher SMO/LMO interfaces. The same interfaces that have extra states have an enhanced ferromagnetic moment at low temperatures.[2]

[1]C. Aruta et al., Phys. Rev. B 80 (2009).
[2]S. May et al., Phys. Rev. B 77 (2008).

12:51PM B34.00009 Induced Ti magnetism at titanate / manganite interfaces

J. GARCIA-BARRIOCANAL, F.Y. BRUNO, A. RIVERA-CALZADA, C. LEON, J. SANTAMARIA, GFMC. Dpto. Física Aplicada III, Universidad Complutense de Madrid, 28040 Madrid, Spain, J.C. CEZAR, P. THAKUR, N.B. BROOKES, European Synchrotron Radiation Facility (ESRF), 6 rue Jules Horowitz, B.P. 220, F-38043 Grenoble Cedex, France, J.W. TAYLOR, J.A. DUFFY, S.B. DUGDALE, C. UTFELD, S.R. GIBLIN, ISIS Facility, Rutherford Appleton Laboratory, Chilton, Oxfordshire, OX11 0QX, United Kingdom., T. NAKAMURA, K. KODAMA, Japan Synchrotron Radiation Research Institute, SPring-8, 1-1-1 Kouto, Sayo, Hyogo 679-5198, Japan, S. OKAMOTO, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6071, USA — We show evidence of induced magnetism resulting from the electronic (charge) or orbital reconstruction occurring at the interface. We show a novel form of Ti magnetism at the interface between $SrTiO_3$ (STO) and $LaMnO_3$ (LMO) [1] as evidenced by evidenced by a strong XMCD signals at Ti and Mn edges. The magnetic alignment (ferromagnetic or antiferromagnetic) of Ti and Mn moments can be tuned by structural parameters.

[1] J. Garcia-Barriocanal et al. Nature Comm. **1**:82 doi: 10.1038/ncomms1080 (2010)

1:03PM B34.00010 Orbital Reflectometry and the Electronic Structure of Oxide Interfaces

EVA BENCKISER, Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart — The occupation of d-orbitals has a key influence on the physical properties of transition-metal (TM) oxides.[1] Due to the strong hybridization with neighboring oxygen ions, the electronic structure is very sensitive to changes in the TM-oxygen bond distances induced by strain and/or by the chemical bonding to other ions with different electronic configuration. Both effects might be important in oxide heterostructures,[2] but thus far it has been difficult to probe atomic-scale modulations of the orbital occupation in a quantitative manner.[3] We present results from polarized soft x-ray resonant reflectivity, which demonstrate that it is possible to derive quantitative, spatially resolved orbital polarization profiles. We show that this method is sensitive enough to resolve differences of $\sim 3\%$ in the occupation of Ni e_g orbitals in adjacent atomic layers of a $LaNiO_3$-$LaAlO_3$ superlattice, and the experimental findings are in good agreement with electronic-structure calculations. The possibility to quantitatively correlate theory and experiment on the atomic scale opens up new perspectives for orbital physics in oxide heterostructures.

[1]Tokura, Y. & Nagaosa, N. Science **288**, 462-468 (2000).
[2]Han, M. J., Marianetti, C. A. & Millis, A. J. Phys. Rev. B **82**, 134408 (2010).
[3]Chakhalian, J. *et al.* Science **318**, 1114-1117 (2007).

1:39PM B34.00011 Source oxidation problem in oxide-MBE environment and its solution

NAMRATA BANSAL, YONG-SEUNG KIM, SEONGSHIK OH[1], Rutgers University — Maintaining stable fluxes for multiple source elements is a challenging task when the source materials have significantly different oxygen affinities in a complex-oxide MBE environment. Although this problem has been known to the complex oxide MBE community since the late 1980s, a detailed study and solution is still lacking. Here, using Sr as a test source, because of its easy oxidation and popularity in complex oxides, we investigated the source-oxidation problem in a number of different conditions. We found that the source oxidation was less for higher flux rates, unmelted source shape, and extended port geometry. The extended port geometry was also found to eliminate the flux transient, usually observed in a standard port, after opening the source shutter. Furthermore, a crucible aperture insert scheme was found to be very effective in suppressing the source oxidation. In this scheme, a disk-shaped aperture was mounted inside the crucible and we found that it blocks most of the oxygen species coming to the source. However, the depth of the aperture disk was critical for its performance. We will discuss how these configurations suppress source oxidation and lead to significantly enhanced stability of Sr-flux in harsh oxidation conditions.

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1:51PM B34.00012 Growth of SrTiO3(110) film with oxide molecule beam epitaxy[1] , JIANDONG GUO, ZHIMING WANG, FANG YANG, JIAGUI FENG, FENGMIAO LI, Institute of Physics, Chinese Academy of Sciences — In the past decade, a tremendous amount of evidence has shown that thin films, superlattices and heterointerfaces of oxides display a rich diversity of glamorous properties that is related, but not identical to that in the bulk. To understand the underlying physical mechanism, it is essential to construct the oxide heterostructures under control with atomic precision. We have studied the $SrTiO_3$(110) surface that bears intrinsic instability of reconstruction in addition to the broken symmetry due to the surface polarity, which provides us an additional degree to tune the properties of the epitaxial material by manipulating the termination layer of the substrate. Beyond the termination, we are able to tune the stability of a series of surface reconstructions and realize the reversible phase transitions between them. By applying the knowledge to the homoepitaxy, we develop an easy method to coordinate the metal evaporation sources with required flux rate ratio precisely during the oxide MBE growth. We further simplify the growth by controlling the shutter of the Sr source. The atomically well defined grown surface is characterized by scanning tunneling microscopy.

[1]This work was supported by Chinese NSF (10704084) and MOST (2006CB921300 and 2007CB936800).

2:03PM B34.00013 Oxygen Doping Study of Cuprate/Manganite Thin-Film Heterostructures[1] , HAO ZHANG, University of Toronto, J.Y.T. WEI, University of Toronto and Canadian Institute for Advanced Research, WEN HE GONG, Brockhouse Institute for Material Research, McMaster University, GIANLUIGI A. BOTTON, Canadian Centre for Electron Microscopy — Recent studies of thin-film heterostructures comprising superconducting cuprates and ferromagnetic manganites have revealed a range of novel physical phenomena. These phenomena are believed to involve complex interfacial interactions between competing order parameters [1], and appear to be highly sensitive to carrier doping [2]. To further examine these phenomena, we carry out a systematic oxygen-doping study of cuprate/manganite multilayer thin films, grown epitaxially by pulsed laser-ablated deposition. Our samples are characterized by electrical transport and magnetization measurements, as well as x-ray diffraction and several microscopy probes including SEM and TEM. We also make cation substitution in the cuprate layer, in order to study the effects of carrier doping across the interface.

[1] For example, see J. Hoppler *et al.*, Nature Materials **8**, 315 (2009).
[2] V. Peña *et al.*, Phys. Rev. Lett. **97**, 177005 (2006).

[1]Work supported by NSERC, CFI/OIT and the Canadian Institute for Advanced Research

Monday, March 21, 2011 11:15AM - 2:15PM –
Session B35 DCMP: Topological Insulators: Theory I C140

11:15AM B35.00001 Classification of Gapped Topological Phases in 1D Interacting System , XIE CHEN, Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA, ZHENG-CHENG GU, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106, USA, XIAO-GANG WEN, Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA — Topological phases exist in quantum many-body systems beyond the usual symmetry breaking understanding of phase and phase transition. While a full classification of topological insulators and superconductors has been given for non-interacting fermions, the question of what phases exist for strongly interacting systems and how to identify them seems hard. Here we give a full classification of 1D gapped phases with possible topological and symmetry breaking order in both spin and fermion systems, based on the local unitary equivalence relation between short-range correlated matrix product states, which represent well the class of 1D gapped ground states. We find that in certain symmetry classes, the classification result for non- interacting systems is changed when strong interaction is allowed. Understanding about 1D system also allows us to obtain some simple results for topological phases in higher dimensions when certain symmetries are present.

11:27AM B35.00002 Classification of topological insulators and superconductors using KR theory , ABHISHEK ROY, University of Illinois, Urbana-Champaign — Kitaev's periodic table[1] provided a classification of topological insulators and superconductors. The classes are indexed by dimension and symmetries. We present a method of arriving at the table using KR theory. This gives a unified and systematic method of constructing model Hamiltonians for each class, as well as those for boundaries and defects. We motivate the formulae for the topological invariants and explain the diagonal periodicity in the invariants.

[1]A. Kitaev, Proceedings of the L.D.Landau Memorial Conference Advances in Theoretical Physics, June 22-26, 2008

11:39AM B35.00003 The classification of topological insulators and superconductors , CHING-KAI CHIU, MICHAEL STONE, TAYLOR HUGHES, University of Illinois at Urbana-Champaign — We use the process of band crossings during quantum phase transitions to explain the periodic table of topological insulators and superconductors. This is achieved by showing how irreducible representations of the real and complex Clifford algebras are related to the 10 Altland-Zirnbauer symmetry classes of Hamiltonian matrices which are associated with time reversal, particle-hole, and chiral symmetries. The representation theory not only reveals why a unique topological invariant $(0, Z_2, Z)$ exists for each specific symmetry class and dimension, but also shows the interplay between quantum phase transitions, topologically protected boundary modes, and topological invariants.

11:51AM B35.00004 Chern Numbers Hiding in Time of Flight Images[1] , INDUBALA SATIJA, ERHAI ZHAO, PARAG GHOSH, George Mason university, NOAH BRAY-ALI, Joint Quantum Institute, National Institute of Standard and Technology — Since the experimental realization of synthetic magnetic fields in neural ultracold atoms, transport measurement such as quantized Hall conductivity remains an open challenge. Here we propose a novel and feasible scheme to measure the topological invariants, namely the chern numbers, in the time of flight images. We study both the commensurate and the incommensurate flux, with the later being the main focus here. The central concept underlying our proposal is the mapping between the chern numbers and the size of the dimerized states that emerge when the two-dimensional hopping is tuned to the highly anisotropic limit. In a uncoupled double quantum Hall system exhibiting time reversal invariance, only odd-sized dimer correlation functions are non-zero and hence encode quantized spin current. Finally, we illustrate that inspite of highly fragmented spectrum, a finite set of chern numbers are meaningful. Our results are supported by direct numerical computation of transverse conductivity.

[1]NBA acknowledges support from a National Research Council postdoctoral research associateship

12:03PM B35.00005 Topological Nature of Phonon Hall Effect[1] , LIFA ZHANG, JIE REN, JIAN-SHENG WANG, BAOWEN LI, National University of Singapore — We provide a topological understanding on phonon Hall effect in dielectrics with Raman spin-phonon coupling. A general expression for phonon Hall conductivity is obtained in terms of the Berry curvature of band structures. We find a nonmonotonic behavior of phonon Hall conductivity as a function of magnetic field. Moreover, we observe a phase transition in phonon Hall effect, which corresponds to the sudden change of band topology, characterized by the altering of integer Chern numbers. This can be explained by touching and splitting of phonon bands.

[1]This project is supported in part by grants R-144-000-257-112 and R-144-000-222-646 of NUS.

12:15PM B35.00006 Effects of Metallic Contacts on Topological Insulator Surface States , JIMMY HUTASOIT, TUDOR STANESCU, West Virginia University — We study the effect of the coupling between a time-reversal invariant topological insulator and a metal. The coupling of the surface states to the metal is studied both numerically, using a tight-binding model, and analytically within a two-dimensional effective theory. The original surface state described by a massless Dirac fermion acquires a non-trivial spectral profile upon interaction with the metal. This results in the broadening of the surface modes and a shift in the position of the Γ- point, which may sink into the valence band at strong coupling.

12:27PM B35.00007 Spin active scattering at the interface between a metal and a topological insulator , ERHAI ZHAO, George Mason University, CHUN ZHANG, National University of Singapore, MAHMOUD LABABIDI, George Mason University — We present theoretical results for the spin-active scattering and local spectrum at the interface between a metal and a three-dimensional topological band insulator. We show that there exists a critical incident angle at which complete (100%) spin flip reflection occurs and the spin rotation angle jumps by π. We discuss the origin of this phenomena, and systematically study the dependence of spin-flip and spin-conserving scattering amplitudes on the interface transparency and metal Fermi surface parameters. The interface spectrum contains a well-defined Dirac cone in the tunneling limit, and smoothly evolves into a continuum of metal induced gap states for good contacts. We also investigate the complex band structure of Bi_2Se_3.

12:39PM B35.00008 Floquet Topological Insulator in Semiconductor Quantum Wells , NETANEL LINDNER, GIL REFAEL, California Institute of Technology, VICTOR GALITSKI, University of Maryland — Topological phase transitions between a conventional insulator and a state of matter with topological properties have been proposed and observed in mercury telluride - cadmium telluride quantum wells. We show that a topological state can be induced in such a device, initially in the trivial phase, by irradiation with microwave frequencies, without closing the gap and crossing the phase transition. We show that the quasi-energy spectrum exhibits a single pair of helical edge states. The velocity of the edge states can be tuned by adjusting the intensity of the microwave radiation. We discuss the necessary experimental parameters for our proposal. This proposal provides an example and a proof of principle of a new non-equilibrium topological state, Floquet topological insulator, introduced in this paper. arXiv:1008.1792

12:51PM B35.00009 A study of localized states in topological insulators , KUN WOO KIM, TAMAR PEREG-BARNEA, GIL REFAEL, California Institute of Technology — Perturbative and Semiclasscial approaches are employed to find the localized state of the toplogical insulators both on sample edges and defects in the bulk. The models used are massive Dirac with either one or two valleys. The topology is provided by the mass term which has either a momentum dependence or a different sign on the two Dirac points. A semiclasscial Hamiltonian is deduced by following a certain classical path and the Hamilton-Jacobi equation determines the dynamics. Our semiclassical results reproduce the lattice model's chiral edge modes and allow us to investigate impurity bound states. These bound states also appear in a T-matrix calculation.

1:03PM B35.00010 Zero modes in the bulk of the Topological Insulators induced by disorder or dislocations , DAVID SCHMELTZER, City College of New York — The enigma of the finite conductivity which comes from the bulk of the Topological Insulators (T.I.) is solved by showing that domain walls in the T.I. bind protected zero modes. We consider two scenarios: a)-Dislocations: -We solve the massive Dirac equation (which corresponds to the T.I. in four and two dimensions) in a curved space generated by the coordinates transformation induced by a single dislocation or a single disclination. We examine the condition for the protected zero modes caused by Torsion and Curvature. b) Disorder:-We use the Keldish formalism to study the effect of disorder and interaction of the T.I. We identify an effective Non-Linear Sigma model with a Maxweell and Chern-Simon term which correspond to the different phases: regular metal, regular insulator, topological insulator and protected metals.

1:15PM B35.00011 Zero energy modes in heterostructures , TUDOR PETRESCU, STEPHAN RACHEL, KARYN LE HUR, Physics Department, Yale University — Zero energy gapless modes have been realized in 1-dimensional domain walls of 2-dimensional systems. In the case of single- or bi-layer graphene, such a quantum wire can be realized by inverting the sign of the gap across a one dimensional interface, without time-reversal symmetry breaking. With the experimental realization of artificial graphene, previously unrealistic additional terms in the Hamiltonian such as staggered potential or artificial gauge fields can be exploited towards the same goal. We classify these terms and study the interplay of disorder effects and boundary conditions.

1:27PM B35.00012 Protected Entanglement Spectrum in Disordered Topological Insulators , EMIL PRODAN, Yeshiva University, TAYLOR HUGHES, University of Illinois at Urbana-Champaign, ANDREI BERNEVIG, Princeton University — The topological insulating phase is robust against disorder. However, the phase diagram of a topological insulator, more precisely the boundary between the trivial and topological phases, can be strongly reshaped by the disorder. It is therefore important to devise methods that can efficiently map the extent of the topological phase in the presence of disorder. This talk will describe two such methods and presents several applications. First, it is shown that, in the topological phase, the entanglement spectrum remains extended while in the trivial phase it becomes localized, in the presence of disorder. The localized/delocalized character of the entanglement spectrum has a clear signature in the level statistics, which can be used to efficiently map the boundary between topological and trivial phase. The second method is based on efficient real space calculations of the bulk invariants that do not involve twisted boundary conditions. In fact, it is shown that both methods involve only data encoded in the ground states of the systems.

1:39PM B35.00013 Theory of Inversion Symmetric Topological Insulators , TAYLOR HUGHES, University of Illinois at Urbana-Champaign, EMIL PRODAN, Yeshiva University, B. ANDREI BERNEVIG, Princeton University — We analyze translationally-invariant insulators with inversion symmetry that fall outside the current established classification of topological insulators. These insulators exhibit no edge or surface modes in the energy spectrum and hence they are not edge metals when the Fermi level is in the bulk gap. However, they do exhibit protected modes in the entanglement spectrum localized on the cut between two entangled regions. There is a direct connection between the inversion eigenvalues of the Hamiltonian band structure and the mid-gap states in the entanglement spectrum. We also analyze the linear response of these insulators and provide examples of when the inversion eigenvalues determine a non-trivial charge polarization, a quantum Hall effect, an anisotropic 3D quantum Hall effect, or a magneto-electric polarization.

1:51PM B35.00014 Topological Properties of Insulators with Inversion Symmetry , ARI TURNER, YI ZHANG, ROGER MONG, ASHVIN VISHWANATH, UC Berkeley — There are many phases of insulators with inversion symmetry (with no other symmetry required). In particular, certain inversion parities cannot change unless there is a phase transition. I will show how to use these parities to classify phases of topological insulators and explain which combinations of these parities have physical consequences (e.g. for the magnetoelectric effect). Many of these results can be derived by pictorial arguments using the entanglement spectrum.

2:03PM B35.00015 Computing topological invariants without inversion symmetry , ALEXEY SOLUYANOV, DAVID VANDERBILT, Rutgers University — We consider the problem of calculating the weak and strong topological indices in noncentrosymmetric time-reversal (T) invariant insulators. In 2D we use a gauge corresponding to hybrid Wannier functions that are maximally localized in one dimension. Although this gauge is not smoothly defined on the two-torus,[1] it respects the T symmetry of the system and allows for a definition of the Z_2 invariant in terms of time-reversal polarization.[2] In 3D we apply the 2D approach to T-invariant planes. We illustrate the method with first-principles calculations on GeTe and HgTe under [100] and [111] strain. Our approach is different from the one suggested previously by Fukui and Hatsugai[3] and should be easier to implement in *ab initio* code packages. Time permitting, we will also discuss methods for decomposing the band space into T-paired Chern subspaces, and for carrying out a general construction of a Wannier representation for Z_2 insulators.

[1]A. A. Soluyanov and D. Vanderbilt, arXiv:1009.1415
[2]L. Fu and C. L. Kane, Phys. Rev. B **74**, 195312 (2006)
[3]T. Fukui and Y. Hatsugai, J. Phys. Soc. Jpn. **76**, 053702 (2007)

Monday, March 21, 2011 11:15AM - 2:15PM –
Session B36 GERA: Photovoltaics: Novel Approaches and System Issues C142

11:15AM B36.00001 Surpassing the classical light-trapping limit in thin film solar cells , JEREMY MUNDAY, DENNIS CALLAHAN, HARRY ATWATER, California Institute of Technology — We describe a methodology for designing thin film solar cells that have light-trapping intensity and absorption enhancements that exceed the classical, ergodic light-trapping limit. From thermodynamic arguments, Yablonovitch and Cody determined the maximum absorption enhancement in the ray optics limit for a bulk material to be $4n^2$, where n is the index of refraction of the absorbing layer. Stuart and Hall expanded this approach to study a simple waveguide structure; however, for the waveguide structures they considered, the maximum absorption enhancement was $< 4n^2$. Using a combination of analytical and numerical methods, we describe why these structures do not surpass the ergodic limit and show how to design structures that can. We present here a physical interpretation in terms of the waveguide dispersion relations and optical density of states. We further describe the necessary criteria for surpassing the classical limit and provide examples of waveguide structures with absorption enhancements in excess of $4n^2$.

11:27AM B36.00002 Resonance shifting: A simple, all-optical method for circumventing the reabsorption problem in luminescent concentrators , NOEL GIEBINK, GARY WIEDERRECHT, Argonne National Lab, MICHAEL WASIELEWSKI, Northwestern University — Luminescent concentrators (LSCs) were developed over three decades ago as a simple route to obtain high concentration ratio for photovoltaic cells without tracking the sun. In principle, high concentration ratios >100 are possible for commonly used chromophores. In practice, however, there is typically an overlap between the chromophore absorption and emission spectra that, although small, ultimately leads to unacceptable reabsorption losses, limiting the concentration ratio to ∼10 and hence the utility of LSCs to date. We introduce a simple, all-optical means of avoiding reabsorption loss by "resonance shifting" from a bilayer cavity that consists of an absorber/emitter waveguide lying upon a low refractive index layer supported by a transparent substrate. Emission is evanescently coupled into the substrate at sharply defined angles and hence, by varying the cavity thickness over the device area, the original absorption resonance can be avoided at each bounce, allowing for extremely low propagation loss to the substrate edges and hence an increase in the optical concentration ratio. We validate this concept for absorber/emitter layers composed of both a typical luminescent polymer and inorganic semiconductor nanocrystals, demonstrating near-lossless propagation in each case.

11:39AM B36.00003 Computational Design of All-Carbon Photovoltaics , MARCO BERNARDI, JEFFREY C. GROSSMAN, Massachusetts Institute of Technology, GROSSMAN GROUP TEAM — We employ ab-initio computational approaches to study interfaces between different carbon nanomaterials (graphene nanoribbons, carbon nanotubes, graphene fragments) with different structures and surface chemistries. The presence of suitable type-II band alignment at these interfaces and significant light-absorption in the visible and infrared make all-carbon heterojunctions appealing as the active material in next-generation flexible photovoltaic devices, particularly given their greatly enhanced stability compared with polymer-based cells. Results for a wide range of carbon nanomaterials interfaces will be presented, and we will discuss possible applications of such a technology, extending the analysis to the thin-film device scale.

11:51AM B36.00004 Continuum and KMC simulations of realistic bulk heterostructure solar cell photovoltaic devices , KANOKKORN PIMCHAROEN, DANIEL OLDS, PHILLIP DUXBURY — Design of novel solar cell architectures is significantly assisted by reliable continuum device models, and computational methods capable of solving these models in one, two and three dimensions. We are developing computational methods for these models and are validating them using Kinetic Monte Carlo simulations in the same morphologies. We present simulations using idealized morphologies to test approximations in the continuum models, and we present results for bulk heterostructure morphologies deduced by refining digital nanostructures to experimental neutron relectometry and small angle scattering data. In particular we discuss the ability of one dimensional device models to capture the physics of photovoltaic response of realistic bulk heterostructures.

12:03PM B36.00005 Computational Materials Design for High Efficiency Photovoltaic Solar Cells and Transparent Conducting Sulfides , HIROSHI KATAYAMA-YOSHIDA, YOSHIMASA TANI, KAZUNORI SATO, Osaka University — Based on the first-principles electronic structure calculations we propose computational materials design for high efficiency and low price (In free) solar cell materials based on CuInSe2. Firstly, to avoid the use of In, we try to substitute In by Zn and Sn, or by Ga. The electronic structure calculations are performed by using the KKR-CPA method. To calculate band gap energy correctly, we use self interaction corrections proposed by Filippetti et al. It is found that the direct band gap does not collapse and there appears no deep impurity state in the gap, thus it should be possible to avoid In without any deterioration of photovoltaic effect. From the calculations of mixing energy, we predict that the present system favors the spinodal decomposition and we can expect the formation of nano-wire by two dimensional spinodal nano-decomposition. When the nano-wires are formed, we can expect Type 2 band alignment between host material and the nano-wires. Due to this band alignment, efficient electron hole separation is expected leading to highly efficient photovoltaic effect. As an extension of the present design, we also propose a new class of n-type and p-type transparent conducting sulfides with the negative activation energy for the application of high-efficiency photovoltaic solar-cells.

12:15PM B36.00006 Efficient Black Silicon Solar Cells with Multi-Scale Surface Texture , FATIMA TOOR, WILLIAM NEMETH, MATTHEW PAGE, QI WANG, HOWARD BRANZ, HAO-CHIH YUAN, National Renewable Energy Laboratory — A nanostructured, density-graded surface layer can replace conventional quarter-wavelength coatings as the anti-reflection layer in photovoltaics. If the layer is comprised of structures smaller than the wavelength of the incident light and the density is graded across more than about half the wavelength of the light, reflection is strongly suppressed (H. M. Branz et al., APL **94** 2009). We developed an inexpensive liquid etch technique for silicon to produce "black Si" based upon this physics. However, the problem of high carrier recombination within this nanostructured layer must be overcome to improve beyond the present best solar cell with its confirmed 16.8% black silicon sunlight-to-electricity conversion efficiency (H-C. Yuan et al., APL **95** 2009). In this work, we combine the black Si layer with conventional KOH-etched pyramidal surface texture (Y. Xiu et al., Langmuir **24** 2008) at micron-scale. Pyramids contribute anti-reflection based on geometric optics. Combining the pyramids with nanostructures only 100 nm deep provides reflectivity below 2% across a wavelength range from 350 – 1000 nm. To-date, we have obtained a solar cell efficiency of 17% with a V_{oc} of 613 mV, J_{sc} of 35 mA/cm^2 and fill-factor of 78%. These cells have improved blue response compared to the best planar black Si cells.

12:27PM B36.00007 Scalability of Nanocoax PV Architecture , MICHAEL J. NAUGHTON, ZHIFENG REN, KRIS KEMPA, Boston College — The radial junction nanocoax-based nanowire solar architecture offers the prospect of high conversion efficiency with thin film PV, due to enhanced light trapping and ultrathin absorbers. We critique the potential applicability of this structure for various PV media.

12:39PM B36.00008 Physical effects of ultrathin photovoltaic junctions , T. KIRKPATRICK, K. KEMPA, M.J. NAUGHTON, Boston College — Hot carrier photovoltaic cells have potential to increase conversion efficiency beyond the Shockley-Queisser limit. In addition to implementing selective energy filters into the device in order to extract the hot carriers at elevated energies beyond the band edges, a possible requirement, of particular importance for non-crystalline material, is that the device also be constructed ultrathin in order to extract the hot carriers as usable energy on time scales of less than one picosecond, after which thermalisation sets in. Ultrathin amorphous silicon p-i-n junctions have been shown to extract hot carriers as usable energy at fixed short circuit current density for p- and n- region thicknesses of 5 nm, and i-layer thickness less than 50 nm [Appl. Phys. Lett. **95**, 233121 (2009)]. Physical effects on device performance in ultrathin cells, such as optical absorption, scattering, band structure, and transport are discussed.

12:51PM B36.00009 Amorphous Silicon-Carbon Nanostructure Solar Cells , MARIA SCHRIVER, UC Berkeley, WILL REGAN, MATTHIAS LOSTER, ALEX ZETTL — Taking advantage of the ability to fabricate large area graphene and carbon nanotube networks (buckypaper), we produce Schottky junction solar cells using undoped hydrogenated amorphous silicon thin films and nanostructured carbon films. These films are useful as solar cell materials due their combination of optical transparency and conductance. In our cells, they behave both as a transparent conductor and as an active charge separating layer. We demonstrate a reliable photovoltaic effect in these devices with a high open circuit voltage of 390mV in buckypaper devices. We investigate the unique interface properties which result in an unusual J-V curve shape and optimize fabrication processes for improved solar conversion efficiency. These devices hold promise as a scalable solar cell made from earth abundant materials and without toxic and expensive doping processes.

1:03PM B36.00010 Prediction of enhanced photovoltaic performance of amorphous silicon solar cells with filled nanopores , JEFFREY GROSSMAN, JOO-HYOUNG LEE, Massachusetts Institute of Technology — We propose a novel hybrid structure for improving the efficiency of thin-film amorphous silicon solar cells. Using $ab\ initio$ calculations, we demonstrate that nanoporous, amorphous silicon (pa-Si), when filled with polythiophene (PT) inside the pores, forms a staggered gap (type II) heterojunction at the interfaces, where both the highest occupied and the lowest unoccupied molecular orbitals of PT are positioned in energy higher than those of pa-Si. Furthermore, we find that while the absorption coefficient (α) of pa-Si is significantly reduced from that of bulk amorphous Si (a-Si), inclusion of PT recovers α to the values of a-Si and even higher at thicknesses of $\sim 1\mu$m. These results suggest that such a hybrid material, which from a manufacturing standpoint may be substantially easier to scale up than nanowire-based approaches, could greatly enhance the hole mobility in the active layer, which is one of the main reasons for poor efficiency in a-Si solar cells.

1:15PM B36.00011 Optimizing materials for photon-enhanced thermionic emission , JARED SCHWEDE, DANIEL RILEY, IGOR BARGATIN, SAMUEL ROSENTHAL, ROGER HOWE, NICHOLAS MELOSH, ZHI-XUN SHEN, Stanford University — We recently described a novel process for solar energy harvesting called photon-enhanced thermionic emission (PETE) based on a semiconductor cathode and a low-workfunction anode separated by a vacuum gap. Previous work explored the limiting theoretical efficiency of a PETE device, which was shown to exceed the Shockley-Queisser limit on single-junction photovoltaic cells, and described experiments that showed strong evidence the PETE effect. In this presentation, I will describe challenges for making the PETE process efficient, some of which were encountered in these proof-of-concept measurements. I will also describe experimental paths to overcoming these challenges and improving efficiency.

1:27PM B36.00012 Optimization and Characterization of Nanostructured Surfaces for Photon-Enhanced Thermionic Emission and Photoemission cathodes , DANIEL RILEY, VIJAY NARASIMHAN, JOEL JEAN, IGOR BARGATIN, JARED SCHWEDE, ZHI-XUN SHEN, ROGER HOWE, NICK MELOSH, Stanford University — In the cathode of an energy converter based on photon-enhanced thermionic emission (PETE) photoexcited carriers may need to encounter the emissive surface numerous times before having sufficient thermal energy to escape into vacuum and therefore should be confined close to the surface. However, in a traditional planar geometry, a thin cathode results in incomplete light absorption. Nanostructuring has the potential to increase light capture and boost emission by decoupling the lengths associated with photon absorption and electron emission. Nanostructures may complicate the properties of the emissive surface; therefore, the effect of nanostructuring on emission efficiency needs to be studied. _We have recently reported preliminary theoretical results from a suite of simulation tools to capture the full photoemission process: photon absorption, carrier transport within the active material, and electron ballistics following emission. In this work we use the simulation suite to optimize nanostructures for applications including PETE-based solar energy converters, photodetectors and electron sources. The samples are then characterized, and the emission efficiency measured in an ultra-high vacuum test chamber under application-centric conditions.

1:39PM B36.00013 Design and characterization of transparent thin film nanostructure device , UDAY TRIVEDI, UTPAL JOSHI — Indium tin oxide (ITO) is one of the most widely used transparent conducting oxides (TCO) because of its electrical conductivity and optical transparency.We have grown "all oxide" transparent $p-n$ junction thin film nanostructure device by using chemical solution deposition and e-beam evaporation onto SiO_2 substrate. The oxide $p-n$ junction was characterized by GIXRD, AFM, UV-Vis. spectroscopy and I-V measurements. Combined GIXRD and AFM confirm phase pure, mono-disperse 30 nm NiO and ITO nanocrystallites. More than 70% optical transparency is achieved across 160 nm thick $p-n$ junction. The forward bias current is greater than the reverse bias current by approximately a factor of 10^4 in the measured voltage s weeping range. A small leakage current as low as 12 nA was observed at a reverse bias of –5 V. Previously, Tonooka and co-authors [3] reported the average turn on voltage of their n-ZnO / p-Cu-Al-O diode $\sim$ 0.5 V, which is higher than our p-NiO/n-ITO diode. This is mainly because of the large variations in the carrier concentrations as well as larger lattice mismatch between the oxides forming the $p-n$ junction. The observed optical and electrical properties of oxide transparent diode are attributed to the heteroepitaxial nature and carrier diffusion at the junction interface.

1:51PM B36.00014 Interface properties of chalcopyrite heterocontacts , CHRISTIAN PETTENKOFER, ANDREAS HOFMANN, EIKE JANOCHA, CARSTEN LEHMANN, Helmholtz-Zentrum Berlin, E-I4 TEAM — Interface properties of heterocontacts determine the device performance of thin film solar cells. We investigated well defined chacopyrite interfaces and heterocontacts of MBE grown samples by electron spectroscopy to obtain informations on the morphology and electronic properties of the contact phases. In particular CuInSe2 and CuInS2 (001) and (112) surfaces were grown by MBE and studied with respect to contact formation to ZnO, ZnS and ZnSe. Due to Cu back diffusion into the bulk even for stoichiometric samples Cu poor interfaces were observed giving rise to interdiffused Zn3In2X6 (X=S,Se) layers in the contact plane. Band alignments obtained fort the prepared heterocontacts will be compared to models given by Mönch and Wei et al. The influence of contact preparation on the properties of the interface will be discussed in detail.

2:03PM B36.00015 Effects of Back Contact Materials on Substrate Configuration CdTe Solar Cells[1] , NATHAN G.F. REAVER, KRISTOPHER WIELAND, ALVIN D. COMPAAN, Dept. of Physics & Astronomy, University of Toledo — Substrate configuration CdTe photovoltaics has the potential to provide both a reduction in the production costs and improved power to mass ratio. In this study the effect of copper placement in the cells, sequence of $CdCl_2$ treatment, and the effect of back contact material on cell performance was examined. Cells were deposited on a Mo coated conductive substrate, on stainless steel or on TCO coated glass, using RF magnetron sputtering. Three different back contacts were used, copper-gold as used in superstrate configuration cells, Sb_2Te_3, and ZnTe:N. Cells were measured using a solar simulator at one sun to obtain current density vs. voltage curves and cell efficiencies. The structure that gave the best performance was stainless steel/Mo/Sb_2Te_3/CdTe/CdS/ZnO/ZnO:Al, with the best cell having an efficiency of 5.34%.

[1]NGFR acknowledges support from the NSF-REU grant PHY-1004649 to the Univ. of Toledo and the Univ. of Toledo Office of Undergraduate Research.

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B37 DMP: Focus Session: Graphene Growth, Characterization, and Devices: Devices and Contacts C146

11:15AM B37.00001 BN / Graphene / BN RF Transistors , HAN WANG, MIT, THITI TAYCHATANAPAT, Harvard University, ALLEN HSU, PABLO JARILLO-HERRERO, TOMAS PALACIOS, MIT — In this work we demonstrate the first BN/graphene/BN transistor for high frequency RF applications. This sandwich structure allows a significant improvement in the mobility of graphene, which reaches more than 18,000 cm^2/Vs at room temperature. Graphene field effect transistors (GFETs) have been fabricated with L_{DS}= 800 nm and L_G=300 nm. The minimum conduction point of these devices is very close to zero, a result of the negligible substrate doping to the graphene. A current density in excess of 1 A/mm and DC transconductance above 200 mS/mm are achieved for both electron and hole conductions. RF characterization is performed for the first time on this device structure and initial results show a current-gain cut-off frequency f_T=10 GHz. These experimental results have been combined with simulations of the small-signal model to study the scaling potential of these GFETs for high frequency applications. The impact of the access resistances (R_s, R_d), the capacitances (C_{gs}, C_{gd}, C_{ds}), and the transconductance (g_m) on the frequency performance of the GFETs has also been studied. Finally, the fabricated devices have been compared to GFETs fabricated with SiO_2 substrate and Al_2O_3 gate dielectrics. The improved performance obtained by the BN/graphene/BN structure is very promising to enable the next generation of high frequency RF electronics.

11:27AM B37.00002 Bilayer graphene $p-i-n$ tunnel junction controlled by modulated top gate[1] , HISAO MIYAZAKI, SONG-LIN LI, KAZUHITO TSUKAGOSHI, NIMS-MANA, JST-CREST, AKINOBU KANDA, Univ. of Tsukuba, JST-CREST — Ambipolar nature of graphene enables us to set charge polarity for electric transport to be p-type or n-type. We fabricated a bilayer graphene (BLG) with spatially modulated p-type and n-type regions. The spatial modulation was introduced by a pair of gate electrodes; a uniform back (substrate) gate and a top gate with stepwise geometry. The gate electric field between the top and back gate also induces band gap in the BLG. As a result, an insulating region is inserted between the p- and n-regions, realizing a $p-i-n$ junction. The current through the junction showed nonlinearity as a function of the source-drain bias. We identified that the origin of nonlinearity is the tunnel current between the p- and n-regions. The nonlinearity reflects the density of states singularity at the edge of the conduction and the valence band in BLG with the band gap. This observation appends another evidence for electric-field-induced band gap in BLG.

[1]This work was supported in part by a Grant-in-Aid for Scientific Research (No. 21241038) from MEXT of Japan, and by the FIRST Program JSPS.

11:39AM B37.00003 Rectification at the graphene and multi-layer-graphene / semiconductor interface from room temperature up to 900K[1] , SEFAATTIN TONGAY, University of Florida, Nanoscience Institute for Medical and Engineering Technology, TODD SCHUMANN, ARTHUR F. HEBARD, University of Florida, Department of Physics — We report on the formation of Schottky diodes on GaN and SiC using a graphite/graphene electrode as a semimetal contact to the semiconductor. The GaN (SiC) /graphene Schottky barriers display rectifying behavior over a wide temperature range with ideality constant close to unity, implying thermionic emission is the dominant transport across the interface. The diodes display larger breakdown voltages (more than 20V) compared to conventional metal junctions (5V). Advantageously, graphite/graphene is stable up to high temperatures and does not diffuse into the semiconductor. We find that these diodes are stable and rectifying up to 900K and are superior to typical metal Schottky diodes reported for the same semiconductors. High temperature measurements are interesting since graphite semimetal contact starts behaving as Boltzmann gas at temperatures well above Fermi energy (T>>280K). Our results imply that graphene based junctions fabricated on conventional semiconductors are good candidates for both high and low temperature devices.

[1]ONR 00075094 (ST, AFH) and by NSF 0704240 (AFH)

11:51AM B37.00004 Complementary-like semiconducting graphene logic inverters , SONG-LIN LI, HISAO MIYAZAKI, KAZUHITO TSUKAGOSHI, National Institute for Materials Science, Japan, AKINOBU KANDA, University of Tsukuba, Japan — The application of graphene as a post-silicon channel material is an interesting but challenging topic due to its metallic nature and low switching ratio. It is expected that the condition would change if a sizeable band gap is introduced. Here we report the electrical characteristics of the first semiconducting graphene-based logic inverters. Free of doping, the *p*- and *n*- branches in the bipolar graphene transistors are delicately used as the complementary components required in logic devices. Within perpendicular electric fields, large transport band gap (> 100 meV) and high switching ratio (~ 200 at 77 K) are obtained in bilayer graphene channels. Besides, a simple and high capacitive-efficiency top gate with natural alumina dielectric ($\sim 0.9\,\mu F/cm^2$) is adopted and the operating bias is lowered within 2 V. For the first time, > 1 voltage gain are extracted from graphene inverters. Voltage gain up to 8 and 2 are achieved at liquid-nitrogen and room temperatures, respectively. Importantly, a match between input and output voltage levels is realized, indicating the potential for direct cascading between multiple devices for future large-scale integration.

12:03PM B37.00005 Ferroelectric gating of CVD graphene devices[1] , GUANGXIN NI, YI ZHENG, National University of Singapore, KUI YAO, Institute of Material Research and Engineering (IMRE), BARBAROS ÖZYILMAZ, National University of Singapore, DEPARTMENT OF PHYSICS, NATIONAL UNIVERSITY OF SINGAPORE, 2 SCIENCE DRIVE 3, SINGAPORE 117542 TEAM, NANOCORE, NATIONAL UNIVERSITY OF SINGAPORE, 4 ENGINEERING DRIVE 3, SINGAPORE 117576 TEAM, INSTITUTE OF MATERIAL RESEARCH AND ENGINEERING (IMRE), 3 RESEARCH LINK, SINGAPORE 117602 COLLABORATION, NUS GRADUATE SCHOOL FOR INTEGRATIVE SCIENCES AND ENGINEERING, SINGAPORE 117597 TEAM — The recent availability of large area graphene has opened up new possibility in graphene research. We will first discuss experiments, where graphene on the ferroelectric substrate PZT allows the fabrication graphene field effect transistors (GFETs) and graphene memory within ± 1 V operating voltage with maximum doping exceeding 10^{13} cm^{-2}. Ferroelectric substrates may also be of importance for large scale applications. Graphene's exceptional optical and mechanical properties make it suitable also for transparent conductors (TCs). While chemical doping has been proven to be an efficient approach to achieving ultra-low sheet resistance, some challenges remain. Here we propose an alternative way to obtain low sheet resistance of graphene using ferroelectric gating.

[1]Singapore National Research Foundation under NRF RF Award No. NRFRF2008- 07 and by NUS NanoCore.

12:15PM B37.00006 Electrical noise in graphene FETs , NAN SUN, KRISTOF TAHY, GERALD ARNOLD, DEBDEEP JENA, HUILI XING, STEVEN RUGGIERO, University of Notre Dame, DEPARTMENT OF PHYSICS TEAM, DEPARTMENT OF ELECTRICAL ENGINEERING COLLABORATION — We report on the low-frequency electrical noise measured in graphene FETs. Samples were created by e-beam lithography using both exfoliated graphene and epitaxial graphene films on SiC. The observed 1/f noise varies as a function of gate bias, where the noise amplitude follows Hooge's empirical relation ($S_V \sim 1/N$), and the noise spectrum deviates from 1/f behavior at low carrier densities. We discuss this behavior in the context of a model including random telegraph noise generated by slow traps.

12:27PM B37.00007 Development of epitaxial graphene based electronics , WALT DE HEER, Georgia Institute of Technology — Epitaxial graphene (EG) has demonstrated a great potential for novel electronic devices [1]. In micron-sized structures graphene is essentially a gapless semimetal, consequently reasonable on-to-off rations can be achieved, but digital electronics is precluded. There are essentially two methods to introduce a bandgap in graphene. One is to make very small structures [1], and the other is to chemically modify the graphene itself [2]. Electron beam lithography is not commercially viable and the graphene is severely degraded by this method. Graphene's conductivity depends on the doping density. For interconnects, reliable methods need to be developed to highly dope graphene without deteriorating the mobility. Furthermore, metallic interconnects are required for all but the simplest structures and they need to be incorporated without defeating graphene's favorable properties. Finally, in the more distant future, EG device architectures that rely on wave properties of the electrons that go beyond diffusive electronics are envisioned [1]. These will require interconnected, nanoscopic graphene structures. An overview and perspective of these issues will be given. I will present new directions, involving multilayer epitaxial graphene, interconnect schemes, non-conventional patterning methods (templated graphene growth [3] and related methods), as well as methods to chemically modify and dope EG.

[1] Berger et al. "Ultrathin Epitaxial Graphite: 2D Electron Gas Properties and a Route toward Graphene-based Nanoelectronics", J. Phys. Chem. B 108, 2004,19912 (2004); W.A.de Heer http://smartech.gatech.edu/handle/1853/31270
[2] E. Bekyarova, et al, JACS 131, 1336 (2009).
[3] M. Sprinkle, et al., "Epitaxial graphene: Templated graphene growth" Nature NanoTechnology 5, 727, (2010)]

1:03PM B37.00008 Metal selection criteria for enhancing electrical conductance of metal-graphene junctions , MARCELO KURODA, Univ. of Illinois - IBM T.J. Watson, J. TERSOFF, IBM T.J. Watson R.C., DENNIS NEWNS, IBM T.J. Watson, GLENN MARTYNA, IBM T.J. Watson R.C. — We study from first principles the electrical conductance of a junction formed by graphitic films in between metal electrodes. We find that for some metals the junction conductance decays exponentially with the number of graphene layers (thickness of the film) while for others it saturates. These different behaviors are attributed to the presence/absence of Fermi-level states in the metal electrode that couple to those of the graphitic thin film. We also find that the bonding between the metal and graphene atoms at the interface has a significant contribution which is dominant for sufficiently thin films. The study may be proven useful for the design and optimization of epitaxially grown electrical contacts.

1:15PM B37.00009 Influence of Metal Contact on the Operation and Scalability of Graphene Field-Effect-Transistors , PEI ZHAO, University of Notre Dame, QIN ZHANG, CMOS and Novel Devices Group, National Institute of Standards and Technology, DEBDEEP JENA, University of Notre Dame, SIYURANGA O. KOSWATTA, IBM Research Division, T. J. Watson Research Center — We explore the effects of metal contacts on the operation and scalability of 2D Graphene Field-Effect-Transistors (GFETs) using detailed numerical device simulations based on the non-equilibrium Green's function formalism at the ballistic limit. Our treatment of metal/graphene (M/G) contacts captures: (1) the doping effect due to the shift of the Fermi level in graphene contacts, (2) the density-of-states (DOS) broadening effect inside the graphene contacts, and (3) the Metal-Induced-States inside the graphene channel. Our results confirm the asymmetric transfer characteristics in GFETs due to the doping effect by metal contacts. Furthermore, the DOS broadening effect will increases the on-current at higher M/G coupling strengths. Finally, with scaling of the channel length, influence on the minimum current in the off-state is also discussed.

1:27PM B37.00010 Flexible and Transparent Field Emission Devices based on Graphene-Nanowire Hybrid Structures , MUHAMMAD ARIF, KWANG HEO, BYUNG YANG LEE, Department of Physics and Astronomy, Seoul National University, Seoul, Korea, DAVID H. SEO, SUNAE SEO, Semiconductor Devices Lab., Samsung Advanced Institute of Tech., Yongin-Si, Gyeonggi-do, Korea, JIKANG JIAN, Department of Physics, Xinjiang University, Xinjiang 830046, P. R. China, SEUNGHUN HONG, Department of Physics and Astronomy, Seoul National University, Seoul, Korea — Recent developments in wafer scale synthesis and transfer of graphene have made it possible to fabricate electrodes for versatile flexible devices. However, a flexible and transparent graphene-based field emission device has not been explored yet. Herein, we report the fabrication of flexible and transparent field emission devices based on graphene-nanowire hybrid structures. In this work, we successfully grew vertically-aligned Au nanowires on graphene surface using an electrochemical method and utilized it as a cathode. We also utilized a graphene electrode for an anode resulting in a transparent and flexible field emission device. Our field emission devices can be bent down to 22 mm radius of curvature without any significant change in its field emission currents. This flexible and transparent field emission device based on graphene-nanowire hybrid structures will utilized for various applications such as field emission displays, x-ray tubes, and pressure sensors.

1:39PM B37.00011 CVD grown graphene field-effect device arrays with water top gate , BEI WANG, B. KOGER, J. ZHU, Physics Department, The Pennsylvania State University, JUN ZHU TEAM — We synthesize single-layer graphene sheets by chemical vapor deposition (CVD) on copper foil. Large sheets are transferred to Si/SiO_2 wafers using poly(methyl methacrylate) (PMMA). Raman spectroscopy of transferred graphene shows the signatures of high-quality graphene with a very small D band. Graphene field-effect device arrays are fabricated using conventional photolithography. A thin SiO_2 film is deposited on top of the finished devices as the last step. We employ two methods of field effect gating. Gate sweeps of the SiO_2 back gate show large initial hole doping. When a droplet of water is deposited on the device and used as a top gate, the majority of devices show a Dirac point of $\sim$0.3 V and bipolar behavior. The water top gate injects charges much more efficiently than the 290nm SiO_2 back gate. The mobility of the devices is estimated to be a few thousand cm^2/Vs. We discuss transport properties and potential applications of these device arrays.

1:51PM B37.00012 Graphene p-n Junctions via Molecular Functionalization , REN-JYE SHIUE, Academia Sinica, HUNG-CHIEH CHENG, CHIA-CHANG TSAI, YIT-TSONG CHEN, National Taiwan University, WEI-HUA WANG, Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan — An essential challenge in graphene-based electronics is to engineer the carrier type and density and still preserve the transport properties of graphene. We report an experimental investigation of graphene $p-n$ junctions via molecular functionalization. By developing a generic scheme for the chemical functionalization, we have shown that an effective and uniform chemical doping of graphene can be achieved by non-covalent modification of the molecules. The effectiveness and uniformity of the modification is systematically confirmed by optical microscopy, surface potential measurement, and Raman spectroscopic imaging. Furthermore, the chemical doping by molecules is utilized to fabricate the graphene $p-n$ junctions. The transport characteristics of the graphene $p-n$ junctions are investigated by transport and magnetotransport measurements. The signatures of the graphene $p-n$ junctions are presented with high carrier mobility, energy splitting of Dirac points, and non-conventional quantum Hall effect.

2:03PM B37.00013 Device fabrication progress on epitaxial graphene on SiC , YIKE HU, ZELEI GUO, RUI DONG, CLAIRE BERGER, WALT DEHEER, Georgia Tech — Epitaxial graphene on SiC has been demonstrated to be a viable route toward electronic device fabrication. While a top gate is required to locally change doping density and carrier type, specifically for field effect transistors graphene devices, back gating is relevant to globally change carrier and to address the graphene layer at the SiC-graphene interface. Here we report result on back-gating and top-gating epitaxial graphene grown on SiC by the confinement controlled sublimation method. Post-patterning treatments of graphene devices are also discussed.

Monday, March 21, 2011 11:15AM - 2:15PM –
Session B38 DCP: Earle K. Plyler Prize Session I: Spectroscopy A130/131

11:15AM B38.00001 Earle K. Plyler Prize for Molecular Spectroscopy Talk: Coherent Ultrafast Multidimensional Spectroscopy of Molecules; From NMR to X-rays , SHAUL MUKAMEL, University of California, Irvine — Multidimensional spectroscopic techniques which originated with NMR in the 1970s have been extended over the past 15 years to the optical regime. NMR spectroscopists have developed methods for the design of pulse sequences that resolve otherwise congested spectra, enhance selected spectral features and reveal desired dynamical events. The major experimental and computational advances required for extending these ideas to study electronic and vibrational motions on the femtosecond timescale will be surveyed. The response of complex molecules and semiconductor nanostructures to sequences of optical pulses provides snapshots of their structure and dynamical processes. Two-dimensional correlation plots of the signals show characteristic cross-peak patterns which carry information about hydrogen bonding, secondary structure fluctuations of proteins and amyloid fibrils, and coherent and incoherent energy and charge transfer in photosynthetic complexes. Double quantum coherence signals that are induced by correlations among electrons or excitons allow the visualization of correlated wavefunctions. Future extensions to the attosecond regime using xray pulses will be discussed. Since core excitations are highly localized at selected atoms, such signals can monitor the motions of valence electron wavepackets in real space with atomic spatial resolution. Common principles underlying coherent spectroscopy techniques for spins, valence electrons, and core electronic excitations, spanning frequencies from radiowaves, infrared, ultraviolet all the way to hard X-rays will be discussed.

[1] "Coherent Multidimensional Optical Probes for Electronic Correlations and Exciton Dynamics; from NMR to X-rays", S. Mukamel, D. Abramavicius, L. Yang, W.Zhuang, I.V. Schweigert and D. Voronine. Acct.Chem.Res. Acct.Chem.Res. 42, 553-562 (2009).
[2] "Coherent Multidimensional Optical Spectroscopy Excitons in Molecular Aggregates; Quasiparticle vs. Supermolecule Perspectives", D. Abramavicius, B. Palmieri, D. Voronine, F. Sanda and S. Mukamel, Chem. Rev. 109, 2350-2408 (2009).

11:51AM B38.00002 Photoelectron spectroscopy of solvated electrons in liquid tetrahydrofuran and methanol microjets , ALEXANDER SHREVE, University of California, Berkeley — Solvated electrons are an important species in radiation chemistry, biology, and other areas. As the simplest quantum solute, solvated electrons are a critical benchmark to test our understanding of solvation in general. Furthermore, when formed in cells, they are highly reactive and may lead to irreversible damage. It is, therefore, important to understand the energetics associated with electron solvation. To this end, we have undertaken a series of studies directly probe electron vertical binding energies (VBEs) in solvents introduced to vacuum through liquid microjets. Solvated electrons are generated following the excitation of the charge-transfer-to-solvent (CTTS) precursor state of iodide from a millimolar concentration salt included in the solution, detached to vacuum, and measured with our field-free time-of-flight spectrometer. Here we present preliminary results of the measurement of the VBE of electrons solvated in bulk tetrahydrofuran and methanol.

12:03PM B38.00003 The Solvated Electron in Acetonitrile , STEPHANIE DOAN, ARTHUR BRAGG, BENJAMIN SCHWARTZ, Dept. Chem. & Biochem., UCLA — The nature of solvated electrons in liquid acetonitrile is of great interest as it appears that excess electrons in this solvent are stabilized in two forms, a dipole-bound (DB) electron (i.e. a typical solvated electron) and a valence-bound electron (VB) electron (e.g. a solvated CH3CN dimer anion). Previous work has suggested that these two species are in equilibrium and can interconvert. We performed 3-pulse transient hole-burning experiments aimed at better understanding the nature of the VB and DB electrons. We found that photoexcitation of VB electrons produces an increased population of DB electrons, but that exciting DB electrons does not produce VB electrons. This suggests a significant asymmetry in the solvent motions that accompany photoexcitation of the electron: it is easier for a DB electron to relax back into the solvent location from which it came than for the local solvation structure to change enough to create a VB electron, whereas excitation of a VB electron disrupts the local solvent structure to the point where the excited electron can relax into the bulk solvent rather than back to the molecules on which it initially resided.

12:15PM B38.00004 Dynamics of electron solvation in $I^-(CH_3OH)_n$ clusters ($4 \leq n \leq 11$) , RYAN YOUNG, University of California, Berkeley — The dynamics of electron solvation following excitation of the charge-transfer-to-solvent (CTTS) precursor state in iodide-doped methanol clusters, $I^-(CH_3OH)_{n=4-11}$ are studied with time-resolved photoelectron imaging (TRPEI). This excitation produces a $I\cdots(CH_3OH)_n^-$ cluster that is unstable with respect to electron autodetachment, and whose autodetachment lifetime increases monotonically from ~800 fs to 85 ps as n increases from 4-11. The vertical detachment energy (VDE) and width of the excited state feature in the photoelectron spectrum show complex time dependences during the lifetime of this state. The VDE decreases over the first 100-400 fs, then rises exponentially to a maximum with a $\sim$ 1ps time constant, decreasing by as much as 180 meV with timescales from 4-10 ps. The early dynamics are assigned to electron transfer from the iodide to a localized portion of the methanol cluster, while the longer-time changes in VDE are attributed to solvent reordering, possibly in conjunction with ejection of neutral iodine from the cluster. Changes in the observed width of the spectrum largely follow those of the VDEs; the dynamics of both are attributed to the major rearrangement of the solvent cluster during relaxation. The relaxation dynamics are interpreted as a reorientation of at least one methanol molecule and the disruption and formation of the solvent network in order to accommodate the excess charge.

12:27PM B38.00005 Vibronic Enhancement of Exciton Sizes and Energy Transport in Photosynthetic Complexes , ANDREW MORAN, JORDAN WOMICK, BRANTLEY WEST, STEPHEN MILLER, University of North Carolina — This talk investigates the impact of vibronic couplings on the electronic structures and relaxation mechanisms of two cyanobacterial light harvesting proteins, allophycocyanin (APC) and c-phycocyanin (CPC). Both APC and CPC possess three pairs of pigments (i.e., dimers), which undergo electronic relaxation on the sub-picosecond time scale. Electronic relaxation is approximately 10 times faster in APC than in CPC despite the nearly identical structures of their pigment dimers. Femtosecond laser spectroscopies conducted in conjunction with a Frenkel exciton model find that photo-induced electronic relaxation in these two proteins is understood on the same footing only when the vibronic couplings in high-frequency modes are properly taken into account. In addition to incorporating high-frequency intramolecular modes in the spectral density, we simulate electronic relaxation dynamics using a model in which the excitons delocalize in a vibronic basis. General implications of the present findings for energy transport in artificial systems (e.g., crystalline organic semiconductors) are discussed.

12:39PM B38.00006 Nonlinear Coherent Optical Imaging for Biomedicine: The Quest for Ultimate Sensitivity , SUNNEY XIE, Harvard University — Recent advances in nonlinear coherent optical imaging, particularly stimulated Raman scattering microscopy, have allowed highly sensitive label-free imaging of living cells and organisms based on molecular spectroscopy. Using the ultimate sensitivity of nonlinear optical microscopy, the detection of a single-molecule absorption signal at room temperature has been achieved. These unprecedented sensitivities offer exciting possibilities for biomedicine.

1:15PM B38.00007 Optical Control of Conjugated Oligomer Planarity , SERGEI TRETIAK, Los Alamos National Laboratory, JENNY CLARK, Cavendish Laboratory, University of Cambridge, GUGLIELMO LANZANI , Lanzani — Using a sequential photo-excitation mechanism we observe the ultrafast conformational planarization of a large fluorene oligomer at $\sim$ 60fs timescale. Novel non-adiabatic excited state molecular dynamics (NA-ESMD) framework incorporating quantum transitions has been used to rationalize this phenomenon. Simulation show the ultrafast relaxation of the photoexcited wavepacket toward the lowest electronic excited state along the torsional coordinate. The process effectively 'locks' the oligomer into a planar state within 100 fs, with excess energy being dissipated into other vibrational modes. Ultrafast control of molecular conformation, as demonstrated here, could have impacts for molecular conformational switches for memory or molecular electronics.

1:27PM B38.00008 Using 2D Fourier-transform spectroscopy to separate homogeneous and inhomogeneous line widths of heavy- and light-hole excitons in weakly disordered semiconductor quantum wells , STEVEN CUNDIFF, ALAN BRISTOW, TIANHAO ZHANG, MARK SIEMENS, JILA, NIST and University of Colorado, RICHARD MIRIN, NIST-Boulder — Optical two-dimensional Fourier-transform spectroscopy is used to study the heavy- and light-hole excitonic resonances in GaAs quantum wells with weak structural disorder. Homogeneous and inhomogeneous broadening contribute differently to the two-dimensional resonance line shapes, allowing separation of homogeneous and inhomogeneous line widths. The heavy-hole exciton exhibits more inhomogeneous than homogeneous broadening, whereas the light-hole exciton shows the opposite. This situation arises from the interplay between the length scale of the disorder and the exciton Bohr radius, which affects the exciton localization and scattering. Utilizing this separation of line widths, excitation-density-dependent measurements reveal that many-body interactions alter the homogeneous dephasing, while disorder-induced dephasing is unchanged.

1:39PM B38.00009 Oxygen atom roaming and multiple dissociation pathways of NO_3 , MICHAEL GRUBB, MICHELLE WARTER, KURT JOHNSON, SIMON NORTH, Texas A&M University — The role of nitrate radical (NO_3) photolysis in atmospheric has long been known, but mysteries remain regarding the mechanism of the dissociation. In particular, the NO + O_2 channel has proven to be a challenge both theoretically and experimentally. High resolution velocity map ion imaging studies reveal that there are two distinct mechanisms to form the NO + O_2 products. Additionally, the dominant of these mechanisms appears to be the non-traditional state "roaming" mechanism recently identified in formaldehyde dissociation. The roaming mechanism involves large amplitude motion associated with a frustrated radical dissociation before roaming oxygen atom abstraction to form O_2. The identification of roaming in the NO_3 reaction may imply the widespread importance of this type of mechanism in atmospheric chemistry.

1:51PM B38.00010 First Principle Simulations of the Infrared Spectrum of Liquid Water using Hybrid Density Functionals , CUI ZHANG, DAVIDE DONADIO, FRANCOIS GYGI, GIULIA GALLI, Univeristy of California, Davis — We report on calculations of the infrared spectrum (IR) of liquid water carried out using first principle molecular dynamics and the hybrid functional PBE0. We find results in much better agreement with experiment than those obtained using semi-local, gradient corrected exchange correlation functionals. In particular the description of the IR stretching band is greatly improved and in good accord with recent measurements. When adopting the PBE0 functional, substantial improvement is also found in the description of the structural properties of the liquid, consistent with a smaller average number of hydrogen bonds, and a reduced molecular dipole moment, as revealed by our analysis of maximally localized Wannier functions. Finally the average electronic gap of the liquid is increased by 60% with respect to PBE, when computed at the PBE0 level of theory, and is in fair agreement with experiment. Work supported by NSF/OCI-0749217.

2:03PM B38.00011 Nonequilibrium Mixed Quantum-Classical simulations of Hydrogen-bond Structure and Dynamics in Methanol-d Carbon tetrachloride liquid mixtures and its spectroscopic signature , KIJEONG KWAC, EITAN GEVA — Liquid mixtures of methanol-d and carbon tetrachloride provide attractive model systems for investigating hydrogen-bond structure and dynamics. The hydrogen-bonded methanol oligomers in these mixtures give rise to a very broad hydroxyl stretch IR band ($\sim$150 cm^{-1}). We have employed mixed quantum-classical molecular dynamics simulations to study the nature of hydrogen- bond structure and dynamics in this system and its spectroscopic signature. In our simulations, the hydroxyl stretch mode is treated quantum mechanically. We have found that the absorption spectrum is highly sensitive to the type of force fields used. Obtaining absorption spectra consistent with experiment required the use of corrected polarizabile force fields and a dipole damping scheme. We have established mapping relationships between the electric field along the hydroxyl bond and the hydrogen-stretch frequency and bond length thereby reducing the computational cost dramatically to simulate the complex nonequilibrium dynamics underlying pump-probe spectra.

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B39 DBP DPOLY DCP: Focus Session: Single Molecule Biophysics II: Novel Single Molecule Approaches to Biology A124/127

11:15AM B39.00001 Single-image molecular analysis for accelerated fluorescence imaging , YAN MEI WANG, University of Washington — We have developed a new single-molecule fluorescence imaging analysis method, SIMA, to improve the temporal resolution of single-molecule localization and tracking studies to millisecond timescales without compromising the nanometer range spatial resolution [1,2]. In this method, the width of the fluorescence intensity profile of a static or mobile molecule, imaged using submillisecond to milliseconds exposure time, is used for localization and dynamics analysis. We apply this method to three single-molecule studies: (1) subdiffraction molecular separation measurements, (2) axial localization precision measurements, and (3) protein diffusion coefficient measurements in free solution. Applications of SIMA in flagella IFT particle analysis, localizations of UgtP (a cell division regulator protein) in live cells, and diffusion coefficient measurement of LacI in vitro and in vivo will be discussed.

[1] Shawn DeCenzo, Michael C. DeSantis, and Y. M. Wang, "Single-image separation measurements of two unresolved fluorophores," Optics Express, 18, 16628-16639, (2010)
[2] M. DeSantis, S. DeCenzo, J. L. Li, and Y.M. Wang, "Precision analysis for standard deviation measurements of single fluorescent molecule images," Optics Express, 18, 6563-6576, (2010)

11:51AM B39.00002 Super-resolution imaging of multiple fluorescent proteins with highly overlapping emission spectra in living cells , MUDALIGE GUNEWARDENE, University of Maine, FEDOR SUBACH, Albert Einstein College of Medicine, TRAVIS GOULD, Yale University , GREGORY PENONCELLO, MANASA GUDHETI, University of Maine, VLADISLAV VERKHUSHA, Albert Einstein College of Medicine, SAMUEL HESS, University of Maine — Diffraction limits resolution in far field microscopy. Single molecule localization based superresolution imaging has surpassed such limitations and is rapidly gaining popularity, yet limited availability of cell-compatible photoactivatable fluorescent probes with distinct emission spectra have impeded simultaneous visualization of multiple molecular species in living cells. We introduce PAmKate, a monomeric far-red photoactivatable fluorescent protein (PAFP), which has facilitated simultaneous imaging of three PAFPs in biological samples with fluorescence photoactivation localization microscopy (FPALM). Successful probe identification was achieved by measuring the fluorescence emission intensity in two distinct spectral channels spanning approximately 100 nm of the visible spectrum. Raft-, non-raft- and cytoskeleton- associated proteins were simultaneously imaged in both live and fixed fibroblasts co-expressing Dendra2-hemagglutinin, PAmKate-transferrin receptor and PAmCherry1-β-actin chimeras, revealing evidence for specific interactions between membrane proteins and membrane-associated actin structures.

12:03PM B39.00003 Single-image diffusion coefficient measurements of proteins in free solution , SHANNON KIAN ZAREH, MICHAEL DESANTIS, JONATHAN KESSLER, YAN MEI WANG, Washing University in St. Louis, Physics department — Diffusion coefficient measurement of biomolecules is important for particle size determination, reaction rate characterization, and molecular dynamics investigation. Here we present a simple and fast method for determining diffusion coefficient of nanometer- and sub-nanometer-sized fluorophores, such as GFP, in free solution by analyzing their single fluorescence images with sub-millisecond exposure times. In this method, the standard deviation (SD) of a diffusing molecule's intensity profile is used to determine its diffusion coefficient. Our SD vs. diffusion coefficient expression is consistent with our simulation and experimental measurement results, rendering this sub-millisecond-long method to be an improvement of at least 100-fold in temporal resolution over current diffusion coefficient measurement methods, such as single-particle-tracking and FCS.

12:15PM B39.00004 Quantifying kinetics and dynamics of DNA repair proteins using Raster-scan Image Correlation Spectroscopy , SALIM ABDISALAAM, University of Texas at Arlington/UT Southwestern Medical Center, MILAN POUDEL, DAVID CHEN, UT Southwestern Medical Center, GEORGE ALEXANDRAKIS, University of Texas at Arlington/UT Southwestern Medical Center — DNA double strand breaks are potentially dangerous lesions as their incomplete repair may lead to carcinogenesis. In this study the confocal Raster scan Image Correlation Spectroscopy technique is used to study kinetics and dynamics of double stand break repair proteins after γ-irradiation of mammalian cells. Diffusion and binding constants were obtained by fitting with different physical models. Results were compared to ones obtained by creating high density DNA damage with a laser and subsequently performing Fluorescence Recovery after Photobleaching over the damage area. This work presents similarities and differences in double strand break repair response between γ-irradiation versus laser damage. This is of importance to answering the question of whether the popular use of laser induced DNA damage is a sufficient surrogate for predicting the radiation treatment response of cancer cells.

12:27PM B39.00005 Overview of single-molecule methods including high-force, force-fluorescence, and dual-trap studies for probing molecular and cellular machinery , MATTHEW LANG, Vanderbilt University — High force optical trapping, including double trap geometry and simultaneous visualization with single molecule fluorescence imaging enables a wide range of measurement capabilities applicable for probing molecular and cellular machinery. A series of single molecule measurement methods will be presented. Force-fluorescence microscopy enables visualizing amyloid fibers while physically probing their structures including direct unfolding and rupture of fibers with a high force optical trap. Force spectroscopy is employed to probe the strength of single peptide aptamer bonds. A dual-trap geometry allows for direct tracking of unfolding and translocation machinery of the biological motor ClpXP. Force fluorescence microscopy directly visualizes T-cell activation. Automation and flexibility in our instruments coupled with advances in physical assay design strategies are leveraged to access a broad set of molecular and cellular measurement targets.

1:03PM B39.00006 ABSTRACT WITHDRAWN –

1:15PM B39.00007 3D single molecule tracking in thick cellular specimens using multifocal plane microscopy[1] , SRIPAD RAM, E. SALLY WARD, University of Texas Southwestern Medical Center, RAIMUND J. OBER, University of Texas at Dallas — One of the major challenges in single molecule microscopy concerns 3D tracking of single molecules in cellular specimens. This has been a major impediment to study many fundamental cellular processes, such as protein transport across thick cellular specimens (e.g. a cell-monolayer). Here we show that multifocal plane microscopy (MUM), an imaging modality developed by our group, provides the much needed solution to this longstanding problem. While MUM was previously used for 3D single molecule tracking at shallow depths ($\sim$ 1 micron) in live-cells [1], the question arises if MUM can also live up to the significant challenge of tracking single molecules in thick samples. Here by substantially expanding the capabilities of MUM, we demonstrate 3D tracking of quantum-dot labeled molecules in a $\sim$10 micron thick cell monolayer. In this way we have reconstructed the complete 3D intracellular trafficking itinerary of single molecules at high spatial and temporal precision in a thick cell-sample.

[1] Biophys J., 2008, 95:6025-6043.

[1]Funding support: NIH and the National MS Society

1:27PM B39.00008 Single Molecule Analysis of Serotonin Transporter Regulation Using Quantum Dots , JERRY CHANG, Vanderbilt University, IAN TOMLINSON, MICHAEL WARNEMENT, ALESSANDRO USTIONE, ANA CARNEIRO, DAVID PISTON, RANDY BLAKELY, SANDRA ROSENTHAL — For the first time, we implement a novel, single molecule approach to define the localization and mobility of the brain's major target of widely prescribed antidepressant medications, the serotonin transporter (SERT). SERT labeled with single quantum dot (Qdot) revealed unsuspected features of transporter mobility with cholesterol-enriched membrane microdomains (often referred to as "lipid rafts") and cytoskeleton network linked to transporter activation. We document two pools of surface SERT proteins defined by their lateral mobility, one that exhibits relatively free diffusion in the plasma membrane and a second that displays significantly restricted mobility and localizes to cholesterol-enriched microdomains. Diffusion model prediction and instantaneous velocity analysis indicated that stimuli that act through p38 MAPK-dependent signaling pathways to activate SERT trigger rapid SERT movements within membrane microdomains. Cytoskeleton disruption showed that SERT lateral mobility behaves a membrane raft-constrained, cytoskeleton-associated manner. Our results identify an unsuspected aspect of neurotransmitter transporter regulation that we propose reflects the dissociation of inhibitory, SERT-associated cytoskeletal anchors.

1:39PM B39.00009 Casein Kinase 2 Reverses Tail-Independent Inhibition of Kinesin-1[1] , JING XU, ZHANYONG SHU, PREETHA ANAND, BABU REDDY, SILVIA CERMELLI, THOMAS WHISENANT, UC Irvine, STEPHEN KING, University of Missouri-Kansas City, LEE BARDWELL, LAN HUANG, STEVEN GROSS, UC Irvine — Kinesin-1 is a plus-end microtubule-based molecular motor, and defects in kinesin transport are linked to diseases including neurodegeneration. Kinesin can auto-inhibit via a direct head-tail interaction, but is believed to be active otherwise. In contrast, this study uncovers a fast but reversible inhibition distinct from the canonical auto-inhibition pathway. The majority of the initially active kinesin (full-length or tail-less) loses its ability to bind/interact with microtubule, and Casein Kinase 2 (CK2) reverses this inactivation (up to 4-fold) without altering kinesin's single motor properties. Motor phosphorylation is not required for this CK2 -mediated kinesin activation. In cultured mammalian cells, knockdown of CK2 level, but not kinase activity, was sufficient to decrease the force required to stall lipid droplet transport, consistent with a reduction in the number of active motors. We propose that CK2 forms a positive regulating complex with the motor. This study provides the first direct evidence of a protein kinase positively regulating kinesin-transport, and uncovers a pathway whereby inactive cargo-bound kinesin can be activated.

[1]This work is supported by NIGMS grants GM64624 and GM079156 to SPG, GM-74830 to LH, NIH grants GM76516 and GM60366 to LB, and AHA grant 825278F to JX.

1:51PM B39.00010 Asymmetric Friction and Directed Movement of Brownian Motors , OLEG ANDREEV, University of Rhode Island, VLADISLAV MARKIN, University of Texas Southwestern Medical Center, URI TEAM, UTSMC TEAM — It is assumed that a Brownian motor is a system that can rectify thermal fluctuations into directed movement. The intriguing question is how this is achieved: what is the mechanism for transferring random pulses from the environment into directed movement. A number of models have been proposed, which, in general, assume the existence of an "asymmetric flashing potential" that makes the motor's diffusion predominately in one direction. In this work, we introduce a model of Brownian motors based on asymmetric friction rather than on asymmetric flashing potential. We show that asymmetric friction can break the symmetry of a molecule's "random walk" by changing the step size depending on direction. Our model assumes the presence of a symmetrical Brownian force (Gaussian function, average force is 0), an isotropic viscous force, which is proportional to the velocity value but opposite in direction, and an asymmetric friction force, whose value depends on the direction. We present a mathematical model that explains the directed movement for several Brownian motor types.

2:03PM B39.00011 GSK-3 regulates transport of kinesin-1 driven cargos *in vivo* , CHRISTINA LEIDEL, Department of Physics, University of Texas at Austin, CAROLE WEAVER, LUKASZ SZPANKOWSKI, LAWRENCE S.B. GOLDSTEIN, HHMI, Department of Cellular and Molecular Medicine, School of Medicine, Univeristy of California, GEORGE T. SHUBEITA, Department of Physics, University of Texas at Austin, CENTER FOR NONLINEAR DYNAMICS, DEPARTMENT OF PHYSICS, UNIVERSITY OF TEXAS AT AUSTIN COLLABORATION, HHMI, DEPARTMENT OF CELLULAR AND MOLECULAR MEDICINE, UNIV. OF CALIFORNIA COLLABORATION — The Glycogen Synthase Kinase 3 (GSK-3) has been linked to many aspects of the development of Alzheimer's disease and was proposed to play a role in the transport of the Amyloid Precursor Protein (APP) by kinesin-1 motors. Using *Drosophila* embryos and larvae with altered GSK-3 expression, we characterize motor transport of cargos including APP and lipid droplets using DIC microscopy, high-resolution video tracking, fluorescence, and *in vivo* stall force measurements with optical tweezers. By comparing cargo velocities and run lengths we find that GSK-3 is a required negative regulator of *in vivo* transport. Stall force measurements on lipid droplets reveal that enhanced transport under conditions of reduced GSK-3 is a result of a larger number of active motors hauling the cargo. Our findings have implications on the use of GSK-3 inhibitors in treatment of Alzheimer's disease.

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B40 DBP: Lipid Bilayers and Biological Membranes: Dynamics and Thermodynamics

A122/123

11:15AM B40.00001 Correlating Anomalous Diffusion with Membrane Obstacle Structure Using Single Molecule Tracking and AFM[1] , MICHAEL SKAUG, MARJORIE LONGO, ROLAND FALLER, UC Davis — Anomalous diffusion has been observed abundantly in the plasma membrane, but the underlying mechanisms are still unclear. In general, it has not been possible to directly image the obstacles to diffusion in membranes, so the dynamics of diffusing particles are used to deduce the obstacle characteristics. We present a supported lipid bilayer system in which we characterized the anomalous diffusion of lipid molecules using single molecule tracking, while at the same time imaging the obstacles to diffusion with atomic force microscopy. To explain our experimental results, we performed lattice Monte Carlo simulations of tracer diffusion in the presence of the experimentally determined obstacle configurations. We correlate the observed anomalous diffusion with obstacle area fraction, fractal dimension and correlation length. We further discuss our results in the context of confinement models and the generating stochastic process.

[1]Supported by NSF grant CBET 0506602

11:27AM B40.00002 Tracking single Kv2.1 channels in live cells reveals anomalous subdiffusion and ergodicity breaking , AUBREY WEIGEL, BLAIR SIMON, MICHAEL TAMKUN, DIEGO KRAPF, Colorado State University — The dynamic organization of the plasma membrane is responsible for essential cellular processes, such as receptor trafficking and signaling. By studying the dynamics of transmembrane proteins a greater understanding of these processes as a whole can be achieved. It is broadly observed that the diffusion pattern of membrane protein displays anomalous subdiffusion. However, the mechanisms responsible for this behavior are not yet established. We explore the dynamics of the voltage gated potassium channel Kv2.1 by using single-particle tracking. We analyze Kv2.1 channel trajectories in terms of the time and ensemble distributions of square displacements. Our results reveal that all Kv2.1 channels experience anomalous subdiffusion and we observe that the Kv2.1 diffusion pattern is non-ergodic. We further investigated the role of the actin cytoskeleton in these channel dynamics by applying actin depolymerizing drugs. It is seen that with the breakdown of the actin cytoskeleton the Kv2.1 channel trajectories recover ergodicity.

11:39AM B40.00003 Studies of molecular diffusion in single-supported bilayer lipid membranes at high hydration by quasielastic neutron scattering[1] , M. BAI, A. MISKOWIEC, S.-K. WANG, H. TAUB, U. Mo., F.Y. HANSEN, Tech. U. Denmark, T. JENKINS, M. TYAGI, D.A. NEUMANN, NIST, S.O. DIALLO, E. MAMONTOV, K.W. HERWIG, ORNL — Bilayer lipid membranes supported on a solid surface are attractive model systems for understanding the structure and dynamics of more complex biological membranes that form the outer boundary of living cells. We have recently obtained quasielastic neutron spectra from single-supported bilayer lipid membranes using the backscattering spectrometer BASIS at the Spallation Neutron Source. Protonated DMPC membranes were deposited onto SiO_2-coated Si(100) substrates and characterized by AFM. Analysis of their neutron spectra shows evidence of a relatively broad Lorentzian component that we associate with bulk-like water above a freezing temperature of ∼267 K. At lower temperatures, the spectra differ qualitatively from that of bulk supercooled water, a behavior that we attribute to water bound to the membrane. We also find evidence of a narrow Lorentzian component that we tentatively identify with a slower motion (time scale ∼1 ns) associated with conformational changes of the alkyl tails of the lipid molecules.

[1]Supported by NSF Grant No. DMR-0705974.

11:51AM B40.00004 Studies of molecular diffusion in single-supported bilayer lipid membranes at low hydration by quasielastic neutron scattering[1] , A. MISKOWIEC, M. BAI, M. LEVER, H. TAUB, U. Mo., F.Y. HANSEN, Tech. U. Denmark, T. JENKINS, M. TYAGI, D.A. NEUMANN, NIST, S.O. DIALLO, E. MAMONTOV, K.W. HERWIG, ORNL — We have extended our investigation of the quasielastic neutron scattering from single-supported bilayer lipid membranes to a sample of lower hydration using the backscattering spectrometer BASIS at the SNS of ORNL. To focus on the diffusive motion of the water, tail-deuterated DMPC membranes were deposited onto SiO_2-coated Si(100) substrates and characterized by AFM. Compared to a sample of higher hydration, the dryer sample does not have a step-like freezing transition at ∼267 K and shows less intensity at higher temperatures of a broad Lorentzian component representing bulk-like water. However, the broad component of the "wet" and "dry" samples behaves similarly at lower temperatures. The dryer sample also shows evidence of a narrow Lorentzian component that has a different temperature dependence than that attributed to conformational changes of the alkyl tails of the lipid molecules in the wet sample. We tentatively identify this slower diffusive motion (time scale ∼1 ns) with water more tightly bound to the membrane.

[1]Supported by NSF Grant No. DMR-0705974.

12:03PM B40.00005 Diffusion in Single Supported Lipid Bilayers , C.L. ARMSTRONG, McMaster Univeristy, Hamilton, Canada, M. TRAPP, Institut de Biologie Structurale, Grenoble, France, M.C. RHEINSTÄDTER, McMaster University, Hamilton, Canada — Despite their potential relevance for the development of functionalized surfaces and biosensors, the study of single supported membranes using neutron scattering has been limited by the challenge of obtaining relevant dynamic information from a sample with minimal material. Using state of the art neutron instrumentation we have, for the first time, modeled lipid diffusion in single supported lipid bilayers.[1] While we find that the diffusion coefficient for the single bilayer system is comparable to a multi-lamellar lipid system, the molecular mechanism for lipid motion in the single bilayer is a continuous diffusion process with no sign of the flow-like ballistic motion reported in the stacked membrane system. In the future, these membranes will be used to hold and align proteins, mimicking physiological conditions enabling the study of protein structure, function and interactions in relevant and highly topical membrane/protein systems with minimal sample material.

[1]C.L. Armstrong, M.D. Kaye, M. Zamponi, E. Mamontov, M. Tyagi, T. Jenkins and M.C. Rheinstädter, Soft Matter Communication, 2010, Advance Article, DOI: 10.1039/C0SM00637H

12:15PM B40.00006 Membrane stress relaxation by transbilayer cholesterol exchange , MARK L. HENLE, L. MAHADEVAN, Harvard University — Fusion and fission events in the cell membrane play a crucial role in many biological processes, yet the mechanism for inducing the membrane bending deformations required for such events remains poorly understood. In particular, standard membrane elastic models predict a problematically high energy barrier for the strongly curved "neck" region formed during fusion and fission. These models assume that the exchange of lipids between membrane leaflets is negligible. While this is valid for phospholipids, other amphiphilic molecules such as cholesterol undergo rapid flip-flop between leaflets. Such exchange can relax bending stresses in the membrane: By flipping from the compressed to the expanded leaflet, cholesterol can reduce the energy required to bend the membrane. In this talk, we present a coarse-grained energetic model (derived from a simple microscopic description of the membrane) for a two-component lipid bilayer that contains a lipid species that can undergo rapid transbilayer exchange. Using this model, we show that lipid flip-flop dramatically reduces the energetic barriers encountered during membrane fusion and fission events and also plays an important role in determining the deformations induced by external forces such as osmotic pressure.

12:27PM B40.00007 Ethanol enhances collective dynamics of lipid membranes , MARTIN KAYE, MAIKEL RHEINSTADTER, McMaster University, Hamilton, Ontario, Canada — Lipid bilayers have long been considered simple homogeneous passive barriers. However, there is a growing consensus that bilayer composition and properties impact their role in membrane function. One molecule which participates in lipid bilayers is ethanol. Ethanol is principally known to increase membrane permeability, serving as a model drug enhancer. While bilayer permeability was thought to depend solely on structural properties such as the area per lipid, this may be supported by thermal fluctuations in the bilayer core. Thermal motion results in the formation of small voids in the hydrocarbon chains, which may play a role in the transport small molecules through the membrane core. In both inelastic neutron scattering experiments and molecular dynamics simulations we find evidence for a new low-energy dynamic mode in the fluid phase of DMPC bilayers immersed in a 5% water/ethanol solution [1]. The molecular motion associated with this phonon corresponds to coherent displacements of the carbon atoms in the lipid tails both in, and partially normal to, the plane of the membrane. This finding supports the possibility of a fluctuation supported trans-membrane transport process in lipid bilayers.

[1] "Ethanol enhances collective dynamics of lipid membranes", M. D. Kaye, M. Tarek, K. Schmalzl, M. C. Rheinstädter, submitted to Physical Review Letters

12:39PM B40.00008 Vesicle Shape Transformations Driven by Active and Spontaneous Lipid Flip-flop , THOMAS POWERS, Brown University, ELNAZ BAUM-SNOW, University of Connecticut Health Center — The lipid composition of cell membranes is created and maintained in part by flippases, enzymes that translocate lipid molecules from one layer of the bilayer membrane to the other. We study how lipid translocation can affect membrane shape, using a cylindrical vesicle as a simple model system. For a short pulse of flippase activity, in which a fraction of lipids are flipped from one layer to the other, we calculate the fraction of flipped lipids that makes the cylinder unstable to a periodic modulation in its radius, as well as the growth rate of perturbations of different wavenumber. We also study the cases of continuous flippase activity and spontaneous flip-flop.

12:51PM B40.00009 *In vitro* approach to the mechanics of lipid membrane area regulation: vesicle absorption and tube formation , MARGARITA STAYKOVA, DOUGLAS HOLMES, CLARKE READ, HOWARD A. STONE — We have designed an experimental approach that allows us to study the response of supported lipid bilayers to cycles of biaxial expansion and compression. We observed that the bilayer effectively adjusts its area during dilatational or compressive strains in order to reduce its tension. For example, if there is a sufficient lipid reservoir in the form of attached vesicles, then a lipid bilayer may accommodate strains tens of times larger than the critical strain for rupture by expanding its area. Additionally, upon compression the bilayer reduces its area by expelling lipid tubes out of its plane. These observations offer new insights into how cells regulate their surface area in response to various mechanical stimuli, i.e. during physiological volume changes, locomotion, cyclic expansion and compression of the uro- and the alveolar- epithelium, etc.

1:03PM B40.00010 Structural Phase Diagram for Multi-lamellar Tubular Deformations of Lipid Mesophases , LOBAT TAYEBI, ATUL PARIKH, University of California, Davis — Stable multi-lamellar cylindrical tubules protrude readily from concentrated mass of amphiphilic molecules in response to a variety of external stresses. Using energetic considerations, we have developed an phase diagram, predicting various types of morphologies of equilibrium multilamellar tubular deformations that stabilize for a broad range of their bending rigidity and surface tension values. Tubular morphologies are described in terms of core radius(rc) and number of lamellae(N). Results of the calculations reveal that emergent tubular morphologies can be classified into three major classes: (1) thin tethers (small rc and low N); (2) solid tubes (high N); and (3) hollow tubes (large rc and and low N). Experimental validation of these predictions is obtained in experiments involving hydration of dry stack lipids Here, tubular deformations, referred to as myelin figures, of all predicted morphologies form in separate populations. Furthermore, the phase diagram also sheds light on a long-standing question of the determinants of the thickness of such myelin figures.

1:15PM B40.00011 Biomembranes that respond to specific triggers by phase separating , MATTHEW LEROUX, MATTHEW FRANTES, VERNITA GORDON, Center for Nonlinear Dynamics and Department of Physics, University of Texas at Austin — Lipid membranes are widely used as models for the cell membrane and for applications such as encapsulation, delivery, and controlled release. We have recently found that when membranes adhere nonspecifically, the adhesion site favors the nucleation and growth of more-ordered lipid phases. The physics behind this, which works by suppressing membrane fluctuations, should be applicable to specifically-adhering membranes as well. This will allow better experimental models for cell adhesion, which is mediated by transmembrane proteins and associated with lipid heterogeneities, and also indicates a new category of pathways for making 'smart,' responsive materials out of lipid membranes. We are transforming our previous, non-specifically adhering systems into membranes that specifically adhere to a surface via binder molecules. We will determine the thresholds for forming ordered phases as a function of binder stiffness, length, and density, compatibility of the binder structure with the molecular packing of lipids in these phases, and membrane properties such as bending modulus and proximity to a phase transition.

1:27PM B40.00012 Lipid domains in supported SM-Chol membranes measured by GISANS[1] , MIKHAIL ZHERNENKOV, MANISH DUBEY, Los Alamos National Laboratory, BORIS TOPERVERG, Ruhr-Universität Bochum, JAROSLAW MAJEWSKI, MICHAEL FITZSIMMONS, Los Alamos National Laboratory — Cell membranes are known to contain regions (called lipid domains, or rafts) described as sphingolipid-cholesterol assemblies which also may contain a subset of membrane proteins. Currently, the main point of discussion is the methodology to study lipid domains and their sizes. We report on Grazing Incidence Small Angle Neutron Scattering (GISANS) measurements of lipid domains in supported sphingomyelin(SM)-cholesterol(Chol) bilayers in a fully aqueous environment. The model bilayers SM:Chol(2:1), SM:Chol(1:2), and a pure SM were deposited using Langmuir-Blodgett/Langmuir-Schaefer technique at a surface pressure of 10 mN/m and measured at 25 $^{\circ}$C. First measurements revealed short range inhomogeneities of the order of 100 Å in both binary systems. The control measurement of a pure SM bilayer exhibited nearly no GISANS indicating an absence of lipid domains in the SM bilayer. This observation is consistent with the notion that a single component system studied below the liquid-gel transition temperature will not produce lipid domains.

[1]Work was supported by DOE-BES.

1:39PM B40.00013 Structure of the Stern layer in Phospholipid Systems[1] , SWETA VANGAVETI, Iowa State University, ALEX TRAVESSET, Iowa State University and Ames lab — The structure of the Stern layer in Phospholipid Systems results from a subtle competition of salt concentration, ionic valence, specific ionic-phospolipid interactions and pH. It becomes very challenging to develop a rigorous theory that encompasses all these effects, yet its understanding is extremely relevant for both model and biological systems, as the structure of the Stern layer determines the interactions of phospholipids with proteins or electrostatic phase separation (rafts). In this talk we will present our theoretical model for the Stern Layer and discuss how all these effects are included. Particularly emphasis is made to Phosphoinositides and Phosphatidic acid.

[1]This work is supported by grant NSF DMR-0748475.

1:51PM B40.00014 Modeling Signal Transduction and Lipid Rafts in Immune Cells , ASHOK PRASAD, Dept. of Chemical and Biological Engr, Colorado State University — Experimental evidence increasingly suggests that lipid rafts are nanometer sized cholesterol dependent dynamic assemblies enriched in sphingolipids and associated proteins. Lipid rafts are dynamic structures that break-up and reform on a relatively short time-scale, and are believed to facilitate the interactions of raft-associated proteins. The role of these rafts in signaling has been controversial, partly due to controversies regarding the existence and nature of the rafts themselves. Experimental evidence has indicated that in several cell types, especially T cells, rafts do influence signal transduction and T cell activation. Given the emerging consensus on the biophysical character of lipid rafts, the question can be asked as to what roles they possibly play in signal transduction. Here we carry out simulations of minimal models of the signal transduction network that regulates Src-family kinase dynamics in T cells and other cell types. By separately treating raft-based biochemical interactions, we find that rafts can indeed putatively play an important role in signal transduction, and in particular may affect the sensitivity of signal transduction. This illuminates possible functional consequences of membrane heterogeneities on signal transduction and points towards mechanisms for spatial control of signaling by cells.

2:03PM B40.00015 Calcium-mediated rigidity in PIP2 lipid domains , WOUTER G. ELLENBROEK, Dept. of Applied Physics, Eindhoven Univ. of Technology and Dept. of Physics & Astronomy, Univ. of Pennsylvania, ANDREA J. LIU, Dept. of Physics & Astronomy, Univ. of Pennsylvania — In lipid mixtures containing the highly negatively charged lipid PIP2 (a crucial component in cell membrane mechanics) multivalent ions such as calcium can drive the formation of PIP2-rich domains by mediating attractions between the lipids. Although the existence of ion-mediated attractions is well known in macromolecular systems, their form is poorly understood because they result from strong correlations between the charged molecules and ions. Within a numerical model of a lipid monolayer, we analyze the mechanics of PIP2-rich domains. We show that they are liquid-like at moderate values of the PIP2-charge but rigid at higher PIP2-charge. We use a recently introduced method to extract the effective pair interaction between the charged lipids in the many-body system, in which the calcium ions and remaining lipids are integrated out.

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B41 DPOLY DBP: Focus Session: Supramolecular Self-Assembly–Controlling Network and Gel Formation I A115/117

11:15AM B41.00001 Bio-mimetic metal-ligand crosslinks yield self-healing polymer networks with near-covalent elastic moduli , NIELS HOLTEN-ANDERSEN, University of Chicago, MATTHEW HARRINGTON, Max Planck Institute for Colloids and Interfaces, HENRIK BIRKEDAL, University of Aarhus, BRUCE LEE, PHILLIP MESSERSMITH, Northwestern University, HERBERT WAITE, University of California, Santa Barbara , KA YEE LEE, University of Chicago — Growing evidence supports a load-bearing role for metal-polymer interactions in biological protein networks. In particular, the strength of the coordinate bonds in metal-ligand coordination complexes combined with their capacity to reform after breaking has been proposed as a source of the high toughness and potential self-healing in certain natural materials. Some of the highest stabilities among metal-ligand coordination complexes are found between Fe3+ and catechol ligands at alkaline pH where the tris-catecholato-Fe3+ stoichiometry prevails, yet the effect of such crosslinks on material properties has not been fully characterized due to the low solubility of Fe3+ at high pH. Inspired by the pH jump experienced by marine biomaterials during secretion, we have developed a simple method to control catechol-Fe3+ inter-polymer crosslinking via pH. The resulting gels display elastic moduli (G') that approach covalently crosslinked gels as well as self-healing properties.

11:27AM B41.00002 Controlling Mechanical Properties of Bis-leucine Oxalyl Amide Gels , WILLIAM CHANG, DANIEL CARVAJAL, KENNETH SHULL, Northwestern University — is-leucine oxalyl amide is a low molecular weight gelator capable of gelling polar and organic solvents. A fundamental understanding of self-assembled systems can lead to new methods in drug delivery and the design of new soft material systems. An important feature of self-assembled systems are the intermolecular forces between solvent and gelator molecule; by changing the environment the gel is in, the mechanical properties also change. In this project two variables were considered: the degree of neutralization present for the gelator molecule from neutral to completely ionized, and the concentration of the gelator molecule, from 1 weight percent to 8 weight percent in 1-butanol. Mechanical properties were studied using displacement controlled indentation techniques and temperature sweep rheometry. It has been found that properties such as the storage modulus, gelation temperature and maximum stress allowed increase with bis-leucine oxalyl amide concentration. The results from this study establish a 3-d contour map between the gelator concentration, the gelator degree of ionization and mechanical properties such as storage modulus and maximum stress allowed. The intermolecular forces between the bis-leucine low molecular weight gelator and 1-butanol govern the mechanical properties of the gel system, and understanding these interactions will be key to rationally designed self-assembled systems.

11:39AM B41.00003 4D Structural Dynamics of Sheared Collagen Networks[1] , RICHARD AREVALO, DANIEL BLAIR, JEFFREY URBACH, Georgetown University — Soft biopolymer networks undergo substantial bulk stiffening when subject to shear strain. This nonlinear rheological signature has been observed for a wide range of semiflexible and stiff biopolymers, but the underlying geometric fiber rearrangements have not been measured and the resulting stress propagation through the network has not been experimentally assessed. We apply steady shear strains to collagen gels adhered to a thin elastic polyacrylamide gel substrate embedded with fluorescent displacement markers, while simultaneously imaging the three-dimensional network with a coupled confocal-rheometer. We observe dramatic network realignment towards the shear gradient driven by the nonaffine stretching, buckling, and rotation of constituent fibers and simultaneously measure stress inhomogeneities at the collagen-polyacrylamide interface. These observations elucidate the physical mechanisms governing strain-stiffening and our recent observation of the system-size dependence of this effect.

[1]This work is supported by the NSF under DMR: 0804782

11:51AM B41.00004 Molecular Dynamics Modeling of Actin Network Formation , RONALD PANDOLFI, PETER BECICH, UC Merced, LAM NGUYEN, FSU, LINDA HIRST, UC Merced — Actin filaments are ubiquitous and critical in cellular functions. The polymer protein F-actin is a semi-flexible filament that forms networks in the presence of binding proteins (i.e. α-actinin, filamin, fascin). Molecular dynamics modeling and simulation of the formation of these networks has revealed the dependence of network structure on the ratio of G-actin monomers to cross-linkers, cross-linker shape, and filament length. In this study we focus on the effects of filament length on the assembled system. Comparative experimental work informs the accuracy of the modeled systems. Fourier analysis of the simulated networks allows quantitative characterization of the network structure.

12:03PM B41.00005 Polyelectrolyte-Surfactant Complexes: A New Class of Organogelators , KEVIN CAVICCHI, YUQING LIU, The University of Akron, GUSTAVO GUZMAN, Universidad Nacional de Colombia — Polyelectrolyte-surfactant complexes (PE-SURFs) are a class of polymers generated by neutralizing a polyelectrolyte with an oppositely charged surfactant. It has been found that PE-SURFs composed of polystyrene sulfonate and long chain alkyl dimethyl amines act as good organogelators for a range of hydrophobic, organic solvents. Thermo-reversible organogels are formed by heating and cooling PE-SURF/solvent solutions. The gel transition temperature is influenced by the degree of polymerization, the length of the alkyl side-chain, the solubility parameter of the solvent, and the concentration of the gelator. Freeze-drying and scanning electron microscopy characterization of the resultant xerogels shows the formation of rod- and plate-like network morphologies depending on the system parameters. This behavior is consistent with gelation driven by the self-assembly of the amphiphilic PE-SURFs into micellar networks.

12:15PM B41.00006 Self-Assembly of DNA–Block Copolymer Micelles , WEI QU, Northwestern University, XUAN JIANG, HAI-QUAN MAO, Johns Hopkins University, ERIK LUIJTEN, Northwestern University — Cationic–hydrophilic block copolymers have been developed as a potential carrier for use in gene delivery, displaying good transfection efficiency and biocompatibility. The cationic blocks effectively condense the DNA into a core surrounded by a protective and stabilizing corona formed by the hydrophilic blocks [Jiang *et al.*, J. Control. Release **122** 297–304 (2007)]. Although the DNA condensation induced by the cationic blocks can be understood from energetic considerations, the formation of micelles with distinct morphologies is more complicated, as it involves several competing interactions. We employ computer simulations to model this interplay of driving forces. By correlating our simulation results with experimental observations, we provide an understanding of the self-assembly process and determine the key structural and experimental parameters that influencing the morphology of the DNA–block copolymer micelles.

12:27PM B41.00007 LL37-DNA complexes and auto-immune diseases , FAN JIN, University of California, Los Angeles, LORI K. SANDERS, University of Illinois, Urbana -Champaign, WUJING XIAN, University of California, Los Angeles, MICHEL GILLIET, University of Texas, Houston, GERARD C. L. WONG, University of California, Los Angeles, DEPARTMENT OF IMMUNOLOGY, UNIVERSITY OF TEXAS, HOUSTON COLLABORATION — LL37 is an alpha-helical host defense peptide in humans. Recent work has shown that Toll-like receptor-9 (TLR9), an intracellular receptor in plasmacytoid dendritic cells (pDCs) of the immune system that normally responds to pathogen nucleic acids, can be pathologically triggered by self DNA in the form of DNA-LL37 complexes. Synchrotron small-angle x-ray scattering (SAXS) measurements reveal an unanticipated form of self-assembly between DNA and this positively charged macroion. We examine the generality of this with other macroions, and propose a new geometric criterion for immune cell activation.

12:39PM B41.00008 Stiffness of DNA nanotubes: insights for the design of dsDNA materials , PAUL WEITEKAMP, Physics Department, UCSB, DANIEL SCHIFFELS, Physics Department, U Munich, ALEX ITEEN, DEBORAH FYGENSON, Physics Department, UCSB — DNA is increasingly used as a material in the design and construction of elaborate structures with nanoscale precision and functionalities. Whether self-assembled from tiles of short, synthetic oligomers or woven from purified genomic strands, most DNA nanostructures are based on parallel arrays of double-stranded DNA (dsDNA) held together by Holliday junction-like cross-links. There is considerable evidence that the double-helices thus intertwined are largely B-form in structure, but the mechanical integrity of the resulting nanostructures has gone largely unexplored. Here we present a systematic study of the stiffness of DNA nanotubes varying parameters such as helix number, cross-link density and strand complexity. We find stiffness is a useful reporter of structural quality for nanotubes and extract design principles for optimizing mechanical integrity of dsDNA materials.

12:51PM B41.00009 Peptide assemblies: from cell scaffolds to immune adjuvants[1] , JOEL COLLIER, University of Chicago — This talk will discuss two interrelated aspects of peptide self-assemblies in biological applications: their use as matrices for regenerative medicine, and their use as chemically defined adjuvants for directing immune responses against engineered antigens. In the first half of the presentation, the design of peptide self-assemblies as analogues for the extracellular matrix will be described, with a focus on self-assemblies displaying multiple different cell-binding peptides. We conducted multi-factorial investigations of peptide co-assemblies containing several different ligand-bearing peptides using statistical "design of experiments" (DoE). Using the DoE techniques of factorial experimentation and response surface modeling, we systematically explored how precise combinations of ligand-bearing peptides modulated endothelial cell growth, in the process finding interactions between ligands not previously appreciated. By investigating immune responses against the materials intended for tissue engineering applications, we discovered that the basic self-assembling peptides were minimally immunogenic or non-immunogenic, even when delivered in strong adjuvants. -But when they were appended to an appropriately restricted epitope peptide, these materials raised strong and persistent antibody responses. These responses were dependent on covalent conjugation between the epitope and self-assembling domains of the peptides, were mediated by T cells, and could be directed towards both peptide epitopes and conjugated protein antigens. In addition to their demonstrated utility as scaffolds for regenerative medicine, peptide self-assemblies may also be useful as chemically defined adjuvants for vaccines and immunotherapies.

[1]This work was funded by NIH/NIDCR (1 R21 DE017703-03), NIH/NIBIB (1 R01 EB009701-01), and NSF (CHE-0802286)

1:27PM B41.00010 Multiscale peptide self-assembly , JUSTIN BARONE, DEVIN RIDGLEY, Virginia Tech — Here, we demonstrate a hierarchical peptide self-assembly process from the nanometer to the micrometer scale. The process begins by mixing a short hydrophobic peptide and a longer α-helix peptide. Cross-β nanostructures spontaneously form that then aggregate into nanometer fibrils and then micron-sized fibers. FT-IR and Raman spectroscopy show unraveling of α-helices and packing of aliphatic side groups as the major events leading to β-sheet and large fiber formation. A thermodynamic model is presented that uses conformational change and hydrogen bond formation to describe free energy change.

1:39PM B41.00011 Intermolecular Hydrogen Bonding in Peptide and Modified Jeffamine Organogels , DANIEL SAVIN, ADAM RICHARDSON, School of Polymers and High Performance Materials, University of Southern Mississippi — In these studies, we present two systems whereby supramolecular assembly results in rigid organogels. First, a series of AB diblock copolymers consisting of poly(Lysine(Z)) (P(Lys(Z)) blocks were synthesized and found to form stable, rigid organogels in THF (ca. 1 - 1.5 wt.% solutions) and chloroform at room temperature. In these systems, the protecting group on the P(Lys) side-chains remains intact and gel formation results from the assembly of the solventphobic P(Lys(Z)) chains through intermolecular beta-sheet formation. The non-peptide block was found to have an effect on organogel properties due to interfacial frustration, which disrupts H-bonding. Second, Jeffamine polymers were modified in a facile way to incorporate intermolecular H-bonding groups to yield networks able to gel various solvents as well as mineral and canola oil. We present the physical and rheological properties of the organogels produced.

1:51PM B41.00012 Designing responsive peptide hydrogels using peptide-responsive polymer conjugates , ALBERTO SAIANI, School of Materials, The University of Manchester, ANTON MASLOVSKIS, ALINE MILLER, School of Chemical Engineering, The University of Manchester — Self-assembly represents a simple and efficient route to the construction of large, complex structures. Peptide self-assembly in particular offers the possibility to design new functional bio-materials that find application in drug delivery and tissue engineering. The β-sheet motif is are of particular interest as short peptides can be designed to form β-sheet rich fibres that entangle and consequently form hydrogels. These hydrogels can be functionalised using specific biological signals and can also be made responsive through the use of enzymatic catalysis and/or conjugation with responsive polymers. In this presentation we will focus on the design of the latter using peptide-responsive polymer conjugates. The main objective is to create hydrogels possessing an internal transition resulting from the conjugation with the responsive polymer in the gel state that can be used as a trigger for example the release of a drug.

2:03PM B41.00013 Stimuli-Responsive Peptide-based Triblock and Star Copolymers , JACOB RAY, SANDEEP NAIK, ASHLEY JOHNSON, JACK LY, DANIEL SAVIN, School of Polymers and High Performance Materials, University of Southern Mississippi — Stimuli-responsive copolymers demonstrate diverse aggregation behavior in aqueous solution. In general, the molecular architecture and the balance of hydrophilic and hydrophobic volumes influence morphology. This study involves polypeptide-based ABA linear triblock and AB2 star copolymer (which structurally resemble phospholipids) amphiphiles. Model systems for this study are poly(L-lysine)-b-poly(propylene oxide)-b-poly(L-lysine) (KPK) triblocks and poly(L-glutamate) (PE) based star copolymers. Extensive studies with KPK systems have resulted in morphological transitions by modifying pH, and we hypothesize that a change in individual chain conformation is the driving force for these transitions. Preliminary results for PE-based star copolymers with various hydrophobic moieties suggest polymersome (vesicle) formation. Light scattering (dynamic and static) and TEM were used to determine aggregate size and morphology as a function of pH; furthermore, circular dichroism (CD) spectroscopy was used to measure helix-to-coil transitions of the polypeptide blocks.

Monday, March 21, 2011 11:15AM - 2:15PM –
Session B42 DPOLY: Polyelectrolytes, Conformations, Assembly, and Dynamics A302/303

11:15AM B42.00001 Scaling behavior of single chain dimension of polystyrene sulfonate[1] , QINGBO YANG, JIANG ZHAO, Institute of Chemistry, Chinese Academy of Sciences — Scaling behavior of single chain of polystyrene sulfonate (PSS-) has been studied by fluorescence correlation spectroscopy. The scaling power index of the hydrodynamic radius of the PSS- single chain in aqueous solutions was found to depend on the salt condition in the solution and a systematic investigation on salt concentration and salt valency has been conducted. The results clearly demonstrate the change in conformation of PSS- chain due to its interaction with the counterions.

[1]Project supported by National Natural Science Foundation of China (NSFC).

11:27AM B42.00002 Bridging induced by multivalent counterions in polyelectrolyte brush , NICOLAS LAUGEL, ROBERT FARINA, Lawrence Berkeley National Lab, PHILIP PINCUS, Materials Research Laboratory, University of California in Santa Barbara, MATTHEW TIRRELL, Dept of Bioengineering, University of California in Berkeley — When the counterions of a polyelectrolyte brush are multivalent, significant changes in its behavior are observed. One example is its shrinkage at values of ionic strengths where osmotic pressure would be expected to keep chains extended. This effect could be explained through the existence of a bridging phenomenon, with the multivalency of each counterion enabling attractive interactions with more than one polymeric charge at a time. Here we present a variational and phenomenological free energy model in a description of the charged brush as an homogeneous layer subject to classical energy contributions related to both chains and counterions. Two mean-field order parameters are introduced to describe counterion condensation and bridging. The model predicts an abrupt collapse of the brush height upon very fine changes in values of the parameters value which is reminiscent of the experimentally observed behavior.

11:39AM B42.00003 Collapse of single polyelectrolytes in a.c. electric fields , CHUNDA ZHOU, ROBERT RIEHN, NC State University — Experimental and theoretical studies of single polyelectrolyte molecules under alternating electric fields have concluded that stretching is the near-universal response. We confined fluorescently stained λ-DNA (48.5 kbp, $\approx$16 μm contour length) in TBE buffer solution in 500 nm x 10 μm microchannels and applied alternating electric fields ranging from 0 kV/cm to about 2 kV/cm. We observed that DNA molecules collapsed under these conditions, in contrast to the literature reports. We observed single molecules with a fluorescence microscope, and analyzed the radius of gyration of each molecule in each frame. The threshold of the electric field at which DNA molecules start to collapse depends on both the concentration of TBE buffer solutions and the frequencies of the alternating electric fields. In particular, the critical electric field for collapse increases as the frequency increases. In our experiment, DNA molecules were suspended in 0.25x TBE, 0.5x TBE, 1x TBE and 2x TBE buffer solution, and the frequency was 100 Hz, 200 Hz, 300 Hz, 450 Hz, 675 Hz or 800 Hz. The critical electric field ranged from 0.5 kV/cm to 1.5 kV/cm. We believe the phenomenon is due to aggregation of density fluctuations within the polymer coil, which is not described in traditional homogeneous coil models.

11:51AM B42.00004 Conformation of Randomly Sulfonated Pentablock Ionomers in Dilute Solution: Molecular Dynamic Simulation Study , DIPAK ARYAL, DVORA PERAHIA, Clemson University, GARY S. GREST, Sandia National Laboratories — As part of our efforts to define the factors that control the structure and dynamics of structures ionic polymers, the conformation of a pentablock copolymer that consists of randomly sulfonated polystyrene, an ionomeric block, bound to poly-ethylene-r-propylene end caped by poly-t-butylstyrene has been studied in dilute solutions using molecular dynamic simulations. Multi-block copolymers offer a means to tailor several properties into one molecule, taking advantage of their rich phase diagram together with unique properties of specific blocks. We varied the solvent quality for the different blocks and followed the changes in conformation. The spatial configuration of the pentablock as well as the dynamics of the polymer was studied. We find that, independent on the solvent, the higher the sulfonation level, the lower R_g. The static and dynamic structure factors were calculated and compared in an implicit poor solvent, water and a common solvent. These data are compared with results obtained from neutron scattering.

12:03PM B42.00005 Polyelectrolyte Dendrimer Conformations from Mean Field Theory , THOMAS LEWIS, VENKAT GANESAN, University of Texas at Austin — The unique architecture of dendrimers has led to research in a wide array of applications including drug delivery. It is widely accepted that non-charged dendrimers exhibit a dense-core radial density profile in order to balance entropic and excluded volume forces. The use of polyelectrolyte dendrimers in drug delivery has been suggested as a way to attain internal cavities within the dendrimer, which can be tuned by varying salt concentration and pH of the solution. In order to gain insight into the equilibrium behavior of both annealed and quenched polyelectrolyte dendrimers, we have developed and numerically solved a Self-Consistent Field Theory approach for charged dendrimer molecules in an implicit solvent. We then use this method to examine the effects of pH, salt concentration, and generation number upon the conformations of these molecules.

12:15PM B42.00006 Controlling the swelling and wettability of weak polyelectrolyte brushes , RICHARD GURTOWSKI, BENXIN JING, ELAINE ZHU, University of Notre Dame — Weak polyelectrolytes (PE) of tunable ionization shows great potential as "smart" polymer materials for diverse applications from drug delivery to energy storage. However, the conformational dynamics of surfaced-tethered weak PE chains remain inadequately understood due to the complexity of their dynamic charge states in response to solvation and surface immobilization conditions. In this work, we investigate the wetting and swelling characteristics of poly(2-vinyl pyridine) (P2VP) brushes grafted to a gold substrate by AFM and water contact angle measurements. We observe the collapse of P2VP brushes, accompanied with increased surface hydrophobicity, as increasing solution pH across a critical transition pH, which is considerably lower than the pKa of free P2VP chains in bulk solution. Surprisingly, the broadness of the transition pH range shows a strong dependence with brush thickness, but not grafting density, suggesting a distribution of chain ionization along grafted P2VP brushes. We further manipulate P2VP brush structures by applying ac-electric fields across the brushes to make tunable and switchable polymer surfaces.

12:27PM B42.00007 Light- and pH Switchable Supramolecular Nanoparticles through Electrostatic Self-Assembly , FRANZISKA GROEHN, University Erlangen-Nuremberg, IMMANUEL WILLERICH — Supramolecular structures that can respond to external triggers are of high interest for example for nanotechnology or drug delivery. Recently we have introduced an approach to electrostatic self-assembly for the formation of supramolecular particles in solution: polyelectrolytes and multivalent stiff organic counterions build well-defined and stable nano-objects. In addition to electrostatics, secondary interactions between counterions such as pi-pi stacking directs the association. Aggregates with narrow size distribution and varying shape such as spheres, cylinders, vesicles and networks result. PH-responsive assemblies can be repeatedly switched "on" and "off" through pH. Furthermore, light is an elegant, non-invasive stimulus offering possibilities for new functional nanostructures. By electrostatic self-assembly, supramolecular particles can be built the size of which can be triggered by light. For example, assemblies of dendrimer macroions and divalent azobenzene counterions can respond to light with a size increase from 30 nm to 165 nm radius. Detailed characterization by static and dynamic light scattering, AFM, SANS and zeta-potential measurements as well as thermodynamic studies yield insight into driving forces and structural control in the self-assembly process.

12:39PM B42.00008 Tunable morphologies from charged diblock copolymers , MONOJOY GOSWAMI, BOBBY SUMPTER, Oak Ridge National Laboratory — Molecular Dynamics (MD) simulations are carried out to understand the physical aspects of different bulk morphologies formed in charged diblock copolymers. It has been seen that the bulk morphologies formed by charged block copolymers, 75 vol % fluorinated polyisoprene (FPI) - 25 vol% sulfonated polystyrene (PSS) with 50% sulfonation are substantially different from their diblock counterparts. In this study we show how the bulk morphologies change from the uncharged diblock counterparts and also how morphology can be tuned with volume fraction of the charged block and with a change in dielectric constant. A physical understanding based on the underlying strong electrostatic interactions between the charged block and counterions is obtained. The 75/25 diblock shows hexagonal morphologies with the minority blocks (PSS) forming the continuous phase due to charge percolation and the FPI blocks arranged in hexagonal cylinders. Some long-range order can be sustained even by changing the dielectric of the medium. Diverse and atypical morphologies are readily accessible by simply changing the number distribution of the charges on PSS block.

12:51PM B42.00009 Finite size effects in polyelectrolyte adsorption: A simulation study , MARIA SAMMALKORPI, PAUL R. VAN TASSEL, Dept. of Chemical Engineering, Yale University — In recent experiments, we have uncovered conditions where polyelectrolyte adsorption to a conducting surface may become continuous in the sense of scaling linearly with time over hours [1]. This discovery of continuous layer growth offers an enticing possibility of nanoscale thin film growth in a single step process, but also brings forth questions of the underlying mechanisms. Here, we present a molecular Monte Carlo simulation study aimed at understanding mechanistically the continuous adsorption process and, more broadly, polyelectrolyte adsorption in general. Our system consists of two parallel polymer chains composed of charged tangent spheres above a surface of variable dielectric discontinuity between the substrate and the solution, and spherical counterions and salt ions. We find that counter ion correlations act to enable the formation of stable polymer-polymer binding and aggregation. We discuss the sensitivity of the attractive regime to a Coulombic coupling parameter and to finite ion size, and the implications of finite size effects and charge distribution both in the polyelectrolytes and in the ions, and implications to experimental observations. [1] A. P. Ngankam and P. R. Van Tassel, Proc. Nac. Acad. Sci. 104, 1140-1145 (2007); C. Olsen and P. R. Van Tassel, J. Colloid and Interface Science 329, 222-227 (2009).

1:03PM B42.00010 Thermal Properties of Linearly and Exponentially Growing Layer-by-Layer Assemblies , AJAY VIDYASAGAR, JODIE LUTKENHAUS, Texas A&M University — Polyelectrolyte multilayer thin films have received significant attention for assembling various nanostructured coatings, but their thermochemical properties are challenging to measure. Here, we present results regarding the thermochemical properties of two different "model" layer-by-layer (LbL) assemblies. The LbL process involves alternate deposition of positively and negatively charged polymers resulting in interpenetrating networks of layers with fine structural control. Films may grow linearly or exponentially, and each type of growth is expected to give varied internal structure. Poly(allylamine hydrochloride)/poly(styrene sulfonate) (PAH/PSS) multilayers assembled without (or with) added salt are selected as the linear (or exponential) "models." Other systems explored include hydrogen bonding and PAH/poly(acrylic acid) multilayers. In general, linear growth takes place due to charge overcompensation leading to thinner films than exponential growth, where interdiffusion of polyelectrolytes is a major driving force forming much thicker films. Calorimetry and ellipsometry were used to determine glass transition and crosslinking temperatures. A standing hypothesis is that linear (or exponential) growth is observed for glassy (or rubbery) multilayers. The aim of this work is to understand the origin of linear versus exponential growth in polyelectrolytes with respect to their thermal properties.

1:15PM B42.00011 Polyelectrolyte gel dynamics during volume phase transitions , MITHUN MITRA, JING HUA, MURUGAPPAN MUTHUKUMAR, University of Massachusetts, Amherst — We will address the dynamics of the elastic modes of a polyelectrolyte gel near the first-order volume phase transition. The role of the neutralizing plasma on the modulus of the polyelectrolyte gel will be discussed.

1:27PM B42.00012 Field theoretic simulations of the interfacial properties of complex coacervates , ROBERT RIGGLEMAN, University of Pennsylvania, GLENN FREDRICKSON, University of California, Santa Barbara — Many biological processes and emerging technologies, such as wet adhesives and biosensors, rely on the association between oppositely charged polyelectrolytes. Such association is driven not only by the electrostatic interactions between the polyelectrolytes, but there is also a substantial entropy gain associated with counterion release upon complexation. In some cases, the association between oppositely charged polymers can lead to a solid precipitate while others can result in a fluid phase rich in polyelectrolytes (coacervate phase) coexisting with a polyelectrolyte-dilute solvent phase. For many of the applications seeking to exploit coacervation, characterization of the interface between the solvent phase and the coacervate is of paramount importance. In this talk, we will present the results of field-theoretic simulations for a coarse-grained polyelectrolyte model that exhibits complex coacervation. Our simulations sample the fully-fluctuating fields in three-dimensions and provide a detailed characterization of the interface between the solvent and the coacervate phase for symmetric polyelectrolytes (where both the polycations and the polyanions carry identical charge densities) as a function of salt concentration and strength of the electrostatic fields. Finally, we characterize the interfacial properties for a select set of asymmetric conditions.

1:39PM B42.00013 Electrohydrodynamics of polyelectrolytes using Lattice-Boltzmann simulations without electrostatics , OWEN A. HICKEY, JAMES L. HARDEN, University of Ottawa, CHRISTIAN HOLM, University of Stuttgart, GARY W. SLATER, University of Ottawa — In computer simulations of polyelectrolyte electrophoresis, the effects of long-ranged hydrodynamics are often ignored due to the high computational cost. However, the hydrodynamic interactions often play a key role in the physics and can lead to some surprising phenomena. We present hybrid Molecular Dynamics simulation methods to study the electrohydrodynamics of polyelectrolytes using a Lattice-Boltzmann (LB) fluid. By applying a local slip between the monomer beads and the LB fluid we are able to reproduce realistic dynamics for free solution electrophoresis as well as the correct stall force for a polyelectrolyte subject to an electric field. Simulations also demonstrate how a net-neutral object, such as a block polyelectrolyte, can have a non-zero net force due to hydrodynamic interactions and that the force can even be perpendicular to the applied electric field.

1:51PM B42.00014 Thermophoresis of a polyelectrolyte[1] , JENNIFER KREFT PEARCE, AUDREY HAMMACK, ANDREW LASTER, JAMES LEE, SETH NORMAN, University of Texas at Tyler — Thermophoresis, the migration of a species due to a temperature gradient, has been shown to be a possible mechanism for manipulating molecules in microfluidic devices. The mechanism governing thermophoresis is complex making a molecule's Soret coefficient (S_T) and its dependence on different physical factors hard to predict. We experimentally investigate thermophoresis of a polyelectrolyte. For sufficiently high average temperatures, two forms of the molecule are present. We measure the Soret coefficient of both and find that one has positive S_T and the other negative. We also investigate the dependence of S_T on co-dissolved ionic species, specifically NaOH and NaCl.

[1]Acknowledgment is made to the Donors of the American Chemical Society Petroleum Research Fund for support (or partial support) of this research.

2:03PM B42.00015 Charge transport in confined ionic liquids[1] , JOSHUA SANGORO, CIPRIAN IACOB, WYCLIFFE KIPNUSU, FRIEDRICH KREMER, University of Leipzig — Charge transport and glassy dynamics in neat and polymerized ionic liquids confined in nanoporous silica are investigated in a wide frequency and temperature ranges by a combination of Broadband Dielectric Spectroscopy and Pulsed Field Gradient Nuclear Magnetic Resonance (PFG NMR). By applying the Einstein-Smoluchowski relations to the dielectric spectra, diffusion coefficients are obtained in quantitative agreement with independent PFG NMR. The impact of geometrical confinement as well as the pore wall-ionic liquid interactions on the overall ionic mobility is explored for diverse categories of ionic liquids. The results are discussed within the framework of dynamic glass transition assisted charge transport in ionic liquids.

[1]Financial support from the Deutsche Forschungsgemeinschaft under the DFG SPP 1191 Priority Program on Ionic Liquids is gratefully acknowledged.

Monday, March 21, 2011 11:15AM - 2:15PM –

Session B43 DMP DPOLY GERA: Focus Session: Polymers for Energy Storage and Conversion – Nanoscale Structure in Polymer-based Photovoltaics A306/307

11:15AM B43.00001 Association of P3HT and PCBM in solution , TOMEK KOWALEWSKI, Carnegie Mellon University — This abstract not available.

11:51AM B43.00002 Organic solar cells: a theoretical study of the effects of polymer side-chains , NICOLAS BERUBE, HELENE ANTAYA, MICHEL COTE, Universite de Montreal — Organic photovoltaic cells received a great interest in the last few years as they offer an environmentally clean and low-cost solution to the world's rising energy needs. One of the main problems limiting the efficiency of an organic solar cell device is the strong binding energy of the excitons, typically situated about a few hundreds of meV, which is ten to one hundred times more than in inorganic devices. Another limiting factor can be the misalignment of the the HOMO (Highest Occupied Molecular Orbital) and the LUMO (Lowest Unoccupied Molecular Orbital) energy level of the different components of the solar cell. In this presentation, we will discuss how different modifications on organic polymers' side-chains can affect and improve their electronic properties. Our calculations, based on density-functional theory using the B3LYP functional, indicate a HOMO and LUMO lowering of more than 1 eV in various organic polymers like poly-isothianaphtene (pITN) and poly-thienothiophene (pTT), and various side-chains like aldehyde-based ones. Preliminary calculations on oligothiophenes also show a lowering of the exciton binding energy.

12:03PM B43.00003 Perylene Diimide Based "Nanofabric" Thin Films for Organic Photovoltaic Cells[1]

, AUSTIN CARTER, JUNE HYOUNG PARK, Dept. of Physics, The Ohio State University, YONG MIN, Dept. of Chemistry, The Ohio State University, ARTHUR EPSTEIN, Dept. of Physics and Chemistry, The Ohio State University — We report progress in using a perylene diimide (PDI) nanofabric as an effective electron accepting nanostructure for organic photovoltaics (OPV). A key challenge in OPV continues to be the recovery of electrons after charge separation due to the relatively poor mobility of C60 and related materials. A series of PDI compounds and complexes have been synthesized and used to fabricate nanofibers and thin films using solution and vacuum deposition techniques. Overlaping PDI-based nanofibers form a fast electron-transporting "nanofabric" that has been characterized (AFM, PL, UV-vis, etc.) and can be blended with electron donating materials. A solution-processible OPV configuration containing a nanofabric heterojunction (FHJ) of poly(3-hexylthiophene) and the PDI nanofabric was investigated. We observed a significant improvement in power-conversion efficiency due in part to expansion of the interfacial area and the presence of high mobility electron pathways to the LiF/Al electrode.

[1]This work is supported by the Wright Center for Photovoltaic Innovation and Commercialization, the Institute for Materials Research and the Center for Affordable Nanoengineering of Polymeric Biomedical Devices.

12:15PM B43.00004 Influence of Annealing and Blending of Photoactive Polymers on Their Crystalline Structure

, MATTHIAS A. RUDERER, STEFAN M. PRAMS, MONIKA RAWOLLE, QI ZHONG, PETER MUELLER-BUSCHBAUM, TU Muenchen, Physik-Department LS E13, Chair of Functional Materials, James-Franck-Str. 1, 85747 Garching (Germany), JAN PERLICH, STEPHAN V. ROTH, HASYLAB at DESY, Notkestr. 85, 22603 Hamburg (Germany) — Thin photoactive polymer films of poly(3-octylthiophene-2,5-diyl) (P3OT) and poly(2,5-di(hexyloxy)cyanoterephthalylidene) (CN-PPV) are investigated. With X-ray reflectivity measurements, linear concentration-thickness dependence is found for both. Grazing incidence wide-angle X-ray scattering (GIWAXS) is used to probe the crystallinity of thin films and to determine characteristic length scales of the crystalline structure. Moreover, the orientation of the crystalline parts regarding the substrate of both the homopolymer and the blended films is probed with GIWAXS. Temperature annealing is found to improve the crystallization for both homopolymers. In addition, reorientation of the predominant crystalline structures takes place. Blending both polymers reduces or even suppresses the crystallization during spin coating as well as temperature annealing. Absorption measurements complement the structural investigations [1].

[1] M.A. Ruderer et al. J. Phys. Chem. B (2010), doi:10.1021/jp106972s.

12:27PM B43.00005 ABSTRACT WITHDRAWN –

12:39PM B43.00006 Bio-Inspired electro-photonic structure for organic and dye sensitized solar cells[1]

, RENE LOPEZ, Department of Physics and Astronomy, University of North Carolina at Chapel Hill, Chapel HIll, NC, 27599 — A major challenge in solar cell technology dwells in achieving an efficient absorption of photons with an effective carrier extraction. In all cases, light absorption considerations call for thicker modules while carrier transport would benefit from thinner ones. This dichotomy is a fundamental problem limiting the efficiencies of most photovoltaics. One pathway to overcome this problem is to decouple light absorption from carrier collection. We present solutions to this problem applying bio-inspired nanostructures to two different types of systems: organic photovoltaic (OPV) and dye sensitized solar cells (DSSC). For OPV devices based on poly-3-hexylthiophene:[6,6]-phenyl-C61-butyric acid methyl ester (P3HT:PCBM), we describe a 2-D photonic crystal geometry that enhances the absorption of polymer-fullerene photonic cells $\sim$ 20% relative to conventional planar cells. Remarkably, the photonic crystal cell offers the possibility to increase photocurrents by improvements in optical absorption and carrier extraction simultaneously, and particularly through the excitation of photonic resonant modes near the band edge of organic PV materials. We also present an optical method to extract charge transport lengths from device photoactive layers. For DSSCs we introduce a new structural motif for the photoanode in which the traditional random nanoparticle oxide network is replaced by vertically aligned bundles of oxide nanocrystals. We have used a pulsed laser deposition system to ablate titanium oxide targets to obtain the porous and vertically aligned structures for enhanced photoelectrochemical performance. Absorption studies show that in optimized structures for titanium oxide, there is a 1.4 times enhancement of surface area compared to the best sol-gel films, Incident-Photon-Conversion-Efficiency values are better than 3 times thicker sol-gel films, and $\sim$ 92% Absorbed-Photon-Conversion-Efficiency values have been observed when sensitizing with the N3 dye (Ru(dcbpyH)2(NCS)2). The direct pathways provided by the vertical structures appear to indeed provide for enhanced collection efficiency for carriers generated throughout the device.

[1]This work is supported by the UNC-EFRC: DOE DE-SC0001011, the NSF Solar: DMR-0934433, the UNC-Chapel Hill Institute for the Environment, and the ACS-PRF Grant No. 49187-DNI10.

1:15PM B43.00007 The Poly(3-hexylthiophene) / ZnO (10-10) interface: structure and energetics

, JIE JIANG, SOHRAB ISMAIL-BEIGI, Yale University — The poly(3-hexylthiophene) (P3HT) polymer on ZnO system is of significant interest for hybrid nanoscale solar energy research and applications. Using density functional theory and periodic supercells, we study the P3HT/ZnO interface where sulfur atoms on the P3HT side chains are used to anchor the polymer onto the ZnO (10-10) surface. We discuss the structure and energetics of the binding modes for low and high polymer coverage. We then apply the Frenkel-Kontorova model to study the likely polymer structures in practice (e.g. dislocation formation to release strain energy). We end with a discussion of the band energy alignment across the interface.

1:27PM B43.00008 Photovoltaic Device Performance Enhancement by Interfacial Decoration of Bulk-Heterojunctions with Semiconducting Nanocrystals

, THEODORE J. KRAMER, IOANNIS KYMISSIS, IRVING P. HERMAN, Columbia University — We have developed a facile method for decorating the donor-acceptor interface of organic bulk-heterojunctions (BHJs) with semiconducting nanocrystals (NCs). Using nano-scale phase separation of a poly(3-hexylthiophene)/polystyrene copolymer blend, followed by selective removal of the polystyrene, we are able to expose a nano-scale network of poly(3-hexylthiophene) [P3HT] fibers. These fibers are subsequently decorated with cadmium selenide (CdSe) NCs prior to back filling the structure with thermally evaporated C_{60}. Optical characterization techniques have confirmed that NCs located at the donor-acceptor interface show enhanced charge transfer to the surrounding medium compared to NCs randomly dispersed in similar BHJs. Photovoltaic (PV) devices made using this technique show improved external efficiencies compared to similar planar PV structures. This technique provides an elegant mechanism for improving the performance of organic BHJs by tailoring their spectral absorption using semiconducting NCs.

1:39PM B43.00009 Semiconducting Nanocomposites via Directly Grafting Conjugated Polymer onto Quantum Rods

, LEI ZHAO, XINCHANG PANG, ZHIQUN LIN, NANOFM TEAM — Nanocomposites of poly(3-hexylthiophene) (P3HT)-cadmium selenide (CdSe) nanorod (NR) were synthesized by directly grafting P3HT onto bromobenzylphosphonic acid (BBPA) functionalized CdSe NR, dispensing with the need for ligand exchange chemistry. The grafting was accomplished by Heck coupling as well as a newly developed catalyst-free click reaction. The resulting P3HT-CdSe NR nanocomposites possess a well-defined interface, thereby significantly promoting the dispersion of CdSe within the P3HT matrix and facilitating the electronic interaction between them. The success of grafting was confirmed by the NMR and DLS, and the occurrence of charge transfer at P3HT/CdSe NR interface was demonstrated by the UV-vis absorption and photoluminescence (PL) measurements as well as the time-resolved PL study. Similar grafting density was yielded using these two methods. The nanocomposites prepared by the catalyst-free click reaction was found to exhibit a faster charge transfer. To the best of our knowledge, this is the first study of grafting conjugated copolymer directly onto the elongated semiconductor nanomaterials. As such, it provides insight into rational design and fabrication of organic-inorganic nanohybrid solar cells with improved power conversion efficiency.

1:51PM B43.00010 Directed assembly of core-shell hybrid nanomaterials for polymer photovoltaics[1] , SHANJU ZHANG, CANDICE PELLIGRA, LISA PFEFFERLE, CHINEDUM OSUJI — The creation of large-area aligned nanohybrid films/arrays remains a challenge in the fabrication of ordered heterojunction photovoltaics. We demonstrate a bottom-up approach based on the directed assembly of lyotropic inorganic-organic core-shell nanohybrids. Semiconductor nanowires are prepared by solvothermal synthesis. Diameter and length of the nanowires are controlled by various reaction parameters. Core-shell nanohybrids are prepared by grafting conjugated polymers onto the nanowires. Effect of the nanowire diameter on the polymer coating is demonstrated. We show that high aspect ratio nanohybrids spontaneously form nematic phases in liquid media. These systems show isotropic, bi-phasic and nematic phases on increasing concentration in reasonable agreement with Onsager's theory for rigid rods. Suspensions are readily processed to produce films with large-area monodomains. With a decrease of nanowire diameter, the polymers in the nanohybrids tend to form ordered crystalline layers, in which the conjugated backbone is aligned along the nanowire long axis. The corresponding optoelectronic properties are discussed.

[1]The work is supported by NSF SOLAR program.

2:03PM B43.00011 Interconnected and nano-perforated lamellar sheets of metal oxides produced using novel block copolymer templates , PAUL ZAVALA-RIVERA, KEVIN CHANNON, VINCENT NYUGEN, EASAN SIVANIAH, NATARAJ SANNA KOTRAPPANAVAR, University of Cambridge, S.A. AL-MUHTASEB, Qatar Univeristy — Recently, our group has investigated the development of a novel bicontinuous nanostructure using block copolymers. This has lead to the creation of various bicontinuous, mesoporous, and interconnected metal oxides sheets. The high surface area produced by the 3D nanostructure has shown a considerable improvement in efficiency in the method of preparation. The main transformations from polymer scaffold to inorganic matrices produced by our group include the use of oxide of titanium, and a number of other sol-gel transformations. The application of these nanostructures is shown in the development of photovoltaic devices. We highlight future applications in electronic, memory, energy storage and production devices.

Monday, March 21, 2011 11:15AM - 2:15PM –
Session B44 DPOLY: Physics of Copolymers I A309

11:15AM B44.00001 Controlling Cellular Endocytosis at the Nanoscale , GIUSEPPE BATTAGLIA, The Krebs Research Institute, Department of Biomedical Science, University of Sheffield, Sheffield, UK — One of the most challenging aspects of drug delivery is the intra-cellular delivery of active agents. Several drugs and especially nucleic acids all need to be delivered within the cell interior to exert their therapeutic action. Small hydrophobic molecules can permeate cell membranes with relative ease, but hydrophilic molecules and especially large macromolecules such as proteins and nucleic acids require a vector to assist their transport across the cell membrane. This must be designed so as to ensure intracellular delivery without compromising cell viability. We have recently achieved this by using pH-sensitive poly(2-(methacryloyloxy)ethyl-phosphorylcholine)- co -poly(2-(diisopropylamino)ethyl methacrylate) (PMPC-PDPA) and poly(ethylene oxide)-co- poly(2-(diisopropylamino)ethyl methacrylate) (PEO-PDPA) diblock copolymers that self-assemble to form vesicles in aqueous solution. These vesicles combine a non-fouling PMPC or PEO block with a pH-sensitive PDPA block and have the ability to encapsulate both hydrophobic molecules within the vesicular membrane and hydrophilic molecules within their aqueous cores. The pH sensitive nature of the PDPA blocks make the diblock copolymers forming stable vesicles at physiological pH but that rapid dissociation of these vesicles occurs between pH 5 and pH 6 to form molecularly dissolved copolymer chains (unimers). We used these vesicles to encapsulate small and large macromolecules and these were successfully delivered intracellularly including nucleic acid, drugs, quantum dots, and antibodies. Dynamic light scattering, zeta potential measurements, and transmission electron microscopy were used to study and optimise the encapsulation processes. Confocal laser scanning microscopy, fluorescence flow cytometry and lysates analysis were used to quantify cellular uptake and to study the kinetics of this process in vitro and in vivo. We show the effective cytosolic delivery of nucleic acids, proteins, hydrophobic molecules, amphiphilic molecules, and hydrophilic molecules without affecting the viability of cells or even triggering inflammatory pathways. Finally we show how size, surface chemistry and surface topology of the vesicles affect their interaction with the cell membrane and hence their cellular uptake.

References:
C. Lo Presti, M. Massignani, T. Smart, H. Lomas, and G. Battaglia *J. Mater. Chem.* (2009) 19, 3576-3590 H. Lomas, I. Canton, S. MacNeil, J. Du, S.P. Armes, A.J. Ryan, A.L. Lewis and G. Battaglia *Adv. Mater.* (2007). 19, 4238-4243
M. Massignani, I. Canton, N. Patikarnmonthon, N. J. Warren, S. P. Armes, A. L. Lewis and G. Battaglia, *Nature Prec.*, 2010, http://hdl.handle.net/10101/npre.2010.4427.1 M. Massignani, C. LoPresti, A. Blanazs, J. Madsen, S. P. Armes, A. L. Lewis and G. Battaglia *Small*, 2009, 5, 2424-2432.
M. Massignani, T. Sun, A. Blanazs, V. Hearnden, I. Canton, P. Desphande, S. Armes, S. MacNeil, A. Lewis and G. Battaglia *PLoS One*, 2010, 5, e10459.

11:51AM B44.00002 Microphase Separation in Block-Random Copolymers of Styrene and Hydrogenated Isoprene[1] , BRYAN S. BECKINGHAM, Princeton Univesity, RICHARD A. REGISTER, Princeton University — The capacity to synthesize block-random copolymers, which are block copolymers with one or more random copolymer blocks, allows for continuous tuning of the interblock segregation strength, χ, through the composition of the random copolymer. The ability to tune χ effectively decouples the block copolymer molecular weight from its order-disorder transition temperature. By lithium-initiated anionic polymerization with added triethylamine, we synthesize near-monodisperse and near-symmetric block-random copolymers of styrene and isoprene: PI-PSrI (50% wt. styrene). In comparison to PS-PI diblock copolymers, the number of unfavorable segmental contacts in the disordered state is decreased and hence the effective interblock χ is reduced. Isoprene-hydrogenated derivatives of these block-random copolymers exhibit microphase separation into well-ordered lamellae and display sharp thermally-induced order-disorder transitions via small-angle x-ray scattering. The observed reduction in χ, as gauged by the molecular weight required to achieve a desired T_{ODT}, matches well with the mean field prediction.

[1]This work was supported by the National Science Foundation Polymers Program (DMR-1003942).

12:03PM B44.00003 Micellization kinetics of diblock copolymers in a homopolymer matrix: A self-consistent field study[1] , RAGHURAM THIAGARAJAN, DAVID MORSE, Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455 — Self-consistent field theory is used to calculate free energy barriers and reaction rates for the spontaneous association and dissociation of micelles formed of block copolymers in a homopolymer matrix. The barriers are prohibitively large for copolymers of typical molecular weights when the unimer (free surfactant) concentration is near the equilibrium critical micelle concentration. As a result, polymeric micelles normally cannot reach true thermodynamic equilibrium. The rates of association and dissociation are, however, sensitive to unimer concentration, making it possible to form or destroy micelles at observable rates in sufficiently highly supersaturated or subsaturated solutions, respectively, even when both reactions are suppressed near the equilibrium CMC. The barrier to disassociation is particularly sensitive to unimer concentration, and vanishes when the unimer concentration is only slightly (e.g., tens of percent) below the equilibrium CMC.

[1]This work was supported by UMN MRSEC (support for Raghuram Thiagarajan) using computer resources provided by both the Minnesota Supercomputing Institute and the UMN MRSEC.

12:15PM B44.00004 Manipulating the structural conformation of block copolymer micelles using co-solvent mixtures , ELIZABETH G. KELLEY, THOMAS P. SMART, MILLICENT O. SULLIVAN, THOMAS H. EPPS, III, Department of Chemical Engineering, University of Delaware — The internal structure of poly(butadiene-*b*-ethylene oxide) (PB-PEO) block copolymer micelles was manipulated through the use of co-solvent mixtures. In aqueous solutions, the PB-PEO block copolymers self-assembled into monodisperse, spherical micelles with well-defined PB cores surrounded by PEO coronas. The addition of tetrahydrofuran (THF) to the micelle solution improved the solvent quality for the PB block and resulted in the swelling of the micelle cores. The average micelle size decreased with increasing THF content as shown by dynamic light scattering, small angle X-ray scattering, and cryogenic transmission electron microscopy. The distribution of PB in the micelles was studied using nuclear magnetic resonance spectroscopy and small angle neutron scattering. Finally, the spherical micelles disassembled in co-solvent mixtures containing greater than 72 vol% THF. This result was consistent with phase behavior studies of PB homopolymer, which indicated that PB is soluble in water-THF mixtures up to a similar THF solution composition.

12:27PM B44.00005 Molecular Exchange in Ordered Diblock Copolymer Micelles[1] , SOO-HYUNG CHOI, TIMOTHY LODGE, FRANK BATES, University of Minnesota — Previously, molecular exchange between spherical micelles in dilute solution (1 vol% polymer) was investigated using time-resolved small-angle neutron scattering (TR-SANS). As the concentration of spherical micelles formed by the diblock copolymers increases, the micelles begin to overlap and eventually pack onto body-centered cubic (BCC) lattice. In this study, concentrated, ordered micelles (15 vol% polymers) prepared by dispersing isotopically labeled poly(styrene-*b*-ethylene-*alt*-propylene) in an isotopic squalane mixture was investigated to understand the micellar concentration dependence of the molecular exchange. Perfectly random mixing of isotopically labeled micelles on the BCC lattice was confirmed by SANS patterns where the interparticle contribution vanishes, resulting in an intensity that directly relates to the exchange kinetics. The measured molecular exchange process for the concentrated, ordered system is qualitatively consistent with the previous observations, but the rate is more than an order of magnitude slower than that for the dilute, disordered system.

[1]Infineum(IPrime), MRSEC(NSF), NIST

12:39PM B44.00006 Kinetics of Pressure Jump for Block Copolymer Phase Transition in Selective Solvent , YONGSHENG LIU, RAMA BANSIL, Boston University, MILOS STEINHART, Institute of Macromolecular Chemistry, CZ Republic — Synchrotron based time-resolved small angle x-ray scattering (SAXS) was used to study the kinetics of the order-disorder transition (ODT) in a 30% (w/v) solution of a diblock copolymer of poly(styrene – isoprene) (SI 18-12) in diethyl phthalate, a selective solvent for the PS block using pressure jump methods. Time resolved pressure jump SAXS experiments were done to study the kinetics of disorder to BCC phase transition and the reverse transition. The results show that the ODT temperature increases at about 20C/kbar with pressure. Analysis of Percus-Yevik model following pressure jumps and pressure ramps will be presented. The analysis shows that core radius of micelles are independent of pressure, but hard sphere radius increases with pressure.

12:51PM B44.00007 Transition Behavior of Hydrogen Bonding mediated Block Copolymer complex , SUDHAKAR NAIDU, HYUNGJU AHN, HOYEON LEE, DU YEOL RYU, Yonsei University, YONSEI UNIVERSITY TEAM — We have investigated transition behavior for block copolymer (BCP) complexes composed of a lamella-forming polystyrene-block-poly(2-vinylpyridine) (PS-b-P2VP) and phenyl acetamide derivatives. Influence of small molecules on transition temperatures such as order-to-disorder transitions (ODT) were analyzed by by in-situ small angle x-ray scattering (SAXS) and depolarized light scattering (DPLS). The importance of the availability for H-bonding mediation to control over transition behavior for BCP mixtures with the functional molecules was shown by changing the annealing temperatures. Non-covalent interactions between the nitrogen units of P2VP block and small molecules enhances nonfavorable segmental interactions between two block components, leading to a significant increase in d-spacing for BCP mixtures.

1:03PM B44.00008 Phase Behavior of Binary Mixtures of Block Copolymers having Hydrogen Bonding , SUNG HYUN HAN, JIN KON KIM, Pohang University of Science and Technology — The phase behavior of binary mixtures of high molecular weight polystyrene-*block*-poly(2-vinyl pyridine) (PS-*b*-P2VP) and low molecular weight polystyrene-*block*-poly(4-hydroxystyrene) (PS-*b*-PHS) copolymers was investigated by using small angle X-ray scattering and transmission electron microscopy. Both block copolymers exhibited lamellar microdomains. When the weight fraction of PS-*b*-PHS in the blend was less than 0.1, lamellar microdomains are maintained. However, with increasing amount of PS-*b*-PHS, the microdomains are transformed to hexagonally-packed cylindrical microdomains, and body-centered cubic spherical microdomains. This is attributed to the hydrogen bonding between P2VP and PHS blocks.

1:15PM B44.00009 Highly Localized Optically Induced Melting Transitions in Block Copolymers , AZAR ALIZADEH, EUGENE BODEN, XIALEI SHI, VICTOR OSTROVERKHOV, DANIEL BRUNNELLE, VICKI WATKINS, CHARLES KERBAGE, MATTHEW MISNER, BRIAN LAWRENCE, GE GLOBAL RESEARCH, NISKAYUNA, NY 12309 TEAM — Semi-crystalline block copolymers are well known to exhibit confined crystallization and/or melting phase transitions in sub-50 nm domains. Confined crystallization within these nano-domains is favored under the following conditions: 1) the crystallizable block forms discrete spherical or cylindrical domains; 2) the glass transition temperature of the matrix block is above the crystallization and melting temperatures of the crystallizable minority block; and 3) the block constituents form a strongly segregating system, such that the phase separation dominates the crystallization process. Here we report on optically induced highly localized crystalline-to-amorphous phase transitions in a composite medium comprised of a semi-crystalline block copolymer and a heat generating dye. We use an optical probe-pump and a Bragg reflective grating to both induce and detect the optically induced phase transitions in these block copolymers. We show that extremely fast and localized melting in these block copolymers can be achieved by exposing the samples to very short (5-20 ns) pulses of light. This study provides a new insight on the timescale of melting transitions in polymeric materials.

1:27PM B44.00010 Self-Assembly of Lamellar Microphases in Linear Gradient Copolymer Melts[1] , NICHOLAS B. TITO, Dartmouth College, SCOTT T. MILNER, The Pennsylvania State University, JANE E. G. LIPSON, Dartmouth College — The ability to create 'designer copolymers' with tunable properties by tailoring their monomer composition has garnered recent interest in their molecular self-assembly. Here we investigate lamellar microphases in linear gradient binary copolymer melts using a variety of techniques, including solutions of self-consistent field equations, scaling theory, and analysis of the strong-segregation limit. The Flory scaling theory predicts the scaling of the equilibrium lamellar width L_{eq} as a function of comonomer incompatibility as characterized by χ. From the strongly segregated limit there are conformational fluctuations, and it is the tradeoff between the entropic effect of these relative to repulsive comonomer interactions that determines L_{eq}. We discover that $L_{eq}\ /R_g \quad \sim (\chi N)^{1/6}$; remarkably, this is the same result as for symmetric diblock copolymers, although for quite different physical reasons.

[1]Work supported by the National Science Foundation and the Petroleum Research Fund.

1:39PM B44.00011 Kinetics and Dynamics of HEX to Gyroid Transition of a Diblock Copolymer in Selective Solvent , JULIAN SPRING, YONGSHENG LIU, RAMA BANSIL, Boston University — Synchrotron based time-resolved small angle x-ray scattering (SAXS) was used to study the kinetics of the formation of a gyroid phase in solutions of a poly (styrene -isoprene) diblock copolymer in dimethyl phthalate, a selective solvent for the polystyrene block. From temperature ramp measurements on an 80% (w/v) sample, a hexagonally-packed cylinders (HEX) phase was identifed below 95 C,while a gyroid formed above 95C. The kinetics of the transitions from HEX to gyroid was examined using temperature jump and ramp experiments over the temperature range of 50-150C. In addition, x-ray photon correlation spectroscopy was used to study the dynamics of the HEX and Gyroid phases, as well as the transition regime. Analysis of the time evolution of the Bragg peaks to follow the kinetics of the transition between these phases will be presented, in addition to analysis of the dynamics of this sample throughout the phase space under investigation. The formation of the Gyroid structure was also modeled using Molecular Dynamics (MD) simulations, and the results of these simulations will also be presented.

1:51PM B44.00012 Dynamics of Cloud Point Transitions in Dilute Solutions of Gradient Copolymers with Prescribed Gradient Strengths , KEITH GALLOW, YUEH-LIN LOO, Princeton University — We have investigated dilute solutions of gradient copolymers comprising hydroxyethyl methacrylate and dimethylaminoethyl methacrylate with different gradient strengths undergoing their cloud point transitions. The gradient strength defines the maximum difference in instantaneous compositions along the polymer backbone. Isothermal dynamic light scattering tracks the fractions of unimers and aggregates with which the half times characterizing this transition can be quantified. We find the temperature dependence of this transition to depend on gradient strength, ranging from -2.22 decades/$^\circ$C for a random copolymer to -0.75 decades/$^\circ$C for a gradient copolymer of comparable molecular weight and overall composition but a gradient strength of 0.52. The progressively shallower temperature dependence of this transition with increasing gradient strength suggests of a nucleation and growth mechanism of aggregate formation.

2:03PM B44.00013 Effect of Macromolecular Architecture on the Morphology of Polystyrene/Polyisoprene Block Copolymers , CALEB DYER, The University of Tennessee, PARASKEVI DRIVA, Oak Ridge National Laboratory, SCOTT SIDES, Tech-X Corporation, BOBBY SUMPTER, JIMMY MAYS[1], MARK DADMUN[2], Oak Ridge National Laboratory, FENG ZUO, FRANK BATES, University of Minnesota — The molecular architecture of branched block copolymers has been shown to dramatically effect morphological behavior. A study of four polystyrene/polyisoprene block copolymers with varying architecture (branched $PSPI_2$, PS_2PI, PS_2PI_2, and linear PSPI), and constant composition and molecular weight is presented. The morphologies of each sample were determined using SCFT simulations and, experimentally using SAXS and TEM. The PS_2PI_2miktoarm star exhibits the same morphology as the lineardiblock but with a reduction in the domain size. The PS_2PI and $PSPI_2$ copolymers demonstrated different morphologies from the diblock copolymer, a result of the architectural asymmetry. The results were then compared to Milner's theoretical predictions and found to be in good agreement. These results, therefore, provide detailed insight into the effect of copolymer architecture on the morphological behavior of block copolymers.

[1]Affiliated also with The University of Tennessee
[2]Affiliated also with The University of Tennessee

Monday, March 21, 2011 11:15AM - 2:15PM –
Session B45 DAMOP GQI: Optomechanics at the Quantum Limit A310

11:15AM B45.00001 Sideband cooling micromechanical motion to the quantum ground state , JOHN TEUFEL, NIST Boulder, TOBIAS DONNER, JILA, University of Colorado and NIST, DALE LI, NIST Boulder, KONRAD LEHNERT, JILA, University of Colorado and NIST, RAYMOND SIMMONDS, NIST Boulder — Accessing the full quantum nature of a macroscopic mechanical oscillator first requires elimination of its classical, thermal motion. The flourishing field of cavity opto- and electromechanics provides a nearly ideal architecture for both preparation and detection of mechanical motion at the quantum level. We realize such a system by coupling the motion of an aluminum membrane to the resonance frequency of a superconducting, microwave circuit. By exciting the microwave circuit below its resonance frequency, we damp and cool the membrane motion with radiation pressure forces, analogous to laser cooling of trapped ions. The microwave excitation serves not only to cool, but also to monitor the displacement of the drum. A nearly shot-noise limited, microwave Josephson parametric amplifier is used to detect the mechanical sidebands of this microwave excitation and quantify the thermal motion of the oscillator as it is cooled with radiation pressure forces to its quantum ground state.

11:27AM B45.00002 Cavity Cooling of A Mechanical Resonator in Amorphous Systems[1] , LIN TIAN, University of California, Merced — The quantum backaction force generated by a cavity coupled with a mechanical resonator can be exploited to achieve sideband cooling of the mechanical mode. By applying a red-detuned driving, the quantum ground state of the mechanical mode can be reached in the resolved-sideband regime, which has recently be demonstrated in experiments. However, in many of these materials, surface defects or adsorbates can couple with the mechanical mode and impair the cavity cooling. These defects can be treated as quantum two-level system (TLS). The mechanical vibration changes the local strain tensor and generates coupling with the TLS via the deformation potential. In this work, we study the cavity cooling of the mechanical mode in the presence of a TLS. By applying the adiabatic elimination technique widely used in quantum optics, we derive the cooling master equation for the resonator-TLS system in the eigenbasis of this system. Our results show that the stationary phonon number depends non- monotonically on the energy of the TLS. We also show that the cooling depends strongly on the decoherence rate of the TLS.

[1]This work is supported by the DARPA/MTO ORCHID program through AFOSR, NSF-DMR-0956064, NSF-CCF-0916303, and NSF COINS program.

11:39AM B45.00003 Quantum Interactions of a Torsional Nanomechanical Resonator with a Single Spin[1] , BRIAN D'URSO, SHONALI DHINGRA, University of Pittsburgh — While the motions of macroscopic objects may ultimately be governed by quantum mechanics, the distinctive features of quantum mechanics can be hidden by thermal excitations and coupling to the environment. We present a system consisting of a torsional nanomechanical resonator with quantum behavior introduced to the system by coupling the resonator with a single spin through a uniform external magnetic field. The spin originates from a nitrogen vacancy (NV) center in a diamond nanocrystal which is positioned on the resonator. The quadratic coupling is maximized by utilizing a low moment of inertia resonator and an avoided level crossing. This coupling results in quantum non-demolition (QND) measurements of the resonator and spin states, enabling a bridge between the quantum and classical worlds. Furthermore, it provides a high-fidelity readout of the NV center spin and a potential means of observing the discrete states of the resonator. We will describe the potential for these measurements and report on the experimental progress made towards observing this coupling in the torsional resonator-NV system.

[1]This work is funded by a DARPA Young Faculty Award.

11:51AM B45.00004 Characterization of an oscillator's mechanical impedance using photon pressure , PAUL WILKINSON, GORDON SHAW, JON PRATT, NIST Physical Measurements Lab — In recent years, there has been much progress in coupling optical cavities to mechanical oscillators, especially in the pursuit of the quantum ground state of a macroscopic oscillator. Photon pressure due to reflection is of particular interest, and such experiments must be carefully designed to minimize competing contributions. Typically, such unwanted contributions are estimated or modeled. We describe an experimental approach to place an upper bound on unwanted contributions. A fiber coupled superluminous light emitting diode is modulated at an optical power of 6.5 mW rms, driving a highly reflective cantilever at a displacement of over 10 nm rms at resonance (Q=4900) in vacuum (10-5 Torr). The optomechanical transfer function is measured and fit to a simple harmonic oscillator model. The stiffness of the oscillator determined from the fit (k=16.6 +/- 1.3 N/m) is found to be in good agreement with that obtained by calibration against our SI-traceable nanoindenter (k=17.4 +/- 0.5 N/m). We characterize the modal stiffness, mass, and dissipation of the first two eigenmodes of our oscillator with SI traceability. The quantitative agreement in our experiment indicates that our oscillator is actuated by photon pressure, and that all other contributions to the force must sum to less than 11%.

12:03PM B45.00005 Multi-stability in an optomechanical system with two-component Bose-Einstein condensate[1] , YING DONG, Department of Physics and Astronomy, and Rice Quantum Institute, Rice University, Houston, Texas 77251-1892, USA, JINWU YE, Department of Physics, The Pennsylvania State University, University Park, PA 16802, USA, HAN PU, Department of Physics and Astronomy, and Rice Quantum Institute, Rice University, Houston, Texas 77251-1892, USA — We investigate a system consisting of a two-component Bose-Einstein condensate interacting dispersively with a Fabry-Perot optical cavity where the two components of the condensate are resonantly coupled to each other by another classical field. The key feature of this system is that the atomic motional degrees of freedom and the internal pseudo-spin degrees of freedom are coupled to the cavity field simultaneously, hence an effective spin-orbital coupling within the condensate is induced by the cavity. The interplay among the atomic center-of-mass motion, the atomic collective spin and the cavity field leads to a strong nonlinearity, resulting in multi-stable behavior in both matter wave and light wave at the few-photon level.

[1]This work is supported by the NSF, the Welch Foundation (Grant No. C-1669) and by a grant from the Army Research Office with funding from the DARPA OLE Program. J. Ye is supported by NSF DMR-0966413.

12:15PM B45.00006 Optomechanical down-conversion , SIMON GROEBLACHER, SEBASTIAN HOFER, WITLEF WIECZOREK, MICHAEL VANNER, University of Vienna, Austria, KLEMENS HAMMERER, Leibniz University Hannover, Germany, MARKUS ASPELMEYER, University of Vienna, Austria — One of the central interactions in quantum optics is two-mode squeezing, also known as down-conversion. It has been used in a multitude of pioneering experiments to demonstrate non-classical states of light and it is at the heart of generating quantum entanglement in optical fields. Here we demonstrate first experimental results towards the optomechanical analogue, in which an optical and a mechanical mode interact via a two-mode squeezing operation. In addition, we make use of the fact that large optomechanical coupling strengths provide access to an interaction regime beyond the rotating wave approximation. This allows for simultaneous cooling of the mechanical mode, which will eventually enable the preparation of pure initial mechanical states and is hence an important precondition to achieve the envisioned optomechanical entanglement.

12:27PM B45.00007 Photothermally induced dynamics in partially coated loaded microcantilevers , SHOMEEK MUKHOPADHYAY, UMAR MOHIDEEN, University of California, Riverside — Cooling of microcantilevers in a Fabry-Perot cavity either by radiation pressure or using the photothermal effect has attracted significant attention lately. We present ongoing experimental results on partially coated microcantilevers which are either loaded (gold sphere) or have a coating only at the tip. In particular, we will compare the results with that of recent work on fully coated cantilevers.

12:39PM B45.00008 Micro-optomechanical trampoline resonators[1] , BRIAN PEPPER, DUSTIN KLECKNER, UC Santa Barbara, PETRO SONIN, EVAN JEFFREY, University of Leiden, DIRK BOUWMEESTER, UC Santa Barbara, University of Leiden — Recently, micro-optomechanical devices have been proposed for implementation of experiments ranging from non-demolition measurements of phonon number to creation of macroscopic quantum superpositions. All have strenuous requirements on optical finesse, mechanical quality factor, and temperature. We present a set of devices composed of dielectric mirrors on Si_3N_4 trampoline resonators. We describe the fabrication process and present data on finesse and quality factor.

[1]The authors gratefully acknowledge support from NSF PHY-0804177 and Marie Curie EXT-CT-2006-042580.

12:51PM B45.00009 Proposal for detecting measurement-induced entanglement between remote mechanical oscillators , KJETIL BORKJE, ANDREAS NUNNENKAMP, STEVEN M. GIRVIN, Yale University — In optomechanical systems where an optical cavity mode interacts with a mechanical oscillator, the light leaking out of the cavity has sidebands at the mechanical frequency. The photon statistics of these sidebands contain information about the mechanical oscillator. We consider driving two similar optical cavities, containing one mechanical system each, in such a way that the mechanical oscillators are laser cooled close to the ground state. When the output fields of the two cavities are made indistinguishable by combining them on a beamsplitter, the detection of sideband photons can lead to measurement-induced entanglement between the two non-interacting mechanical oscillators. We show how this short-lived entanglement between remote mechanical oscillators can be verified through measurements of higher-order coherences of the optical output field.

1:03PM B45.00010 Investigation of radiation pressure shot-noise in a microwave circuit optomechanical system , JENNIFER HARLOW, JILA, University of Colorado and NIST, JOHN TEUFEL, RAYMOND SIMMONDS, NIST, KONRAD LEHNERT, JILA, University of Colorado and NIST — We examine the possibility of measuring the radiation pressure shot-noise of microwave light. When the motion of a nanomechanical oscillator is coupled to the microwave energy stored in a resonant circuit, the oscillator experiences a radiation pressure force. That force must have a random component associated with the quantum nature of the microwave field, a mechanical manifestation of the microwave photon. The variance of this random component increases with increasing circuit excitation power. Until recently, reaching powers where radiation pressure shot-noise would dominate over other random forces was unfeasible due to relatively weak optomechanical coupling and technical power limitations of microwave circuits. However, the recent advent of a mechanical oscillator coupled strongly to a microwave circuit [1] will enable exploration of this regime. We discuss the most favorable circuit parameters and measurement strategy for studying radiation pressure shot-noise.

[1] J. D. Teufel, et al, Circuit cavity electromechanics in the strong coupling regime, arXiv:1011.3067v1.

1:15PM B45.00011 Levitated Quantum Nano-Magneto-Mechanical Systems , MAURO CIRIO, JASON TWAMLEY, GAVIN K. BRENNEN, Centre for Engineered Quantum Systems, Macquarie University, Sydney Australia, GERARD J. MILBURN, Centre for Engineered Quantum Systems, University of Queensland, Brisbane, Australia — Quantum nanomechanical sysems have attracted much attention as they provide new macroscopic platforms for the study of quantum mechanics but may also have applications in ultra-sensitive sensing, high precision measurements and in quantum computing. In this work we study the control and cooling of a quantum nanomechanical system which is magnetically levitated via the Meissner effect. Supercurrents in nano-sized superconducting loops give rise to a motional restoring force (trap), when placed in an highly inhomogenous magnetic field and can yield complete trapping of all translational and rotational motions of the levitated nano-object with motional oscillation frequencies $\nu \sim 10 - 100$MHz. As the supercurrents experience little damping this system will possess unprecendented motional quality factors, with $Q_{motion} \sim 10^9 - 10^{13}$, and motional superposition states may remain coherent for days. We describe how to execute sideband cooling through inductive coupling to a nearby flux qubit, cooling the mechanical motion close to the ground state.

1:27PM B45.00012 Measurement of Casimir force with transparent conducting oxides , ALEXANDR BANISHEV, CHIA-CHENG CHANG, UMAR MOHIDEEN — The Casimir force plays an important role in micro- and nano electro mechanical systems (MEMS and NEMS) fabrication, because it can easily exceed the electrostatic forces used for actuating the systems at small electrode separation distances. The reduction of the Casimir force in devices is a complicated problem that needs to be scientifically investigated to open opportunities for the full exploitation of MEMS and NEMS technology. One of the ways to tune the Casimir force is to properly choose the materials of which the interacting surfaces are made. According to the Lifshitz theory, the interaction between two objects depends on their dielectric permittivity. In that case the transparent dielectrics attract less than reflective materials. This can be used to decrease the Casimir force when the design requires a smaller short range interaction. To achieve low Casimir forces and avoid uncontrolled electrostatic forces as present in dielectrics, transparent but conductive materials can be used. An ideal choice is conductive Indium Oxide such as very low doped Indium Tin Oxide (ITO). In this report we present the results of the Casimir force using transparent electrodes such as Indium Tin Oxide coated SiO_2 plate.

1:39PM B45.00013 Precision measurements of the Casimir force at Low temperatures[1] , RODRIGO CASTILLO-GARZA, UMAR MOHIDEEN, Physics and Astronomy Dept. UC Riverside — We will present research involving the precision measurement of the Casimir force at low temperatures. The role of material losses in this force and its incorporation into the Lifshitz theory remains unresolved. The Casimir force results from the modification of the zero point photon spectrum due to the presence of boundaries. The problem arises when the Casimir force is calculated at non zero temperature, where the role of thermal photons have to be included to that of the zero point photons. We plan to address this problem by measuring the Casimir force for different materials as a function of the temperature. Currently we are involved in making precision measurements of the Casmir force at 6K, 77K, and 300K with a micro cantilever based system that we have designed and built at UC-Riverside. The high sensitivity of this instrument will provide us with the resolution to advance our understanding of the interactions of both virtual photons and real photons when confined to a semi-infinite cavity made out of real metals. The constructed apparatus will also provide a deeper understanding of the role vacuum fluctuations play when the cavity constituents are made of a combination of dielectric, superconductor, and metal surfaces.

[1]The support of UCMEXUS, NSF and DOE is acknowledged.

1:51PM B45.00014 Strong interactions of single atoms and photons near a dielectric boundary[1] , N.P. STERN, D.J. ALTON, T. AOKI, H. LEE, E. OSTBY, K.J. VAHALA, H.J. KIMBLE, California Institute of Technology, Pasadena, CA 91125, USA — Quantum control of strong interactions between a single atom and photon has been achieved within the setting of cavity quantum electrodynamics (cQED). To move beyond proof-of-principle experiments involving one or two conventional optical cavities to more complex scalable systems that employ $N > 1$ microscopic resonators requires localization of atoms on distance scales ~ 100 nm from a resonator's surface where an atom can be strongly coupled to a single intracavity photon while at the same time experiencing significant radiative interactions with the dielectric boundaries of the resonator. As an initial step into this new regime of cQED, we use real-time detection and high-bandwidth feedback to select and monitor motion of single Cesium atoms through the evanescent field of a microtoroid[2]. Direct temporal and spectral measurements coupled with simulations reveal both the significant role of Casimir-Polder attraction and the manifestly quantum nature of the atom-cavity dynamics, here in a regime of strong coupling, setting the stage for trapping atoms near micro- and nano-scopic optical resonators.

[1]Work supported by NSF PHY-0652914 and the NSSEFF.
[2]D. J. Alton, *et al, Nature Physics* (2010); available as arXiv:1011.0740.

2:03PM B45.00015 Distinct single photons strongly interacting at a single atom in a waveguide , PAVEL KOLCHIN, RUPERT F. OULTON, XIANG ZHANG, University of California at Berkeley — We propose a waveguide QED system where two distinct single photons can interact strongly. The system consists of a single ladder-type three level atom coupled to a waveguide. We show that the nonlinear interaction can be tremendously enhanced by the strong coupling of the cascade atomic transitions to the waveguide mode simultaneously. As a result, a control photon tuned to the upper transition induces a π phase shift and tunneling of a probe photon tuned to the otherwise reflective lower transition. Waveguide QED schemes could be an alternative to high quality cavities or dense atomic ensembles in quantum information processing.

2:00PM - 2:00PM –
Session C1 APS: Poster Session I (2:00pm - 5:00pm) Hall D

C1.00001 POLYMERS AND SOFT MATTER I –

C1.00002 Helical Ordering in Chiral Diblock Copolymers – the Effect of Chirality , WEI ZHAO, SUNG WOO HONG, GREGORY GRASON, THOMAS RUSSELL, University of Massachusetts Amherst — Introducing molecular chirality into the segments of block copolymers can influence the nature of the resultant morphology. Such an effect was found for poly(styrene-b-L-lactide) (PS-b-PLLA) diblock copolymers where hexagonally packed PLLA helical microdomains (H* phase) form in a PS matrix. However, molecular ordering of PLLA within the helical microdomains and the transfer of chirality from the segmental level to the morphological scale is still not well understood. We used a coarse-grained model to describe the interactions between segments of chiral blocks, and calculated the bulk morphologies of chiral AB diblock copolymers using self-consistent field theory (SCFT). We also performed in situ grazing incidence small angle x-ray scattering experiments to investigate the formation of the helical microdomains by changing solvents. Experiments confirmed that the H* phase is a kinetically trapped, metastable morphology below the melting point of PLLA block, while the SCFT explores the range of thermodynamic stability of helical structures in the phase diagram of chiral block copolymer melts.

C1.00003 ABSTRACT WITHDRAWN –

C1.00004 Crystallization of a Cyanurate Trimer in Nanopores , YUNG P. KOH, SINDEE L. SIMON, Texas Tech University — Nanoconfinement is known to depress the melting temperature through the well-known Gibbs-Thompson equation. Less well studied is the influence of nanoconfinement on crystallization kinetics. In this work we investigate crystallization of a cyanurate trimer using differential scanning calorimetry. The material shows cold crystallization and melting in the bulk state. Under the nanoconfinement of controlled pore glasses (CPG), cold crystallization and melting shift to lower temperatures, following the shift in the glass transition temperature. More importantly, however, the crystallization kinetics slow down and no crystallization occurs in 13 nm-diameter pores. Isothermal crystallization studies indicate that the Avrami exponent is approximately 2.0 for both bulk and nanoconfined samples. The time scale for crystallization is over one order of magnitude longer for samples confined in 50-nm pores in spite of the fact that samples were crystallized the same distance from T_g.

C1.00005 Chemical Composition Distribution of Partially Brominated Polystyrenes , WAYNE POWERS, Rensselaer Polytechnic Institute, YOUNG KUK JHON, JAN GENZER, North Carolina State University, CHANG RYU, Rensselaer Polytechnic Institute, RENSSELAER POLYTECHNIC INSTITUTE TEAM — Interaction chromatography has been employed to estimate the chemical composition distribution of partially brominated polystyrenes. In particular, random blocky and truly random partially brominated polystyrenes (b-PBrxS and r-PBrxS) differ in the dispersity of their chemical composition distributions, because of the limited accessibility of styrene segments for the bromination at temperature below theta temperature. First, the adsorption-based IC technique was used to fractionate b-PBrxS and r-PBrxS of the same average mole fraction of bromine. Then, these fractions were reinjected, and the peak position of each fraction was analyzed. In addition, the average chemical composition of each brominated polystyrene fraction has been analyzed separately via neutron activation analysis (NAA). The results of this analysis clearly supports that the chemical composition distribution b-PBrxS is narrower than that of r-PBrxS.

C1.00006 Controlled Orientation of Block Copolymer Microdomains on Modified Solid Surfaces , WEIYIN GU, SUNG WOO HONG, THOMAS RUSSELL, University of Massachusetts-Amherst — The interfacial interactions between block copolymers (BCP) and a substrate are important for the self-assembly of BCPs in thin films, especially in terms of orientation of BCP microdomains. A simple, rapid, and robust technique for controlling the alignment of BCP microdomains on modified surfaces is described. End-functionalized poly(styrene-b-ethylene oxide)s (PS-b-PEOs) with different block ratios were end-grafted onto Si substrates creating BCP brushes. Thin films of cylindrical forming PS-b-PEO were prepared on the surface of anchored BCP brushes and thermally annealed. When the fraction of styrene, f, of the anchored BCP was 1, no features were observed in thin film of a PS-b-PEO placed on the surface of the anchored brush due to preferential interaction of the PS block with the brush. When f was varied from 0.3 to 0.7, hexagonally packed cylindrical microdomains oriented normal to the substrate were formed having long range lateral ordering.

C1.00007 Studies on Morphology of PCPDTBT/Fullerene Bulk Heterojunction Organic Photovoltaics , YU GU, THOMAS RUSSELL, University of Massachusetts-Amherst — Low-bandgap conjugated polymer, poly[2,6-(4,4-bis(2-ethylhexyl)-4H-cyclopenta[2,1-b;3,4-b']-dithiophene)-alt-4,7-(2,1,3-benzothiadiazole)] (PCPDTBT), has been used in the active layer of the bulk heterojunction (BHJ) solar cells. Though PCPDTBT has a desirable bandgap, the power conversion efficiency (PCE) of the corresponding solar cells is still lower than the expectation. Grazing incidence wide angle X-ray scattering (GI-WAXS) showed that PCPDTBT is amorphous. Dynamic secondary ion mass spectrometry (DSIMS) and small angle neutron scattering (SANS) confirmed that PCPDTBT and [6,6]-phenyl C61-butyric acid methyl ester (PCBM) were uniformly distributed in the active layers. It is likely that the intimate mixing of the two components leads to a recombination of the free charges and the relatively low PCE. With additives, like 1,8-diiodooctane, the crystallinity of PCPDTBT increases and the PCBM segregates, which leads to improved device performances.

C1.00008 Morphology Evolution of Molecular Weight Dependent P3HT: PCBM Solar Cells , FENG LIU, DIAN CHEN, ALEJANDRO BRISENO, THOMAS RUSSELL, UMASS-Amherst — Effective strategies to maximize the performance of bulk heterojunction (BHJ) photovoltaic devices have to be developed and understood to realize their full potential. In BHJ solar cells, the morphology of the active layer is a critical issue to improve device efficiency. In this work, we choose poly(3-hexyl-thiophene) (P3HT) and phenyl-C61-butyric acid methyl ester (PCBM) system to study the morphology evolution. Different molecular weight P3HTs were synthesized by using Grignard Metathesis (GRIM) method. In device optimization, polymer with a molecular weight between 20k-30k shows the highest efficiency. It was observed that the as-spun P3HT: PCBM (1:1) blends do not have high order by GISAXS. Within a few seconds of thermal annealing at 150 $^\circ$ the crystallinity of P3HT increaased substantially and the polymer chains adopted an edge-on orientation. An-bicontinous morphology was also developed within this short thermal treatment. The *in situ* GISAXS experiment showed that P3HT of high molecular weight was more easily crystallized from a slowly evaporated chlorobenzene solution and their edge-on orientation is much more obvious than for the lower molecular weight P3HTs. DSC was used to study the thermal properties of P3HTs and P3HT: PCBM blend. The χ of P3HT-PCBM was also calculated by using melting point depression method.

C1.00009 Elimination of branching in beta-hairpin self-assembling peptides , SAMEER SATHAYE, DARRIN POCHAN, Department of Materials Science and Engineering, University of Delaware, DARRIN POCHAN RESEARCH GROUP TEAM — Nanoscale fibril self-assembly in (VK)4VDPPT (KV)4-NH2 peptides is initiated by intramolecular peptide folding into a beta-hairpin conformation. Once folded, the peptides undergo intermolecular bilayer formation due to hydrophobic collapse of hydrocarbon valine side chains, all located on one face of respective folded beta-hairpins. Subsequent intermolecular hydrogen bonding between folded hairpins leads to fibril formation. A physically crosslinked network structure is formed due to fibrillar entanglement and defects in hydrophobic collapse that nucleate branching points. We attempt to design "lock and key" specificity in the hydrophobic faces of the folded beta-hairpins so that only 1-d fibril formation can occur without any branching. The success of the new peptide designs to rid the system of branching and characteristics of the networks afforded by new peptide sequences and blends thereof will be discussed by various characterization techniques such as Rheological Characterization, Circular Dichroism (CD), Transmission Electron Microscopy (TEM) and Small Angle Neutron Scattering (SANS).

C1.00010 Theory of Nanoparticle Interactions Mediated by Reversibly Binding Polymer Chains , STEPHANIE TRITTSCHUH, GREGORY GRASON, University of Massachusetts Amherst — In stable polymer-nanoparticle composites, particles must be compatibilized with the polymer matrix to overcome entropically- driven, short-range depletion forces that drive particle aggregation. One strategy is to incorporate end-functional groups to polymers that reversibly bind to particle surfaces via donor- acceptor type interactions, such as hydrogen bonding. The addition of reversibly binding chain ends introduces a new length scale for the effective interaction between two particles due to the possibility of inter-particle bridging conformations available to chains at small particle-particle separations. We use self- consistent field theory to explore the effective pairwise particle potential in a melt of reversibly associating chains and examine how changing particle size, chain length and binding affinity shapes the free energy of interaction and alters higher-order inter-particle organization in nanocomposites.

C1.00011 Thio-amide functionalized polymers via polymerization or post-polymerization modification

, ALI OZCAM, NC State University, ADAM HENKE, IVA STIBINGEROVA, JIRI SROGL, Institute of Organic Chemistry and Biochemistry, JAN GENZER, NC State University — Decreasing supplies of fresh water and increasing population necessitates development of advanced water cleaning technologies, which would facilitate the removal of water pollutants. Amongst the worst of such contaminants are heavy metals and cyanides, infamous for their high toxicity. To assist the water purification processes, we aim to synthesize functionalized macromolecules that would contribute in the decontamination processes by scavenging detrimental chemicals. Epitomizing this role thio-amide unit features remarkable chemical flexibility that facilitates reversible catch-release of the ions, where the behavior controlled by subtle red-ox changes in the environment. Chemical tunability of the thio-amide moiety enables synthesis of thio-amide based monomers and post-polymerization modification agents. Two distinct synthetic pathways, polymerization and post-polymerization modification, have been exploited, leading to functional thioamide-based macromolecules: thioamide-monomers were copolymerized with N-isopropylacrylamide and post-polymerization modifications of poly(dimethylaminoethyl methacrylate) and poly(propargyl methacrylate) were accomplished via quarternization and "click" reactions, respectively.

C1.00012 Charged triblock copolymer self-assembly into charged micelles

, YINGCHAO CHEN, KE ZHANG, JIAHUA ZHU, KAREN WOOLEY, DARRIN POCHAN, DEPARTMENT OF MATERIAL SCIENCE AND ENGINEERING UNIVERSITY OF DELAWARE TEAM, DEPARTMENT OF CHEMISTRY TEXAS A&M UNIVERSITY COLLABORATION — Micelles were formed through the self-assembly of amphiphlic block copolymer poly(acrylic acid)-block-poly(methyl acrylate)-block-polystyrene (PAA-PMA-PS). Importantly, the polymer is complexed with diamine molecules in pure THF solution prior to water titration solvent processing-a critical aspect in the control of final micelle geometry. The addition of diamine triggers acid-base complexation between the carboxylic acid PAA side chains and amines. Remarkably uniform spheres were found to form close-packed patterns when forced into dried films and thin, solvated films when an excess of amine was used in the polymer assembly process. Surface properties and structural features of these hexagonal-packed spherical micelles with charged corona have been explored by various characterization methods including Transmission Electron Microscopy (TEM), cryogenic TEM, z-potential analysis and Dynamic Light Scattering. The forming mechanism for this pattern and morphology changes against external stimulate such as salt will be discussed.

C1.00013 Examining the Role of Structure on Charge Transport of Polymer Semiconductors

, KIARASH VAKHSHOURI, Chemical Engineering Department, The Pennsylvania State University, ENRIQUE GOMEZ — Charge carrier mobility in conjugated semi-crystalline polymers depends critically on the crystallinity, orientation of the crystals, and connectivity between ordered regions. However, the complex interplay between these morphological parameters is not fully understood. By varying the thermal annealing parameters and casting solvents, we have systematically studied charge transport within poly(3-hexylthiophene) and poly(2,5-bis(3-alkylthiophen-2-yl) thieno[3,2-b]thiophene) as a function of the crystallinity. It is found that the crystallinity itself does not always correlate with the charge mobility. Our hypothesis is that the crystallization kinetics can alter the number of tie chains, thereby affecting charge transport in semi-crystalline polymer semiconductors.

C1.00014 Towards quantitative structure-function relationships for organic solar cells

, DEREK KOZUB, Department of Chemical Engineering, The Pennsylvania State University, KIARASH VAKHSHOURI, ENRIQUE GOMEZ — Organic solar cells belong to a class of devices where the morphology of the active layer has a large impact on device performance. However, characterization of the morphology of organic semiconductor mixtures remains a challenge. We have utilized Grazing Incidence Small Angle X-Ray Scattering (GISAXS), Resonant Soft X-ray Scattering (RSOXS), and Energy Filtered Transmission Electron Microscopy (EFTEM) to characterize the morphology of polythiophene/fullerene mixtures as a function of processing conditions. GISAXS and RSOXS have been used to determine the domain spacing within the active layer, whereas EFTEM has been used to generate images with high contrast between domains. Furthermore, these techniques have been useful in guiding our attempts to control the nucleation of crystals and perturb the structure of the active layer. By comparing our morphological data with device data, we are developing structure-function relationships relevant to organic solar cells.

C1.00015 Polarization Controlled Photomechanical Behaviors of Polydomain Azobenzene Liquid Crystalline Polymer Networks[1]

, TIMOTHY WHITE, KYUNG MIN LEE, VINCENT TONDIGLIA, HILMAR KOERNER, RICHARD VAIA, TIMOTHY BUNNING, Air Force Research Laboratory — We report the polarization controlled photomechanical behaviors of azobenzene liquid crystalline polymer networks (azo-LCNs) as a function of crosslink density and temperature. High modulus, glassy polydomain azo-LCNs were synthesized by copolymerizing RM257 and 2-azo, initiated by 1 wt% of the inorganic photoinitiator Irgacure 784. Crosslinking density of azo-LCNs increases from 2.09 mol/dm^3 to 7.24 mol/dm^3 with curing time from 1-120 min. Storage modulus and loss tangent of azo-LCNs also increase with crosslinking density. All azo-LCNs are glassy at room temperature. To increasing temperature, E' begins to decrease through T_g to a level dependent on the crosslinking density, and eventually reaching a rubbery plateau region. Interestingly, the bidirectional (forward and reverse) bending angles of the polydomain azo-LCN cantilevers at equilibrium decrease with increasing temperature and crosslinking density. Absorption and bending behaviors of the azo-LCNs with various thicknesses, concentrations and molecular structure of azobenzene monomer will be discussed.

[1]Authors acknowledge support from AFRL/RX and AFOSR

C1.00016 Effects of Sequence Distribution, Concentration and pH on Gradient and Block Copolymer Micelle Formation in Solution

, STEPHEN MARROU, JUNGKI KIM, CHRISTOPHER WONG, JOHN TORKELSON, Northwestern University — Gradient copolymers are a relatively new class of materials with a gradual change in comonomer composition along the copolymer chain length, which have exhibited unique material properties in comparison to random and block copolymers. Here we extend this architecture to amphiphilic systems that form micelles in solvent, as the effect of a nonuniform comonomer sequence distribution is expected to strongly influence critical aggregation phenomena. Utilizing pyrene as a fluorescence probe, we determined that gradient copolymers present an intermediate critical aggregation concentration in comparison to analogous block and random copolymers. The effect of gradient architecture on a pH-sensitive copolymer was also investigated, concluding that gradient sequencing significantly impacts the solubility and critical aggregation pH when compared to block and random copolymers of similar composition, providing further evidence that gradient architectures introduce a powerful means of tuning properties between block and random copolymers.

C1.00017 Temperature dependence of ionic association of lithium triflate in acetate solutions

, DHARSHANI BOPEGE, Department of Physics and Astronomy, University of Oklahoma, Norman, OK 73019, USA, MATT PETROWSKY, ROGER FRECH, Department of Chemistry and Biochemistry, University of Oklahoma, 101 Stephenson Parkway, Norman, OK, 73019, USA, J.M. FURNEAUX, Department of Physics and Astronomy, University of Oklahoma, Norman, OK 73019, USA — Ion transport is studied in polymer and organic liquid electrolytes due to the importance of these systems in rechargeable battery applications. We have used Fourier Transform Infrared Spectroscopy (FTIR) to study the temperature dependence of ionic association in solutions of lithium trifluoromethanesulfonate ($LiCF_3SO_3$, LiTf) dissolved in propyl, hexyl, octyl, and decyl acetates. The IR Spectra were recorded for three salt concentrations (0.1, 0.2, 0.5 mol kg^{-1}) from 0 °C to 80 °C. Two spectral bands were analyzed at each temperature: the CF_3 symmetric bend (δ_s) in the 740-780 cm^{-1} region and the carbonyl stretch in the 1660-1800 cm^{-1} region. Relative intensities of these bands were calculated by a curve fitting procedure. Three different LiTf ionic species were observed in the $\delta_s(CF_3)$ region. The carbonyl band due to coordination with Li ion appears at a lower frequency (1714 cm^{-1}) than the pure carbonyl band (1744 cm $^{-1}$).

C1.00018 Organic Molecules and Network Polymers of Intrinsic Microporosity: Structural Characterization via X-ray Scattering and Simulations[1] , AMANDA G. MCDERMOTT, LAUREN J. ABBOTT, Penn State University, ANNALAURA DEL REGNO, University of Manchester, KADHUM J. MSAYIB, BADER S. GHANEM, RUPERT TAYLOR, MARIOLINO CARTA, NEIL B. MCKEOWN, Cardiff University, PETER M. BUDD, FLOR R. SIPERSTEIN, University of Manchester, CORAY M. COLINA, JAMES RUNT, Penn State University — Like polymers of intrinsic microporosity (PIMs), organic molecules of intrinsic microporosity (OMIMs) are glassy solids featuring a large concentration of pores smaller than 2 nm and large internal surface area as measured by gas sorption experiments. OMIMs are oligomers designed to fill space inefficiently, consisting of several rigid segments joined at one vertex to produce concave faces. Both X-ray scattering patterns and simulations provide insight into the packing geometry and short-range order of these molecules. We also discuss the interpretation of scattering patterns from two- and three-dimensional network PIMs.

[1]Supported by NSF/Materials World Network/EPSRC and the NSF Graduate Research Fellowship Program.

C1.00019 Methyl Methacrylate Polymerization in Nanoporous Matrix: Reactivity and Molecular Weight , HAOYU ZHAO, SINDEE SIMON, Texas Tech University — The influence of nanoconfinement on the free radical polymerization of methyl methacrylate is investigated. Nanoporous controlled pore glass (CPG) is used as a nanoconfining matrix for the polymerization. The reaction is followed by measuring heat flow as a function of reaction time during isothermal polymerization using differential scanning calorimetry (DSC). Preliminary results indicate several interesting effects for polymerization in 110 nm diameter pores: the induction time increases under nanoconfinement, the effective reaction rate constant increases, the effective activation energy is unchanged, and the gel effect or autoaccleration occurs at earlier times after induction. The latter result concerning the gel effect is presumably due to the decrease in diffusivity under nanoconfinement which results in a decrease in the termination rate of free radicals. The cause of the longer induction times and accelerated reaction rates just after induction are under investigation. The influence of nanoconfinement on molecular weight will also be examined.

C1.00020 The Dynamic Heat Capacity of the Potential Energy Landscape of a Simple Chain Model , JONATHAN BROWN, JOHN MCCOY, New Mexico Tech — The dynamic heat capacity of a simple (bead-spring) polymeric model glassformer was computed using molecular dynamics simulations by sinusoidally driving the temperature, and recording the resultant energy. The underlying potential energy landscape of the system was probed by taking a time series of particle positions and quenching them with an energy minimization routine. This shows that the long time relaxation of the model glassformer is the direct result of the dynamics of the potential energy landscape.

C1.00021 Characterization of the Morphology and Rapid Expansion of Swellable Organically Modified Silica , LILIANNA E. CHRISTMAN, AMANDA LOGUE, The College of Wooster, Department of Physics, PAUL L. EDMISTON, The College of Wooster, Department of Chemistry, SUSAN Y. LEHMAN, The College of Wooster, Department of Physics, Wooster OH 44691 — Swellable organically modified silica (SOMS) is a novel sol-gel derived material. SOMS is hydrophobic and selectively absorbs non-polar liquids and immediately swells 5 to 6 times upon absorption. SOMS can be used to remove organic contaminants from water; the contaminant can then be recovered and the SOMS reused. We have investigated the SOMS swelling behavior of neat organic liquids usng macroscopic measurements of the force exerted during expansion and through atomic force microscopy (AFM) of the surface. A powdered SOMS sample was placed in a cylinder with an adjustable piston. Solvent percolated into the cylinder and the piston gradually moved to allow expansion while measuring the force using a load cell. During expansion the SOMS exerted forces up to 150 N per gram of material. AFM shows the surface of the SOMS is textured with cauliflower-like features. In unswollen SOMS, these globules have length scales of a few hundred nanometers, while for SOMS swollen in a solvent the features expand to several micrometers.

C1.00022 ABSTRACT WITHDRAWN –

C1.00023 Self-assembly of PtBA-P3HT multi-arms star-like block copolymer at the air/water interface , LEI ZHAO, XINCHANG PANG, CHAOWEI FENG, ZHIQUN LIN, NANOFM TEAM — A novel PtBA-P3HT multi-arm star-like diblock copolymer (BCP) was synthesized via a combination of atom transfer radical polymerization, quasi-living polymerization and click reaction. The self-assembly of PtBA-P3HT multi-arm star-like BCP at the air/water interface was systematically explored using the Langmuir Blodgett (LB) technique. The hydrophobic star-like BCP has 21 arms, with PtBA as the core and P3HT as the shell. At the air/water interface, the BCP molecules gradually assembled into domains composed of bundle-like structures under surface pressure, and finally formed the network structure in a way controlled by PtBA chain folding and P3HT chain stacking. The photoluminescence measurement showed that the formation of P3HT bundle in LB film led to enhanced luminescence due to the reduced inter-chain coupling.

C1.00024 Glassy dynamics of polymers in thin films and monomolecular layers , MARTIN TRESS, EMMANUEL U. MAPESA, University of Leipzig, ANATOLI SERGHEI, Universite Lyon 1, FRIEDRICH KREMER, University of Leipzig — The glassy dynamics of nanometer thin polymer layers supported on a solid substrate was investigated by Braodband Dielectric Spectroscopy (BDS). The thickness was systematically reduced finally resulting in randomly distributed polymer coils. Highest priority was put on an appropriate sample preparation including an annealing procedure for sufficient long time at elevated temperatures in inert atmosphere to avoid effects due to remaining solvent and chemical degradation. Further, detailed checks of the surface topology by atomic force microscopy (AFM) were performed to verify stability of the samples during the whole measurement. The dynamics is compared to the bulk to trace changes due to the impact of the interface and to give a length scale for the interfacial interactions.

C1.00025 Confinement-Induced Ordering in Dewetting of Polymer Blend Film[1] , MU WANG, XIAO-CHUN CHEN, RU-WEN PENG, GUO-BIN MA, DAJUN SHU, Department of Physics, Nanjing University — Dewetting and phase separation of polymer blend film on a periodically modified substrate can generate unique microstructures. Despite external perturbations in previous studies, polymer film remained continuous with the boundary locating at infinity. It is interesting to investigate dewetting and phase separation process in a confined geometry, such as a fishnet-like environment, where unique self- organization process is anticipated. We report here an effect that polymer blend film of polystyrene(PS) and poly (methylmethacrylate)(PMMA) may evolve to a perfectly ordered droplet array on a periodically excavated silicon substrate, and each droplet possesses a PS kernel surrounded by PMMA cofferdam. The formation of regular pattern depends on initial thickness of polymer film and interstitial separation of microholes on substrate, and a scaling has been revealed. Our observation demonstrates a confinement-induced ordering in dewetting of polymer blend film, and suggests a budget and convenient approach to generate regular polymer microstructures over a large area.

[1]Project supported by NSF of China and MOST of China under Grant Nos. Nos. 50972057, 10874068, 11034005, and 61077023 and 2010CB630705.

C1.00026 Synthesis of polymer brushes by surface-initiated controlled radical polymerization in the presence of free initiators. A Monte Carlo investigation , SALOMON TURGMAN-COHEN, JAN GENZER, North Carolina State University — Simultaneous controlled radical polymerization from free and surface-grafted initiators is studied by means of computer simulations. We model "truly living" reactions by neglecting chain termination and chain transfer. We study the competition between bulk- (i=b) and surface-initiated (i=s) polymers by monitoring the rates of polymerization ($d<N>_i/dt$), the average molecular weight ($<N>_i$), and the polydispersity index (PDI_i) while varying the initiator grafting density (σ), the fraction of surface based polymers (η), and the initial number of free monomers (I_o). We find that $d<N>_B/dt > d<N>_S/dt$ and that $d<N>_S/dt$ decreases with increasing σ. The difference in polymerization rates between the bulk and surface polymerizations results in polymer populations with different $<N>$; this has implications for the experimental determination of σ and $<N>_S$. Although η affects $<N>_S$ and $<N>_B$, it does not influence the PDI. At a specific $<N>_i$, the PDI_i has a value independent of η. In addition, $PDI_S > PDI_B$; this difference increases with increasing σ. We therefore conclude that polymerization conditions that yield bulk polymers with low PDI do not guarantee the same PDI for the surface-initiated polymers.

C1.00027 Directed Dewetting of Thin Polymer Films[1] , SUCHANUN MOUNGTHAI, TRANG PHAM, GUS RAJAENDRAN, GILA STEIN, Univ. of Houston — We present a simple route to generate arrays of microscale polygons by directed dewetting of polystyrene thin films on topographic pre-patterns.[2] Silicon wafers are patterned with arrays of ca. 10 μm wide hexagonal holes using photolithography and wet etching. Patterned substrates are coated with thin films of polystyrene and heated above the glass transition temperature to promote dewetting. The dewetting process is monitored *in-situ* with optical microscopy, and final droplet structures are also imaged with atomic force microscopy. The mechanism of polygon formation is driven by Rayleigh instability; Formation rates and final polygon size are controlled by temperature/viscosity, film thickness, and the geometry of the topographic pre-pattern.

[1]Funded by NSF ECCS 0927147.

[2]Yoon et al., Soft Matter, 2008, 4, 1467-1472.

C1.00028 Reaction-Diffusion Processes in Ultrathin Films of Photoresist[1] , GINUSHA PERERA, GILA STEIN, Univ. of Houston — Projection lithography is the primary technology used for patterning semiconductor devices. High-throughput manufacturing requires imaging materials (resists) that are highly sensitive to radiation, and this demand is satisfied through a process termed chemical amplification (CA). CA resists are comprised of a polymer resin (reactant) and photoacid generator (catalyst); a coupled reaction-diffusion mechanism drives image formation, where image resolution is limited by slow diffusion of the acid catalyst. There is evidence that thin film reaction rates deviate from the bulk behavior, and current models for image formation do not capture such effects. We demonstrate that X-Ray Diffraction can measure spatial extent-of-reaction in ultrathin films of a nanopatterned poly(4-hydroxystyrene-co-tertbutylacrylate) CA resist. The feedback acquired is used to construct predictive models for the coupled reaction-diffusion processes that incorporate the physics of confined polymers.

[1]Funded by NSF ECCS 0927147

C1.00029 Mechanical properties determination of PDMS films on hard substrate using atomic force microscopy , WENWEI XU, TODD SULCHEK, The George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology — Mechanical properties of PDMS thin films adhering on hard substrate were investigated using Atomic Force Microscope (AFM) with a spherical tip. Simulation was implemented using finite element method and was compared to the experiments. The effect of the hard substrate on the mechanical response of the PDMS film becomes significant when the indentation depth exceeds 45% of the sample thickness. This relationship was also verified by comparing Hertz model to the experiments in the whole indentation range. Hertz model is not applicable in the large deformation region because the large deformation violates the assumption on which the Hertz model is based. The point wise Young's modulus as a function of indentation was obtained using Hertz model and also identified the effect of the hard substrate on mechanical responses. Furthermore, the point wise Young's modulus in the linear elasticity region decreases with increasing film thickness, until the sample is thick enough and its modulus reaches that for bulk PDMS. In the point wise Young's modulus plot, the Young's moduli at small indentations were several orders of magnitude higher than those in the linear elasticity region; this phenomenon has been observed in previous research and was also studied in our experiments.

C1.00030 Anisotropic Surface and Interfacial Instabilities in Nanoimprinted Polymer Bilayers , DAE UP AHN, ZHENG ZHANG, YIFU DING, University of Colorado — We illustrate the spontaneous formation of hierarchical polymer patterns driven by surface/interfacial instabilities at mobile and corrugated polymer-polymer interface. Upon thermal annealing of polystyrene (PS) films deposited on (and also confined in) topographic patterns of poly(methylmethacrylate) (PMMA), the PS/PMMA bilayers underwent a sequential event of morphological changes encompassing uniform pattern decay, simultaneous capillary breakup, anisotropic coarsening, and Rayleigh instabilities. Particularly, depending on the geometry of the bilayer pattern, the simultaneous capillary breakup has occurred in different modes. The morphological evolutions and structure formations are unique to the current system, and are drastically different from the polymer film dewettings on a planar surface, a chemically patterned surface, or a topographically patterned rigid surface. Thus, we demonstrate that the direct participations of the viscous topographic interface in the instabilities or assemblies offer a unique strategy to achieve a rich spectrum of highly anisotropic hierarchical structures.

C1.00031 Modification of Silicon Oxide Surfaces with Thermally Annealed Polystyrene Films , STEVEN KALAN, KEVIN CAVICCHI, ALAMGIR KARIM, University of Akron — The modification of silicon with a native oxide surface has been accomplished by annealing thin films of anionically polymerized polystyrene spun-coat from solution at elevated temperature followed by dissolving the film in solvent to leave a thin layer of adsorbed polymer that persisted even after prolonged desorbing in solvent even at elevated temperature. It was found by water contact angle analysis of the samples after washing with organic solvent that annealing is a key step to adsorption of a thin layer of polystyrene on the film surface. X-ray reflectivity analysis also demonstrated that the thickness of the adsorbed layer is proportional to the molecular weight of the polymer. However, the contact angle showed a non-monotonic dependence on molecular weight. The further modification of these surfaces by ultraviolet/ozone treatment will be discussed. This is a novel surface treatment method as it performed with a polystyrene polymer without any additional chemical functionality through straight-forward vacuum annealing and washing with organic solvent.

C1.00032 A closer look on the thermo-responsive behavior of ultrathin pNIPAM films - relating interfacial molecular transitions to macroscopic properties , PATRICK KOELSCH, VOLKER KURZ, Karlsruhe Institute of Technology, STEFAN ZAUSCHER, Duke University — The thermo-responsive behavior of thiol-modified poly(N-isopropylacrylamide) (pNIPAM) films immobilized on gold were probed by in situ broadband sum-frequency generation (SFG) spectroscopy, ellipsometry and capturing bubble contact angle. The pNIPAM films were prepared by atom transfer radical polymerization using a nitro-biphenyl-thiol-SAM on a polycrystalline gold surface as a substrate. Macroscopic properties of the film during the lower critical solution temperature (LCST) are tracked in detail by ellipsometry and capturing bubble contact angle allowing us to measure the thickness and water content within the film as well as the surface energy. These results are correlated with data acquired by in situ SFG spectroscopy, an intrinsic surface specific method probing LCST dynamics on a molecular scale.

C1.00033 Non-Contact Measurements of Stiffness in Confined PS Films by Fluorescence and XPCS

, CHRISTOPHER EVANS, Northwestern University, SURESH NARAYANAN, ZHANG JIANG, Argonne National Lab, JOHN TORKELSON, Northwestern University — Fluorescence is used to detect stiffness in confined polystyrene (PS) films through the intensity ratio (I3/I1) of the dye molecule pyrene. Free-standing PS films show a softening (an increase in I3/I1) when the film thickness decreases below 400 nm, and a stiffening (a decrease in I3/I1) below thicknesses of 200 nm. Silica- and PDMS-supported PS films show no softening but report stiffening for films less than 200 nm thick, a result not in accord with the Tg reductions seen for PS on silica. X-ray photon correlation spectroscopy (XPCS) also reports stiffening in PS on silica through the relaxation times of capillary waves at the polymer surface. A two order of magnitude increase in relaxation time is observed for small in-plane wavevectors (q) in a 30 nm PS film compared to a 120 nm film. Bilayer films of PS supported on various bulk underlayers studied by XPCS indicate that lower substrate modulus leads to faster PS surface relaxation times. These are the first reported non-contact measurements related to stiffness in confined PS on silica.

C1.00034 Interfacial Structure, Dynamics, and Transport of Polyelectrolyte Membrane Materials for Fuel Cells

, CHRISTOPHER SOLES, K. PAGE, S. EASTMAN, S. KIM, S. KANG, National Institute of Standards and Technology; Polymers Division, J. DURA, NIST Center for Neutron Research, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY; POLYMERS DIVISON TEAM, NIST CENTER FOR NEUTRON RESEARCH COLLABORATION — Polymer electrolyte membranes (PEM) fuel cells show promise for a wide range of applications both in the transportation sector and for stationary power production due to their high charge density and low operating temperatures. While the structure and transport of bulk PEMs have been studied extensively, little is known about these materials at interfaces and under confinement, as they exist within the membrane electrode assembly (MEA). Using neutron/ x-ray reflectivity and polarization-modulation infrared reflection-absorption spectroscopy, we have studied the polymer-substrate interfacial structure, swelling, and water transport as function of humidity, surface chemistry, and film thickness. The interfacial structure is highly dependent upon the substrate surface chemistry and the swelling/water diffusivity are suppressed when the PEM is confined to a thin film. This new information will enable researchers to more accurately model the performance of the MEA as current simulations typically rely on bulk property values to predict water and proton transport under these conditions.

C1.00035 Large and Reversible Plasmon Tuning using Ultrathin Responsive Polymer film[1]

, SRIKANTH SINGAMANENI, SAIDE NERGIZ, Washington University in St. Louis — We demonstrate reversible linear and branched aggregation of gold nanoparticles adsorbed on an ultrathin responsive polymer ((poly(4-vinyl pyridine), P4VP) film. P4VP is a weak cationic polymer, which exhibits a reversible coil to globule transition with change in external pH. Atomic force microscopy revealed that in the coiled state (below the isoelectric point of the polymer) of the polymer chains, gold nanoparticles adsorbed on the polymer layer existed as primarily individual nanoparticles. On the other hand, lowering the pH caused the polymer chains to transition from coil to globule state, resulting in aggregation of the nanoparticles into linear and branched chains. Reversible aggregation of the nanoparticles results in a dramatic change in the optical properties of the metal nanostructures. Apart from the large redistribution of the intensity between the individual (530 nm) and coupled (650 nm) plasmon bands, the coupled plasmon band exhibits a shift of nearly 60 nm with change in external pH. The pH triggered aggregation of the nanoparticles and the dramatic change in the optical properties associated with the same can form an excellent platform for colorimetric sensing.

[1]The work reported here is supported by the Siteman Cancer Center at Barnes-Jewish Hospital and Washington University School of Medicine

C1.00036 Mechanical Properties of Nanofibers Revealed by Interaction with Streams of Air

, YINAN LIN, DANIEL CLARK, DARRELL RENEKER, The University of Akron — Measurements of mechanical properties of electrospun nanofibers are needed for process control [1] and for design of structures that are durable, conformal and hierarchical. A new method, complementing measurements made on miniature mechanical testing devices [2], was developed. Electrospun nanofibers were captured directly between two steel rods that functioned "grips." Tensile deformation was applied by separating grips. The stress information was revealed by the deflections of the nanofibers caused by forces from broad streams of air, flowing perpendicularly to the fibers, at measured velocities. Glints of reflected light that revealed the contour of the deflected nanofibers were recorded with a camcorder. Image analysis of the shapes of the nanofibers was combined with scanning electron microscopy measurements of the diameter of the ends to evaluate the mechanical properties. Stress strain curves and hysteresis loops of selected ultrathin electrospun fibers were obtained. Direct comparisons of mechanical properties were made for a wide range of polymers.

[1] Reneker, D. H.; Yarin, A. L. Polymer 2008, 49, (10), 2387-2425.
[2] Naraghi, M.; Chasiotis, I.; Kahn, H.; Wen, Y. K.; Dzenis, Y. Applied Physics Letters 2007, 91, (15), 151901.

C1.00037 Structural Characterization of Nanopatterned Surface Gratings with Grazing Incidence X-Ray Scattering

, ELAINE CHAN, DONG HYUN LEE, DMITRY VORONOV, HOWARD PADMORE, Lawrence Berkeley National Laboratory, TING XU, University of California, Berkeley, THOMAS RUSSELL, University of Massachusetts Amherst, ALEXANDER HEXEMER, Lawrence Berkeley National Laboratory — The fabrication of surface gratings with periodic, nanoscale features is a promising route for templating nanopatterned thin film materials with macroscopic lateral order. These materials can be utilized for constructing novel and improved micro- and opto-electronic devices and x-ray optical elements. To characterize the structural features of the grating substrates and templated thin films, grazing incidence x-ray scattering (GISAXS) is becoming an increasingly desirable and emerging technique because the method provides sufficiently high sensitivity. We investigate herein the structural features of gratings with sawtooth topologies using GISAXS. We characterize the GISAXS patterns of gratings prepared from silicon and sapphire substrates, and examine the emergence of specific features that appear for varying sawtooth aspect ratio and at different incident angle values. These features are further analyzed using theoretical calculations where feasible. In this manner we demonstrate the utility of GISAXS for characterizing the structures of nanopatterned surfaces.

C1.00038 Thermal Programmed Desorption of $C_{32}H_{66}$

, M. CISTERNAS, Pontificia Univ. Catolica de Chile, V. DEL CAMPO, Univ. Tecnica Federico Santa Maria, Chile, A.L. CABRERA, U.G. VOLKMANN, Pontificia Univ. Catolica de Chile, F.Y. HANSEN, Technical Univ. Denmark, H. TAUB, Univ. of Missouri-Columbia — Alkanes are of interest as prototypes for more complex molecules and membranes. In this work we study the desorption kinetics of dotriacontane C32 adsorbed on SiO_2/Si substrate. We combine in our instrument High Resolution Ellipsometry (HRE) and Thermal Programmed Desorption (TPD). C32 monolayers were deposited in high vacuum from a Knudsen cell on the substrate, monitorizing sample thickness *in situ* with HRE. Film thickness was in the range of up to 100 Å, forming a parallel bilayer and perpendicular C32 layer [1]. The Mass Spectrometer (RGA) of the TPD section was detecting the shift of the desorption peaks at different heating rates applied to the sample. The mass registered with the RGA was AMU 57 for parallel and perpendicular layers, due to the abundance of this mass value in the disintegration process of C32 in the mass spectrometers ionizer. Moreover, the AMU 57 signal does not interfere with other signals coming from residual gases in the vacuum chamber. The desorption energies obtained were ΔE_{des}=11,9 kJ/mol for the perpendicular bilayer and ΔE_{des} = 23,5 kJ/mol for the parallel bilayer.
[1] V. del Campo et al., Langmuir **25** (22), 12962 (2009); E. A. Cisternas et al., J. Chem. Phys. **131** (11), 114705 (2009).

C1.00039 Molecular dynamics simulations of dotriacontane films supported on a SiO_2 surface

, SEBASTIAN GUTIERREZ, Pontificia Universidad Catolica de Chile, RAUL ARAYA, TOMAS PEREZ-ACLE, Universidad de Chile, MARIA JOSE RETAMAL, ULRICH G. VOLKMANN, Pontificia Universidad Catolica de Chile — Dotriacontane ($C_{32}H_{66}$, C32) films supported on SiO_2 surfaces were studied using very high-resolution ellipsometry, atomic force microscopy (AFM) and x-ray reflectivity techniques. For almost complete layers a model was proposed [1] in which the C32/SiO_2 interfacial region is characterized by a parallel bilayer and perpendicular layers on top. Recent AFM measurements performed on samples forming sea-weed like structures, showed that for these particular perpendicular "fractal like" layers the heights are lower than the all-trans length of dotriacontane (42.5 Å). To gain insights on the internal molecular ordering and layering of C32 supported on SiO_2 surfaces, we used all-atom molecular dynamics to simulate C32 films at different temperatures. Our results confirm the presence of the parallel bilayer suggesting the existence of a mixed layer on top, formed by molecules with both parallel and perpendicular segments. These findings suggest a different molecular architecture for sea-weed like structures of dotriacontane supported on SiO_2.

[1] H. Mo et al., Chem. Phys. Lett. **377**, 99-105 (2003); U. G. Volkmann, et al., J. Chem. Phys. **116**, 2107 (2002).

C1.00040 Fabricating Stable Superhydrophobic Hierarchical Polyelectrolyte Multilayer Films by Layer-by-Layer Assembly and Nanolithography

, XIAYUN HUANG, NICOLE ZACHARIA — Recent experiment shows that wetting can be controlled by not only the chemical nature but geometrical structure of the surface also. Even for a hydrophilic surface, it can transit into hydrophobic one when manipulating the roughness of surface. It is also of interest to determine if superhydrophobic surfaces can be created from hydrophilic multilayer films because multilayer is easy to be coated on any place by layer-by-layer assembly. Here, we used water-soluble polycations, PAH (poly(allylamine)), and polyions, SPS (sodium poly(styrene sulfonate)), to form polyelectrolyte multilayers. By nanoimprint lithography and in-situ growth of inorganic patterns in between these polyelectrolyte multilayers, we can include some micro-sized and nano-sized structures for different generations. When controlled introducing micro-sized and nano-sized hierarchical structures into multilayers, we can learn how the surface roughness increasing superhydrophobic properties from geometry view fundamentally.

C1.00041 Adhesion of Nanoparticles[1]

, JAN-MICHAEL CARRILLO, University of Connecticut, ELIE RAPHAEL, ESPCI, ANDREY DOBRYNIN, University of Connecticut — We have developed a new model of nanoparticle adhesion which explicitly takes into account the change in the nanoparticle surface energy. Using combination of the molecular dynamics simulations and theoretical calculations we have showed that the deformation of the adsorbed nanoparticles is a function of the dimensionless parameter $\beta \propto \gamma (GR)^{-2/3} W^{-1/3}$, where G is the particle shear modulus, R is the initial particle radius, γ is the polymer interfacial energy, and W is the particle work of adhesion. In the case of small values of the parameter β <0.1, which is usually the case for strongly cross-linked large nanoparticles, the particle deformation can be described in the framework of the classical Johnson, Kendall, and Roberts (JKR) theory. However, we observed a significant deviation from the classical JKR theory in the case of the weakly cross-linked nanoparticles that experience large shape deformations upon particle adhesion. In this case the interfacial energy of the nanoparticle plays an important role controlling nanoparticle deformation. Our model of the nanoparticle adhesion is in a very good agreement with the simulation results and provides a new universal scaling relationship for nanoparticle deformation as a function of the system parameters.

[1]ACS: PRF No. 49866-ND7

C1.00042 ABSTRACT WITHDRAWN –

C1.00043 Pressure Mapping Within a Tribological Contact with Fluorescence Imaging

, MOURAD CHENNAOUI, JANET WONG, Imperial College London, London, UK — In many lubricated applications from gears to MEMS, the operating pressure must be known in order to achieve optimum performance and design. However, due to the small length scale that exists at the tribological contact, placing sensors is unpractical to allow direct pressure measurement. Instead, the pressure is often inferred from indirect techniques such as film thickness measurements, photo-elasticity or the use of micro-transducers. Although these methods lead to good pressure approximations, they generally involve calibrations on well-defined setups. The results obtained can be difficult to interpret or suffer from limited spatial resolutions. In this work, fluorescent molecules in a lubricating fluid are used as probes for in-situ pressure measurements. The change in the probe's photophysical behaviour with pressure is utilised to quantitatively correlate the pressure distribution in a tribological contact such as the one found in elastohydrodynamic lubrication regimes.

C1.00044 Thermal Properties of specific Nonconjugated Conductive Polymers studied using Differential Scanning Calorimetry

, GURUDUTT TELANG, SAPANA SHRIVASTAVA, MRINAL THAKUR, Photonic Materials Research Laboratory, Auburn University, AL 36849 — Differential scanning calorimeter (DSC) has been used to measure the thermal properties of nonconjugated conductive polymers, poly(β-pinene) and trans-1,4-polyisoprene before and after doping with iodine. The measurements have been made over the temperature range of -50 °C to 110°C. The heat capacity of poly(β-pinene) has been observed to increase upon iodine doping. The T_g of undoped poly(β-pinene) and the T_m of undoped trans-1,4-polyisoprene have been measured and were found to be 77 °C and 60 °C respectively. After doping the T_g and T_m transitions were not clearly observable. X-ray diffraction studies have shown the γ-phase crystal structure for trans-1,4-polyisoprene film in the undoped state. These results will be discussed considering the molecular and nano-structures of these materials before and after doping.

C1.00045 Complex fluids with robustly tunable optical properties: experiments and theory[1]

, T. CONG, S.N. WANI, A.S. SANGANI[2], R. SURESHKUMAR[3], Syracuse University, Syracuse, NY, 13244, U.S.A., SYRACUSE UNIVERSITY TEAM — Fluids with tunable optical properties are of fundamental and practical interest. They can be easily processed to manufacture thin films and interfaces for applications such as molecular detection and light trapping in photovoltaics. We use solution phase self-assembly to uniformly distribute various metallic nanoparticles to produce stable suspensions with localized, multiple wavelength or broad-band optical properties. Their spectral response can be robustly modified by varying the species, concentration, size and/or shape of the nanoparticles. Spectral behavior for finite particle concentrations can be predicted by an effective medium theory developed in this work. Structure, rheology and optical properties of these plasmonic suspensions as well as their potential application to high efficiency photovoltaics design will be discussed.

[1]NSF Grant 1049454

[2](Currently at the National Science Foundation, Arlington, VA)

[3]E-mail: rsureshk@syr.edu

C1.00046 Exploiting redox chemistries to manipulate structure and electrical conductivity in polymer acid-doped polyaniline , JACOB TARVER, JOLINE FAN, YUEH-LIN LOO, Department of Chemical and Biological Engineering, Princeton University — Template synthesis of polyaniline on poly(2-acrylamido-2-methyl-1-propanesulfonic acid) yields electrostatically stabilized particles that can be aqueously dispersed and cast into thin films; electrical conductivity in these films scales with inter-particle connectivity. Previous research has shown that solvent annealing with dichloroacetic acid (DCA) induces structural rearrangement of polymer chains and consequently enhances the electrical conductivity by up to two orders of magnitude (from 0.4 to 40 S/cm). Alternatively, the electrostatic interactions between polyaniline and its template can be neutralized through chemical reduction with hydrazine monohydrate, after which the polymer undergoes extensive structural rearrangement; subsequent exposure to nitric oxide leads to reassociation of polyaniline and its polymer acid dopant. Enhanced conductivity is observed following this chemical redox process, and is attributed to extensive polymer chain relaxation and concurrent elimination of the particulate nature of template-synthesized polyaniline.

C1.00047 Electromagnetic transport in magnetorheological elastomer composites[1] , DARIN ZIMMERMAN, KOFI ADU, RICHARD BELL, TIMOTHY HOOPER, GARY WEISEL, The Pennsylvania State University, Altoona College — We present systematic measurements of the electron transport properties and optical response of gold-coated-iron (Au/Fe)-elastomer composite materials. By mixing micron-sized Au/Fe particles with silicone-based liquid elastomer, we produce two types of magnetorheological elastomer composites (MREs): those in which the particles are aligned by an external magnetic field prior to elastomer hardening and those in which the particles are left in random arrangement. By applying modest external stress or an external magnetic field to the two types of post-hardened MREs, we control the transport properties and optical response and observe significant differences in their behavior.

[1]The National Science Foundation; CBET 0755696

C1.00048 Solution Structures of Poly(3-alkylthiophene)[1] , KAIKUN YANG, LIWEI HUANG, NARAYAN CH DAS, HOWARD WANG, State University of New York, Binghamton — Small angle neutron scattering has been used to understand the solution structure of regioregular and regiorandom alkyl-derived polythiophenes, with alkyl side groups varying from 4 to 10 carbons. While poly(3-octylethiophene) (P3OT) remain coil conformations in solution, poly(3-butylthiophene) (P3BT) and poly(3-dodecylthiophene) form gel networks. However, poly(3-hexylthiophene) (P3HT) forms rod-like aggregates over large length scales. At elevated temperatures, all structures dissolve to coil solutions. A temperature dependent study shows that the aggregates (coils, rods and gels) are thermally reversible. The solution structure is reflected in the morphology of as-prepared films cast from the same P3HT solution stored for various time. In general, roughness and large rod-like features in as-cast films increase with storage time. Those long 1D aggregates may form in solution and is responsible for the eventual gelation of P3HT solution, render it useless for casting films for applications.

[1]NSF CMMI -0928865

C1.00049 Generation of conductivity through transfer charge properties, for polyesters and polyamides with characteristic functional groups , CARMEN GONZALEZ, LUIS HERNAN TAGLE, CLAUDIO A. TERRAZA, Pontificia Universidad Catolica de Chile, ANDRES BARRIGA, Universidad de Chile, A.L. CABRERA, ULRICH G. VOLKMANN, Pontificia Universidad Catolica de Chile — Electro-optic properties of σ-conjugated polymers, as polysilylene; are associated with electron conjugation in the silicon atom, which allows a significant delocalization of electrons along of the chain. Thus, the conductivity is intimately connected to the mobility of charge carriers, which in turn depends on the structure and morphology of the system. We report the characterization of polyesters (PEFs) and polyamides (PAFs). Film thicknesses were obtained by ellipsometry. The vibration frequencies of the groups were determined by FT-IR and corroborated by Raman spectroscopy. Structural information was obtained from X-Ray diffraction (XRD). The structural and surface morphology were studied by scanning electron microscope (SEM). Electrical conductivity of the polymers was measured before and after exposure to iodine vapor, for films of different thicknesses. Morphological differentiation was studied by energy dispersive microscopy (EDX), showing a regular distribution of iodine within the polymer. Preliminary conductivity measurements showed adverse effects when oxidation of the polymer films is induced These effects are related to a certain grade of disorder within the system

C1.00050 Structural symmetry breaking of silicon containing polymers and their relation with electrical conductivity and Raman active vibrations , ALEJANDRO CABRERA, CARMEN GONZÁLEZ , LUIS TAGLE, CLAUDIO TERRAZA, ULRICH VOLKMANN, Pontificia Universidad Catolica de Chile, ANDRÉS BARRIGA, Universidad de Chile, ESTEBAN RAMOS, MAXIMILIANO PAVEZ, Pontificia Universidad Catolica de Chile — The incorporation of silicon into the polymeric main chain or side groups can provide an enhancement in chemical, physical and mechanical properties. We report an efficient method for the synthesis of polymers containing silicon in the main chain, from the polycondensation reactions of four optically active carboxylic diacid. The solubility of the polymers, the molecular weight, the glass transition and the thermal stability were studied by standard techniques. Raman spectroscopy was used to probe the conformation of stretching modes as function of the temperature. The conductivity measurements indicated that the alignment of the molecules is a crucial parameter for electrical performance. When the polymers were exposed to iodine, charge transfer increased their mobility and decreased their optical band gaps. These novel properties highlight the possibility to generate alternative active opto-electronics polymers.

C1.00051 Structural Disorder and Thermal Properties of the Alpha' Phase of Poly(l-Lacitc Acid) , JEFFREY KALISH, SHAW LING HSU, University of Massachusetts - Amherst — Poly(lactic acid) samples rich in alpha' or alpha crystals have been characterized using spectroscopic and thermal methods. Cryogenic infrared and Raman spectroscopy were used to probe the differences in chain conformation and packing. Compared to the alpha crystal, the alpha' crystal has weakened specific carbonyl and methyl interactions. Experimental spectroscopic analysis in conjunction with simulation studies have shown that the alpha' crystal has uniform chain conformational disorder. This disorder in chain conformation and packing leads to different crystalline forms with varying stabilities. The difference in thermal stability was quantified by measuring enthalpic change at melting for both crystalline forms by extrapolation of the glass transition as well as by using small molecule extrapolation. Equilibrium melting enthalpy was determined to be 57 J/g for alpha' and 96 J/g for the alpha crystal. The transformation from the less stable alpha' to the more stable alpha phase has been characterized. This analysis provides an explanation for the double melting peaks usually found in the PLLA samples.

C1.00052 Influence of graphene on the crystallization behavior of polyethylene , SHAN CHENG, CHRISTOPHER LI, Drexel University — Recent work on polyethylene(PE)/carbon nanotube nanocomposites demonstrates that CNTs can significantly alter PE crystallization. Graphene, a 2D counterpart of CNT, is an excellent candidate for fabricating polymer nanocomposites. We herein report the influence of graphene on crystallization behavior of PE. High density polyethylene (HDPE) was first crystallized in dilute solution in the presence of dispersed single or few-layer graphene sheets. Epitaxial growth of polyethylene on the basal plane of graphene sheets was observed using transmission electron microscopy. PE/graphene nanocomposites with various graphene loading were then fabricated. Both non-isothermal and isothermal crystallization behavior of these nanocomposites were studied using a differential scanning calorimeter. Multiple melting peaks of the nanocomposite were correlated to homo- and heterogeneous nucleation of PE crystallites. Crystallization kinetics was studied using Avrami equation. The results were compared with cabon nanotube/PE system and the difference will be discussed.

C1.00053 Crystallization effects of carbon nanotubes on semicrystalline isotactic polypropylene[1] , GEORGI GEORGIEV, Assumption College, SCOTT SCHOEN, DEVIN IVY, PEGGY CEBE, Tufts University, ASSUMPTION / TUFTS TEAM — When carbon nanotubes are introduced in isotactic polypropylene (iPP) materials the iPP crystals assemble in a fibrillar instead of spherulitic arrangement. We study the effects of concentration and isothermal vs nonisothermal treatments on the rate of crystal formation. Those nanocomposites provide means of controlling the crystal orientation in polymer materials by aligning the nanotubes and creating materials with novel properties. We used Differential Scanning Calorimetry (DSC) as our primary method of investigation due to its ability to give detailed data on the phase transitions of iPP nanocomposites with low concentrations of CNTs (0-5 percent). We analyzed the crystallization of each sample in the DSC at a range of cooling rates (10-20C/minute). We found that increased concentrations of CNTs speed up the nanocomposites' crystallization and decrease the crystal size distribution.

[1]Assumption College / NSF

C1.00054 Structure and dynamics of solvent-free polymer grafted nanoparticles: A computational study , ALEXANDROS CHREMOS, ATHANASSIOS PANAGIOTOPOULOS, Chemical and Biological Engineering, Princeton University — The structure and dynamics of solvent-free polymer-grafted nanoparticles have been investigated using molecular dynamics simulations. A basic coarse-grained model was used, where the nanoparticle is represented as a single smooth particle with bead- spring polymer chains attached to it. Motivated by the recent advances in nanoparticle ionic materials and nanoparticle organic hybrid materials, we use our model to explore the behavior of these systems over a wide range of parameters and gain insights of their structure and transport properties. In particular, we find that the chain length variation can change the softness of the nanoparticles, so for short chains the system exhibits rich structural characteristics while for long chains display (dilute) liquid-like characteristics. Additionally, we find that by increasing the softness of the particles the structural relaxation of the system becomes less sensitive to temperature variation, indicating a change from the hard-spheres to soft particles. The results confirm the experimental observations that changing the chain length the system can display behavior that spans from glasses to liquids.

C1.00055 A new method to measure the optical trapping energy of nanoparticles , JOSEPH JUNIO, Lehigh University, JACK NG, Hong Kong Univeristy Science and Technology, JOEL COHEN, University of the Pacific, ZHIFANG LIN, Fudan University, H. DANIEL OU-YANG, Lehigh University — A novel method is described for measuring the potential energy of nanoparticles in an optical trap by trapping an ensemble of particles with a focused laser beam. The mechanical force balance between repulsive osmotic and confining gradient-force pressures determines the single-particle trapping potential independent of interactions between the particles. The ensemble nature of the measurement permits evaluation of single-particle trapping energies much smaller than k_BT. Energies obtained by this method are compared with those of single-particle methods as well as with theoretical calculations based on classical electromagnetic optics.

C1.00056 Spontaneous asymmetry in coated spherical nanoparticles in solution and at liquid-vapor interfaces , J. MATTHEW D. LANE, GARY S. GREST, Sandia National Laboratories — Nanoparticles in solution are often stabilized with functional coatings to prevent aggregation. We'll present recent simulations results showing that small spherical nanoparticles produce highly asymmetric coating arrangements, when coated with simple polymer chains. These coatings are not symmetric even when extremely uniform grafting arrangements and full coverages are employed. I will also discuss the geometric properties which dictate the coating shape. When particles are placed in an anisotropic environment, such as the liquid/vapor interface, the asymmetric coatings are amplified and oriented by the surface. Particle shape and its responsive behavior is seen to strongly influence interactions. Implications and examples of controlled self-assembly will be presented.

C1.00057 ABSTRACT WITHDRAWN —

C1.00058 Controlled Evaporative Self-Assembly of Hierarchical Polymer Stripes with Ordered Nanochannels , WEI HAN, MYUNGHWAN BYUN, LEI ZHAO, Iowa State University, JAVID RZAYEV, The State University of New York, ZHIQUN LIN, Iowa State University — A toluene solution of a bottlebrush block copolymer, polystyrene-polylactide (PS-PLA), was confined in a "cylinder-on-flat" geometry, from which the consecutive "stick-slip" motion of the contact line of the PS-PLA solution was effectively regulated as the solvent evaporated, thereby forming gradient stripes at the microscopic scale. Upon subsequent solvent vapor annealing, hierarchically organized structures of PS-PLA were produced in which the lamellar nanodomains normal to the substrate were obtained within the stripes. After mild removal the PLA component, channels at the nanoscale wrere formed with the stripes. This facile approach of combining controlled evaporative self-assembly with subsequent vapor annealing opens up a new avenue to rationally organize and engineer self-assembling building blocks into functional materials and devices in a simple, cost-effective and controllable manner.

C1.00059 Supercritical carbon dioxide induced surface melting/recrystallization process in ultrathin PEO films[1] , NAISHENG JIANG, Stony Brook University, MITSUNORI ASADA, Kuraray Co., Ltd., PETER GIN, SO KING LAM, MAYA ENDOH, Stony Brook University, SUSHIL SATIJA, NIST, TAD KOGA, Stony Brook University — Crystallization of polymeric materials in nanoconfined geometries has attracted considerable attention in the past decade. In this talk, we will show the novel effects of supercritical carbon dioxide as a plasticizer in order to control the melting/crystallization behavior of semicrystalline polymer thin films. Poly(ethylene oxide) (PEO) thin films with thickness of 10nm-100nm were used for this study. In-situ neutron reflectivity technique was utilized to study the swelling behavior of deuterated PEO films in $scCO_2$ at T=50 $^\circ$C, showing the clear evidence of the surface melting phenomenon even below the bulk melting temperature (65 $^\circ$C). The surface structures before and after exposure at the different CO_2 process conditions were then investigated in air by using atomic force microscopy and grazing incidence x-ray diffraction. The results clearly showed that $scCO_2$-induced re-crystallization from the amorphous state via pressure quench results in various surface crystalline structures, depending on temperature, pressure, quench rates, and the film thickness.

[1]We acknowledge the financial support provided by NSF CAREER AWARD under funding number CMMI-0846267.

C1.00060 ABSTRACT WITHDRAWN —

C1.00061 Highly Swollen Porous Microstructures in Polyelectrolyte Multilayers , CHUNGYEON CHO, JEREMY KAISER, NICOLE ZACHARIA — We investigated the creation of porous morphologies from polyelectrolyte multilayers (PEMs) consisting of linear poly(ethylenimine) and poly(acrylic acid), and poly (allylamine hydrochloride) and poly (acrylic acid) as a function of pH and immersion time under post-base assembly treatment. The porous transition is linked to the neutralization of the polycations electrolytes as well as ionization of PAA by the exposing LbL films to high pH. This causes PEMs to undergo spinodal decomposition, creating pores and an increase in film thickness. By using reactive wet stamping technique, we were able to locally cause porosity changes under high pH conditions in the LbL films. Further investigation of the mechanical properties of patterned LbL films was done by performing nano-indentation analysis. The results showed clear difference of physical properties such as hardness and modulus between stamped and unstamped regions based on porous transition.

C1.00062 Morphological Change of Poly(4-*tert*-butylstyrene-*block*-4-*tert*-butoxystyrene) in a Wide Range of Segregation Strength Though Hydrolysis Reaction

, SITI SARAH ABDUL RAHMAN, DAISUKE KAWAGUCHI, YUSHU MATSUSHITA, Department of Applied Chemistry, Nagoya University, Japan — Morphological change of symmetric poly(4-*tert*-butylstyrene-*block*-4-*tert*-butoxystyrene)s (BO) upon hydrolysis reaction was investigated by transmission electron microscopy and small-angle X-ray scattering. Segregation strength, χN (χ: interaction parameter, N: degree of polymerization), which governs the chain dimension, was gradually tuned since poly(4-*tert*-butoxystyrene) (O), a non-polar polymer, can be converted into poly(4-hydroxystyrene) (H), a polar one, through hydrolysis. Samples with different molecular weights and conversion rates of O into H, f_Hs, were prepared. Domain spacing of the lamellar structure, D, increased as f_H increases where it abruptly increased at a critical f_H, indicating that the chain stretched perpendicularly to the lamellar interface. The degree of chain stretching compared to a random coil, D/D_0s (D_0: correlation length at f_H=0), were scaled by χN. Three regimes can be distinguished in the plot of (D/D_0) vs. χN: (I) the weak segregation regime with $D/D_0 \sim$1 that associates with the scaling behavior of $D \sim N^{0.55}$, (II) the intermediate segregation regime with the scaling behavior of $(D/D_0) \sim (\chi N)^{0.34}$, and (III) the strong segregation regime with $D/D_0 \sim$2.3 which corresponds to $D \sim N^{0.67}$.

C1.00063 Frustrated ABC Linear Block-Random Copolymer with a Semicrystalline End Block[1]

, BRYAN S. BECKINGHAM, RICHARD A. REGISTER, Princeton University — The solid-state structure of semicrystalline block copolymers is set either by block incompatibility or by crystallization of one or more blocks. A variety of solid-state morphologies may be observed depending on the block interaction strength, ranging from spherulitic to confined crystallization within preexisting microphase-separated domains. Linear triblock copolymers, polybutadiene-*b*-polyisoprene-*b*-poly(isoprene-*r*-styrene) (A-B-C), are synthesized via lithium-initiated anionic polymerization in cyclohexane. After polymerization of the butadiene block, triethylamine is added to facilitate the random styrene/isoprene copolymerization while also increasing the vinyl content of the polyisoprene block. Selective hydrogenation of the diene units with a Ni-Al catalyst yields a semicrystalline polyethylene endblock, with a frustrated block sequence: $\chi_{BC} > \chi_{AB} >> \chi_{AC}$. For a polymer with block molecular weights of 30-14-14 kg/mol, small-angle x-ray scattering reveals the formation of a well-ordered lamellar melt from which crystallization of the hydrogenated polybutadiene (polyethylene) block proceeds.

[1]This work was supported by the National Science Foundation Polymers Program (DMR-1003942).

C1.00064 Self-Consistent Field Modeling of Diblock Copolymers in Selective Solvents[1]

, RAGHURAM THIAGARAJAN, DAVID MORSE, Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455 — The purpose of my poster is to study the driving forces behind the self-assembly of a diblock copolymer AB, consisting of a solventphilic block (B) and a solventphobic block (A), in selective solvents (S). Micellar transformations between spherical, cylindrical, and bilayer curvatures for a model system are tracked using self-consistent field modeling, in real space, in the dilute regime. The transition from a concentrated regime, $\phi_{\rm AB} \sim 1$, to a dilute regime, $\phi_{\rm AB} \sim 0$, is studied. Phase portrait for the concentrated regime is generated using periodic self-consistent field modeling. The unbinding transition, as seen in the periodic counterpart of self-consistent field theory, is compared with the transformations observed in the dilute regime. The two phase regions in the dilute regime are mapped out for the inverted phases as well.

[1]This work was supported by UMN MRSEC (support for Raghuram Thiagarajan) using computer resources provided by both the Minnesota Supercomputing Institute and the UMN MRSEC.

C1.00065 Synthesis and Characterization of Tapered Block Copolymers

, WEI-FAN KUAN, RAGHUNATH ROY, JONGKEUN PARK, THOMAS EPPS, University of Delaware, Newark, DE 19716 — Tapered block copolymers offer the opportunity to manipulate copolymer segregation strength independent of molecular weight and chemical constituents, which allows the design of materials with improved mechanical properties while retaining the desired phase separated structures. In this work, we focus on the synthesis and characterization of poly(isoprene-*b*-isoprene/styrene-*b*-styrene-*b*-styrene/methyl methacrylate-*b*-methyl methacrylate) [P(I-IS-S-SM-M)] tapered triblock copolymers. P(I-IS-S) tapered diblock copolymers are synthesized using living anionic polymerization and treated as macroinitiators for activator regenerated by electron transfer (ARGET) atom transfer radical polymerization (ATRP). ARGET ATRP is employed to make the SM tapered interface and M block, enabling synthesis of tapered triblocks with low polydispersity ($M_w/M_n <$ 1.2). These materials self-assemble into well-defined nanoscale architectures depending on segment volume fractions and taper dimensions.

C1.00066 Gelation of Copolymers Photo-crosslinked by Pendant Benzophenones

, SCOTT CHRISTENSEN, RYAN C. HAYWARD, University of Massachusetts - Amherst — Copolymers containing pendant benzophenone (BP) groups provide a simple and powerful route to crosslinkable polymer films. While the solution state photo-chemistry of BP is well established, and crosslinking of polymers blended with BP has been studied in detail, the process of crosslinking by covalently attached BP has received comparatively little attention. We have prepared copolymers of BP with several different monomers, and studied gelation as a function of BP content and degree of photochemical conversion. We seek to understand the influence of polymer chemistry on crosslinking efficiency, to guide choices of materials for photo- crosslinkable polymer films and to provide a route for tailoring morphology in polymer blends.

C1.00067 Understanding the phase behavior and equilibration kinetics of PDMS-containing block copolymers

, CHARLOTTE STEWART-SLOAN, EDWIN THOMAS, Massachusetts Institute of Technology — Block copolymers containing both PDMS and an olefin are of interest because they combine high chi parameters which allow for strong segregation on small length scales with a differential etch resistance to oxygen plasma. In order to understand the phase behavior and how it is affected by thermal treatments, low molecular weight diblocks of PS-PDMS and PI-PDMS were examined at different temperatures using synchrotron radiation. The movement and changes in intensity of the peaks present in the SAXS patterns at different temperatures after long equilibration times provides information about the equilibrium structures present in these materials and the evolution of these patterns over time allows insight into structural kinetics. The ODT was determined for three different compositions and the structure equilibration on heating and cooling were investigated. Of particular interest is the evolution of structure at room temperature after high temperature treatment.

C1.00068 Cloud Point Depression in Dilute Solutions of HEMA/DMAEMA Copolymers with Prescribed Composition Profiles and Gradient Strengths

, KEITH GALLOW, Princeton University, YOUNG JHON, JAN GENZER, North Carolina State University, YUEH-LIN LOO, Princeton University — We have synthesized a random copolymer and gradient copolymers of hydroxyethyl methacrylate and dimethylaminoethyl methacrylate whose instantaneous compositions vary linearly and according to hyperbolic tangent (Tanh) functions along the backbones, all having similar molecular weights and overall compositions. The cloud point of the dilute solution of the random copolymer is 20.0°C; the transparent-to-turbid transition occurs over 1.0°C. Dilute solutions of linear gradient copolymers exhibit cloud point depressions of up to 3.5°C and transition breadths of 1-3°C compared to that of the random copolymer. The cloud points of dilute solutions of gradient copolymers with Tanh composition profiles are further suppressed by as much as 9.0°C compared to that of the random copolymer. Our observations demonstrate the importance of monomer sequence distribution in altering the macroscopic solution properties of copolymers.

C1.00069 High area density etching mask for data storage industry based on the block copolymer self-assembly[1]

, XIAODAN GU, THOMAS RUSSELL, University of Massachusetts Amherst, BIN ZHANG, DORSEY PAUL, Western Digital Inc., UNIVERSITY OF MASSACHUSETTS TEAM, WESTERN DIGITAL INC. TEAM — The application of block copolymer as etching mask for data storage industry was investigated. Higher area density silicon oxide pillars from block copolymer template were generated on the media substrate over several inch square areas. Thin film of PS-b-PVP was spin coated and solvent annealed to generate cylindrical micro-domain normal to surface. The film was then reconstructed in the ethanol alcohol to generate the porous cylindrical micro-domain. Polydimethylsiloxane (*PDMS*) was then spin coated onto the porous film surface. The film was heated to facilitate the movement of PDMS into the pores, and then etched with fluorine and oxygen plasmas to remove the polymeric material, leaving only silicon oxide pillars. The effect of pore diameter on the size and quality of silicon oxide pillar was investigated. Larger pores generated higher quality pillars. Areal densities from 0.5 to 2 Teradots per inch square were achieved. The silicon oxide produced had a good ion-etch resistance, enabling pattern transfer the pillar pattern to underlying magnetic media.

[1]MESEC DOE Western DIgital Inc

C1.00070 Orientation Control of Block Copolymer Films on Rough Substrates Prepared by E-beam Lithography

, YOUNGWOO CHOO, HYO SEON SUH, HYUN-MI KIM, MYUNG RAE CHO, YUN DANIEL PARK, KI-BUM KIM, Seoul National University, KOOKHEON CHAR — Several researches on the perpendicularly oriented BCP thin films induced from the underlying substrates with surface roughness have been reported. In the present study, we investigated the effect of each roughness factor, such as period or depth of the roughness, on the orientation of BCP thin films. In order to control such roughness factors systematically, we introduced various lithographic techniques. The hydrogen silsesquioxane (HSQ) patterns with controlled period and depth were prepared by the Atomic Image Projection E-beam Lithography (AIPEL), which were realized by adjusting lithographic parameters of AIPEL. In addition, we also prepared silicon oxide patterns using ordinary e-beam lithography. The line width and period of patterns were finely tuned during the E-beam writing while the depth of the patterns was modified by the reactive ion etching on the patterned substrates. On the substrates with specified roughness, we deposited symmetric PS-*b*-PMMA diblock copolymers and observed the effect of individual roughness factors on the orientation of BCP thin films.

C1.00071 Architectural Effects in Thin Films of Poly(styrene-b-methyl methacrylate) Copolymers[1]

, NIKHILA MAHADEVAPURAM, THAI VU, GILA STEIN, Univ. of Houston — Block copolymer self-assembly offers a simple route to generate nanostructures over large areas. Control over domain orientation is critical for nanopatterning; typically, the lower-surface energy constituent will segregate at the air interface and drive a parallel orientation of cylindrical or lamellar domains. Recent works by Khanna et al.[2] and Matsen[3] suggest that molecular architecture can affect surface energetics and domain orientations. We compared the thin film ordering of lamellar poly(styrene-b-methyl methacrylate) (PS-PMMA) diblock copolymers with PMMA-PS-PMMA triblock copolymers. Films that ranged in thickness from $t = L_0 - 5L_0$ were cast on neutral substrates, annealed under vacuum at 220°C for 2 days, and then measured with grazing-incidence small-angle X-ray scattering. The triblock copolymers adopt a perpendicular domain orientation near the film surface for all thicknesses considered, while the perpendicular domain orientation was only stable for diblock copolymers when $t \leq L_0$. However, triblock thin films contain defects in the film interior that limit their utility.

[1]Funded by NSF ECCS 0927147

[2]Khanna et al., Macromolecules, 39, 9346-9356, 2006

[3]Matsen, Macromolecules, 43, 1671-1674, 2010

C1.00072 From blood dialysis to desalination: A one-size fits all block copolymer based membrane system

, NATARAJ SANNA KOTRAPPANAVAR, Univeristy of Cambridge, PAUL ZAVALA-RIVERA, KEVIN CHONNON, University of Cambridge, SHAHEEN S.A. ALMUHTASEB, Qatar University, EASAN SIVANIAH, University of Cambridge, UNIVERSITY OF CAMBRIDGE TEAM, QATAR UNIVERSITY COLLABORATION — Asymmetric membrane with ultrahigh selective self-assembled nanoporous block copolymer layer were developed successfully on polyimide (PI) support, which demonstrated excellent thermal, chemical and mechanical stability. Membranes with specific nano- structural architectures and optimized cascades of block assemblies on the top selective skin have been used largely for separation of colour from aqueous streams, wastewater treatment, desalination, blood filtration and gas separation with dense layer transformation. A consistent and reliable method of membrane preparation and measuring separation performance has been adopted. A homologous series of ethylene oxide oligomers covering a large range was used to characterise MWCO of Membrane and were able to provide many points to give a comprehensive description of the membrane performance in the nanofiltration range.

C1.00073 Circular Patterns over Large Areas from The Self-Assembly of Block Copolymers Guided by Shallow Trenches

, SUNG WOO HONG, XIAODAN GU, University of Massachusetts Amherst, JUNE HUH, Yonsei University, SHUAIGANG XIAO, Seagate Technology, THOMAS RUSSELL, University of Massachusetts Amherst — We report the fabrication of ultra-dense circular nanoarrays of block copolymer (BCP) microdomains over macroscopic areas. These arrays were generated by the directed self-assembly of BCPs on the topographically patterned substrates, where the trenches with circular shape are patterned on a flat substrate. The width of circular trench and the distance between circular trenches are varied for commensurability issues, and difference BPCs are used to demonstrate the generality of this strategy. When a commensurability condition is satisfied, BCPs on the topographically patterned substrates undergo a grapho-epitaxial self-assembly with solvent annealing, resulting in an areal density amplipication of the circular patterns over large areas. The methodology described here may provide an easy approach to high densities of circularly shaped nanopatterns for data storage applications.

C1.00074 Poly (2-vinyl naphthalene-b-acrylic acid) (P2VN-b-PAA) block copolymer pattern formation, alignment and pattern transfer by reactive ion etching (RIE)

, XIN ZHANG, CHRISTOPHER METTING, R.M. BRIBER, SANG HAK SHIN, BEN JONES, Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742 — P2VN-b-PAA (Mn=30.8-b-24 kDa) lamellar block copolymer was examined for use as a pattern transfer template due to the potential large dry etching contrast between the blocks. As-spun films have a micelle or vertically oriented cylindrical morphology depending on the spinning solvent. Vapor annealing with acetone, a poor solvent for P2VN-b-PAA, resulted rapid reordering to a vertically oriented lamellar morphology within 5 minutes for films <50 nm thick. Films between 30 to 50 nm thick were spin coated onto oxide wafers with interdigitated electrodes to examine if an electric field would align the morphology. The lamellae aligned normal to the electrodes within 1 hour by electric field assisted acetone vapor annealing at field strengths as low as 1V/micron. CF_4 plasma dry etching contrast as high as 1:3.8 (P2VN:PAA) for homopolymer blanket films was measured. The block copolymer pattern was transferred to the silicon substrate in two steps using CF_4 followed by SF_6 RIE.

C1.00075 Methods for Self-Assembly of Rod-Coil Diblock Copolymer Thin Films , SAMANTHA COLLINS, AMANDA KAMPS, MICHAEL FRYD, RUSSELL COMPOSTO[1], SO-JUNG PARK[2], University of Pennsylvania — Long range order in diblock copolymer (BCP) thin films can be induced by solvent annealing. First, thin films of semiconducting BCPs were spin-coated onto base-treated and hydroxyl-terminated silicon substrates. These BCP films were then solvent vapor annealed in inert, solvent-saturated atmosphere. Structure was investigated as a function of substrate end group, film thickness, and solvent annealing duration, and an optimized ordering condition was found. Film thickness was varied to direct the morphology perpendicular to the substrate for potential photovoltaic device applications. Second, BCP thin films were processed by novel thermal gradient annealing as an alternative route to directing long range order in the films. The effect of thermal gradient steepness and temperature range on ordering was analyzed for the optimized thickness determined by solvent annealing.

[1]Senior Author
[2]Senior Author

C1.00076 Nanopatterns in a confined triblock copolymer , JUMI LEE, YEONGMIN JEON, Dankook University, JAEUP KIM, Ulsan Institute of Science and Technology, JUNHAN CHO, Dankook University — Ordered structures in thin films of ABC triblock copolymers are studied experimentally and theoretically in order to be applied to fabrication of nanoscale electronic devices. A field-theoretic simulation method based on the self-consistent field theory is used to generate useful nanopatterns starting with a random configuration of compositions. The main parameters for the phase stability, such as Flory interaction parameters, total chain size, compositions, film thickness, and surface interactions, are considered as controllable variables in the present analysis. By using some typical triblock copolymers, nanopatterns observed in experiments are comparable with those in the simulation.

C1.00077 Hierarchical assembly of coil-rod-coil peptide-based copolymers , NANDULA WANASEKARA, CASEY JOHNSON, LASHANDA KORLEY, Department of Macromolecular Science and Engineering, Case Western Reserve University, Cleveland, OH — Coil-rod-coil block copolymers have been shown to exhibit an array of morphologies, from crystalline lamellae, to novel, three-dimensional tetragonal lattices, depending upon coil length and molecular weight. We have been motivated by recent advances in controlled polymerization techniques and the opportunity to develop bio-inspired copolymer motifs to explore the hierarchical self-assembly of coil-rod-coil peptide-based copolymers with variations in peptidic rod length. Thin films were characterized using atomic force microscopy, x-ray scattering and thermal analysis techniques showing random sphere-like nanostructures with alpha-helix peptide secondary structure. Our goal is to utilize these materials to engineer the interface of hierarchically-designed, nature-inspired elastomers.

C1.00078 Enhanced stability of self-assembled polymer nanostructures by molecular crosslinking , MARK STOYKOVICH, IAN CAMPBELL, BRIAN PEREA, University of Colorado-Boulder — Self-assembled nanostructures of block copolymers have attracted interest for applications in next generation lithography and advanced materials synthesis. Many of these applications require mechanically and chemically robust nanostructures that cannot be achieved by simple diblock copolymer materials alone. Here we have investigated a method to stabilize block copolymer nanostructures after self-assembly in thin films by incorporating cross-linking molecular components within the self-assembled domains. Polymer blends consisting of a majority symmetric PS-block-PMMA copolymer and equal amounts of PS and PMMA homopolymers were prepared and determined to form lamellar phase morphologies. The PS and PMMA homopolymers were synthesized with a small fraction of glycidyl methacrylate monomer which served as the cross-linking agent in the blends. These nanostructures exhibit enhanced solvent and thermal stability, and have been demonstrated for the fabrication of three-dimensional multilayer structures.

C1.00079 Local segmental dynamics of cis-1,4-polybutadiene, polypropylene, and polyethylene terephthalate via molecular dynamics simulations , DAVID WHITLEY, DAVID ADOLF, University of Leeds, UK — NPT molecular dynamics simulations of cis-1,4-polybutadiene, polypropylene, and polyethylene terephthalate have been performed. The simulation pressure was 1 atmosphere for all systems, with all simulation temperatures being well above each polymer's glass transition temperature. The trajectories have been analysed via autocorrelation functions (ACFs) of chord vectors spanning different numbers of chain backbone bonds. Inverse Laplace transformations of these ACFs using the CONTIN algorithm afforded the corresponding distributions of relaxation times (DRTs) for the simulated dynamics. All DRTs illustrated a peak on fast time scales corresponding to short length scale segmental motion and a peak at longer time scales corresponding to longer length scale relaxations. An intermediate peak between the fast and slow peaks appears as the relaxation dynamics of longer chord vectors are analysed. The temperature dependence of the relaxation dynamics has also been investigated.

C1.00080 Coarse-grained modeling of polystyrene at different concentrations using the Iterative Boltzmann Inversion technique , BESTE BAYRAMOGLU, ROLAND FALLER, UC Davis — We present systematic coarse-graining of several polystyrene models and test their performance under confinement and eventually in brush systems. The structural properties of a dilute polystyrene solution, a polystyrene melt and a confined concentrated polystyrene solution at 450K, 1 bar were investigated in detail by atomistic molecular dynamics simulations of these systems. Coarse-graining of the models was performed by Iterative Boltzmann Inversion Technique (IBI), in which the interaction potentials are optimized against the structure of the corresponding atomistically simulated systems. Radial distribution functions, bond, angle and dihedral angle probability distributions were calculated and compared to characterize the structure of the systems. Good agreement between the simulation results of the coarse-grained and atomistic models was observed.

C1.00081 Identifying Entanglement States of Ring Polymers Using Knot Polynomials , JIAN QIN, SCOTT MILNER, ChE at Penn State University — Melts of ring polymers have fixed topologies in the absence of ring opening or reconnecting operations. We identify the topological states by recognizing how rings are knotted with each other, which can be achieved by computing knot invariant polynomials. We used this idea to count the entanglement states of ring polymers, prepared with off-lattice Monte Carlo simulations, in which the system topology is allowed to change by various ring rebridging moves. We project polymer configurations to obtain crossing diagrams, and use algorithms based on knot theory to compute the Jones invariant polynomial. We studied both aperiodic and periodic systems, to estimate the surface effects on entanglements. For the periodic case, we extended the algorithm for aperiodic knots to deal with periodic patterns. These tools enable us to accumulate the probability distribution of topological states for rings of different lengths, from which we determined the entanglement length by identifying the topological entropy as k_B per entanglement strand.

C1.00082 Conformation of a Lennard-Jones Chain in Explicit Solvent: A Solvation Potential Approach[1] , SHISHIR ADHIKARI, MARK TAYLOR, Dept. of Physics, Hiram College, Hiram, OH — The conformation of a polymer chain in solution is intrinsically coupled to the chain's local solvent environment. In much of the theoretical work on polymers in solution the effects of solvent are treated implicitly and explicit chain-solvent coupling is ignored. Although a formally exact treatment of chain-solvent coupling can be constructed, the required many-body solvation potential is not practical to compute. Following on our work with hard-sphere and square-well chain-in-solvent systems [1] here we show that for Lennard-Jones (LJ) systems this many-body solvation potential can be made tractable via an "exact" decomposition into a set of two-site potentials. We use these exact short chain results, combined with the pure solvent potential of mean force, to construct approximate two-site solvation potentials for long LJ-chains. Monte Carlo simulations for full chain-in-solvent systems verify the accuracy of our solvation potential mapping across the full LJ-solvent phase diagram.

[1] J. Chem. Phys. 127, 184901 (2007); J. Polym. Sci., Part B: Polym. Phys. 45, 3319 (2007).

[1]Funding: NSF DMR-0804370

C1.00083 Differential AC/scanning chip nanocalorimeter for in-situ measurements of vapor deposited glasses , MATHIAS AHRENBERG, University of Rostock, KATIE WHITAKER, University of Wisconsin-Madison, HEIKO HUTH, University of Rostock, MARK D. EDIGER, University of Wisconsin-Madison, CHRISTOPH SCHICK, University of Rostock, UNIVERSITY OF ROSTOCK TEAM, UNIVERSITY OF WISCONSIN-MADISON TEAM — We use nanocalorimetry to investigate the formation of extraordinarily stable glasses prepared by vapor deposition. For that purpose we've built a vapor deposition chamber that allows in-situ characterization of vapor-deposited organic molecules down to liquid nitrogen temperature. The use of commercially available nanocalorimeter sensors permits us to measure the temperature at the sample position directly via heater resistivity. The calibration of this method was done with the frequency dependence of the dynamic glass transition temperature of low molecular glass formers such as toluene over a broad frequency range. This was applied to investigate vapor deposition of glass formers as a function of time as well as vapor deposited samples as a function of temperature.

C1.00084 An apparatus for in situ x-ray scattering studies of polymer melts during homogenous uniaxial extensional flow , WESLEY BURGHARDT, RUINAN MAO, Northwestern University — In situ x-ray scattering methods have been broadly applied to study the structural dynamics of polymers and other complex fluids under flow, and can provide deep insights into the microstructural origins of complex non-Newtonian flow characteristics. Most studies in this vein have employed either homogenous shear flow, or processing flows such as fiber spinning which are complicated by inhomogenous deformation histories and/or nonisothermal operation. Here we present the design and implementation of a new apparatus for in situ x-ray scattering studies of polymer melts during homogenous uniaxial extensional flow. The experiment is based on the commercially-available SER extensional flow fixture, which employs two counter- rotating drums to deform a sample strip of polymer melt. This fixture has been incorporated into a custom-fabricated convection oven designed to facilitate x-ray access to the sample, and operation in a typical synchrotron beam line environment. Preliminary data on extensional flow induced orientation of ordered block copolymers will be used to illustrate the capabilities of this device.

C1.00085 Differential dynamic optical microscopy for the characterization of soft matter: liquid crystal dynamics, volume phase transition of hydrogels, and phase transition of binary mixtures , BEOM-JIN YOON, JUNG OK PARK, MOHAN SRINIVASARAO, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332, MICHAEL H. SMITH, L. ANDREW LYON, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA, 30332 — The structure and dynamics of soft matter were studied by differential dynamic optical microscopy. One can retrieve q-space information through image processing and Fourier analysis, even when the feature sizes in real space image are too small to be resolved or even visible in an optical microscope. The temporal sequence of real space images were Fourier transformed, and analyzed for the temporal and spatial fluctuations of power spectrum. Here, we present the results on liquid crystal dynamics and their elastic properties, volume phase transition of hydrogels when their dimensions are sub-micron, and critical opalescence of binary mixtures (water/2,6-lutidine).

C1.00086 Fast Off-Lattice Monte Carlo Simulations with Soft Potentials , JING ZONG, DELIAN YANG, Colorado State University, YUHUA YIN, Nankai University, XINGHUA ZHANG, QIANG (DAVID) WANG, Colorado State University — Fast off-lattice Monte Carlo simulations with soft repulsive potentials that allow particle overlapping give orders of magnitude faster/better sampling of the configurational space than conventional molecular simulations with hard-core repulsions (such as the hard-sphere or Lennard-Jones repulsion).[1] Here we present our fast off-lattice Monte Carlo simulations ranging from small-molecule soft spheres and liquid crystals to polymeric systems including homopolymers and rod-coil diblock copolymers. The simulation results are compared with various theories based on the same Hamiltonian as in the simulations (thus without any parameter-fitting) to quantitatively reveal the consequences of approximations in these theories.

[1] *Q. Wang and Y. Yin*, **J. Chem. Phys., 130**, 104903 (2009).

C1.00087 Kinetic Control for the Morphological Transition of Block Copolymer Micelle Complexes , MISOOK LEE, JINKEE HONG, KOOKHEON CHAR, Seoul National University — The morphology of charged block copolymer micelle complexes, consisting of crew-cut poly(styrene-b-acrylic acid) (PS-b-PAA) and poly(styrene-b-4vinyl pyridine) (PS-b-P4VP) micelles, was controlled by pH of aqueous solvent. The charge densities of corona block segments (PAA and P4VP blocks) dispersed in water were sensitive functions of solution pH. The high pH region (pH $>$ 5.5) is particularly interesting in the present case due to the formation of spherical micelle clusters since the degree of ionization of P4VP blocks is negligible while PAA blocks are fully charged in this regime. These spherical clusters were then slowly transformed into different morphologies when the solution pH was adjusted to the range allowing both of the corona blocks to be oppositely charged. The morphological transitions of micelle blends were also monitored by varying experimental parameters such as blending ratio, blending sequence, and the content of co-solvent when coupled with the effect of solution pH. The present study demonstrates that the kinetic pathway for the formation and transformation of micelle complexes at various solution pH is significantly important for the morphological evolution involving charged micelles.

C1.00088 Multigeometry micelles made from self-assembly of block copolymer mixtures via kinetic control , JIAHUA ZHU, University of Delaware, SHIYI ZHANG, YUN LIN, KE ZHANG, Texas A&M University, CAROLINE MIESCH, TODD EMRICK, University of Massachusetts-Amherst, KAREN WOOLEY, Texas A&M University, DARRIN POCHAN, University of Delaware — Multicompartment/multigeometry micellar structures, due to segregation of unlike hydrophobic domains trapped within the same micelle core, have been produced via self-assembly of block copolymer mixtures in tetrahydrofuran/water solution. The mixture is composed of two/or more block copolymers with distinctive hydrophobic blocks but the same poly(acrylic acid) (PAA) hydrophilic block. By taking advantage of the complexation in the hydrophilic corona between the acid side chains of the PAA block and added organoamine molecules, unlike hydrophobic blocks are trapped in the same micelle core and, consequently, locally segregate into compartments. Through designed kinetic pathways, block copolymer design and mixing ratios, both micelle compartment size and shape could be controlled to form multicompartment spheres, sphere-cylinder hybrid micelles and multicompartment cylinders. New mixtures using PAA-containing block copolymers with additional hydrophilic blocks or end-group functionalization produce multigeometry/multicompartment micelles with patterned surfaces in addition to multicompartment cores.

C1.00089 Nanocomposites Consisting of Nanoparticles with Multidentate PS Brushes Mixed with PS Matrices , HYEMIN LEE, SANGHYUK WOOH, JAEHOON LIM, Seoul National University, MATTHIAS ZORN, RUDOLF ZENTEL, Johannes Gutenberg University of Mainz, KOOKHEON CHAR, Seoul National University — In order to prevent massive phase separation of nanoparticles (NP) in a polymer matrix, the relevant hybridization of NPs with polymer matrices has proven to be an effective method for the high performance of nanocomposites in applications. The surface of inorganic (gold or QD) NPs of various size was modified with polystyrene (PS) polymer brushes, poly(styrene)-block-poly(cysteamine methyl disulfide), by the ligand exchange procedure. The disulfide groups in the PS brushes act as anchoring blocks for NPs. Different PS brushes were prepared with different total molecular weights and mole fractions of disulfide moieties. Compared with NPs dispersed in PS without disulfide anchoring groups, NPs anchored with PS brushes through disulfide groups were uniformly distributed within PS matrices. The dispersion of NPs within a polymer matrix was found to be influenced by the total molecular weight of PS brushes as well as the number of anchoring disulfide groups. Furthermore, the effect of the ratio between relative size of NP and the radius of gyration of a polymer brush as well as the grafting density of PS brushes anchored onto NPs on the NP distribution within a polymer matrix is discussed.

C1.00090 Controlling the Self-Assembly of Inorganic Nanoparticles within Conjugated Rod-Coil Block Copolymers , BRYAN MCCULLOCH, RACHEL SEGALMAN, University of California - Berkeley — Blends of conjugated polymers and inorganic nanoparticles have been investigated for numerous applications however optimization relies on precise control over the nanoscale morphology. We have designed a conjugated rod-coil block copolymer consisting of poly(3-(2'-ethyl)hexylthiophene)-b-poly(2-vinyl pyridine) (P3EHT-b-P2VP) which self assembles into controllable morphologies. Inorganic nanoparticles reside within the P2VP domain due to the favorable interactions between P2VP and the nanoparticle surface as well as the exclusionary effects of the liquid crystalline P3EHT. The nanoparticle location can be tuned by altering nanocrystal surface chemistry. These findings are used to develop a comprehensive understanding of the self assembly processes in conjugated rod-coil block copolymer nanocomposites.

C1.00091 Experimental and computational studies of finite-size effects in nanocomposites , M.P. ROMAN, Dept. of Physics, NC State University, Raleigh, NC 27695, E.W. SKAU, D.R. STEVENS, L.N. DOWNEN, T.J. HOFFMAN, L.I. CLARKE — Polymeric nanocomposites are formed when a nanometer-sized particle is embedded within a supporting matrix. Such composites can also be nanostructured - that is, shaped so that characteristic sample length scales may be similar to at least one dimension of the embedded particle [1]. This is particularly true for long aspect-ratio particles such as nanotubes where the length of the particle can approach or exceed the thickness of a thin nanocomposite film or a nanofiber diameter. In these cases, the formation of a particle network (for instance, for mechanical or electrical conductivity enhancement) is affected. We present experimental electrical conductivity and 3-D continuum Monte-Carlo simulation results on such finite-sized percolation effects, which can occur whenever any dimension of the sample is less than ca. 10 times the longest dimension of the particle.

[1] D. R. Stevens, L. N. Downen, and L. I. Clarke, *Phys. Rev. B* **78**, 235425 (2008).

C1.00092 Nanoparticle Surface Functionalization for Improved Dispersion in Network Composites , ADAM RICHARDSON, OLIVIA MCNAIR, GREGORY STRANGE, MARK EARLY, DANIEL SAVIN, School of Polymers and High Performance Materials, University of Southern Mississippi — Incorporation of inorganic nanoparticles into crosslinked networks has resulted in greater toughening behavior with lower filler content compared to traditional composites. The characteristics that provide these desirable qualities are also responsible for their poor dispersion and, consequently, limiting wide commercial use. This work aims to demonstrate how excellent dispersion can be obtained easily and efficiently in different networks through nanoparticle surface modification. Both epoxy/Jeffamine and thiol-ene based networks were examined with differing molecular weight and chemical functionality tethers. The aggregation behavior of nanocomposite samples were monitored optically and using TEM. Thermomechanical properties were studied using DSC, DMA and MTS. The Tg was dependent on both nanoparticle incorporation and functionality. Toughening was observed in some, but not all, cases.

C1.00093 Effect of Metal-Dielectric Interface on Capacitor Functions of Ag-Polymer Nanocomposites at Low Frequency (< 1 MHz) , ATAUR CHOWDHURY, University of Alaska Fairbanks, ABHIJIT BISWAS, University of Notre Dame, ILKER BAYER, Italian Institute of Technology — Metal-dielectric interfaces greatly influence the capacitor functions of nanodielectric composites. Nanodielectric composites of silver in PMMA were fabricated by electron-beam-assisted vapor phase codeposition at ambient temperature ($\sim 35^\circ$ C) in high vacuum. The fabricated samples containing 15- 65% silver reveal unique interfacial structure as studied by X-ray and atomic force microscopy. The capacitance of the as prepared samples were measured with an Agilent LCR meter at frequencies ranging from 20 Hz to 1 MHz. All nanodielectric composites show similar capacitor characteristic with a capacitor density of about 2.0 nF at 20 Hz to about 0.2 nF at 1 MHz., revealing continuous decrease in capacitor density with increasing frequency. This continuous decrease is a direct result of the interface between the silver granules and the dielectric material. This behavior, however, is in clear contrast with our recent study of BTO-PMMA nanocomposites (A. Biswas, et al., NNL, Vol. 1, 111-118, 2009), which show a stable capacitor function over a wide frequency range (20-80 MHz).

C1.00094 A Robust Model for Predicting Charge Mobility in a Random CNT Composite Sample , JOSHUA BROWN, Louisiana Tech University, PEDRO DEROSA, Louisiana Tech University/Grambling State University — Experimental results have shown that Carbon Nanotube (CNT) concentrations have significant impact on the conductivities of CNT polymer composites. Two charge transport mechanisms have previously been observed in these composites: covalent hopping and tunneling. Using these mechanisms as a foundation a robust Monte Carlo simulation has been realized. The simulation first creates a CNT composite sample under different initial conditions such as concentration, tortuosity and length. The charge mobility of the sample is then predicted under an applied electric field for CNT concentrations below and above the percolation threshold.

C1.00095 Effect of Single-Walled Carbon Nanotubes on Glass Transition Behavior in Polystyrene , BRIAN GRADY, University of Oklahoma, WARREN FORD, ABHIJIT PAUL, Oklahoma State University — Our group previously investigated (Macromolecules, 2009, 42, 6152) the effect of nanotube addition on the glass transition temperature (Tg) and the heat capacity change at the glass transition (Delta Cp). Tg increased with nanotube addition by $\sim 7^\circ$C at 1 wt% added nanotubes, while the delta Cp had the same qualitative behavior, but with a $\sim$20% decrease instead of an increase. We have extended this work to polymer grafted-to nanotubes, with polystyrene molecular weights of 2800, 15,000 and 50,000 g/mol; the weight fractions of grafted chains were approximately the same. For the two higher grafting densities, Tg showed the same qualitative behavior but quantitatively the increase in Tg was closer to 9°C. Composites with 50 K grafted nanotubes were statistically identical in terms of the Tg and Delta Cp, although the latter at high nanotube concentrations (20 wt%) did show some anomalous behavior. The decrease in Delta Cp for composites made with the nanotubes having the highest grafting density was linear with added grafted nanotubes to a maximum of a $\sim$35% decrease. Delta Cp for the materials made with 15 K grafted nanotubes showed either a small decrease, or no change in Delta Cp.

C1.00096 Deformation and fracture of Coarse-grained Model of Filled Rubber Composites , KATSUMI HAGITA, National Defense Academy, HIROSHI MORITA, AIST, MASAO DOI, University of Tokyo, HIROSHI TAKANO, Keio University — We presented a result of coarse-grained Molecular Dynamics simulation of filled polymer melts with Sulfur-crosslink under deformation based on the Kremer-Grest Model. Under uni-axial deformation (extension) by setting Poisson's ratio to less than 0.5, facture of this polymer nanocomoposites occurs due to volume increase for increasing the strain. In order to study facture behavior, we use the original Lennard Jones potential formula (with attractive part) as interaction between polymers. The size of simulation box under periodic boundary conditions (PBC) is set to about 133nm. We put 2048 fillers, 5120 polymer chains of 1024 particles, and many crosslink into the PBC box. Due to the crosslink, all polymer chains are connected to one network gel. One filler consists of 320 particles of the C320 fullerene structure. A repulsive force from the center of the filler is applied to the particles of C320 in order to make a sphere whose diameter is about 7nm. We can observe the fracture occurs due to void created near surface of fillers for the case that interaction between polymer and filler is relatively non- attractive. Various cases of Poisson's ratio and interaction between polymer and filler are examined.

C1.00097 SEMICONDUCTORS —

C1.00098 Photocatalytic Activity of TiO_2 Thin Films Obtained by the Sputtering RF in Wastewater

, JAIRO ARMANDO CARDONA BEDOYA, WILMER ASMED SANCHEZ VELANDIA, MIGUEL IBAN DELGADO ROSERO, ALEX ENRIQUE FLORIDO CUELLAR, Universidad del Tolima, Facultad de Ciencias, Depto. de Física, ORLANDO ZELAYA ANGEL, JULIO G. MENDOZA ALVAREZ, Centro de Investigación y de Estudios Avanzados, IPN, Depto. de Física — The photocatalytic activity of TiO_2 thin films in wastewater, under an UV irradiation, is studied. The films were prepared on corning glass substrates by the sputtering RF technique. We present evidence on the photocatalytic degradation, carried out by advanced oxidation processes (AOPs) in domestic wastewater pretreated with UASB (upflow anaerobic sludge blanket) reactors. TiO_2 films were illuminated with ultraviolet light during a time of 4 hours ($\lambda \cong 264$ nm). We could see the effect of degraded operation in the absorbance measurement using UV-VIS spectrophotometry. The results show an increased rate of degradation of the wastewater by 30% compared to the values reflected biologically treated wastewater by anaerobic reactors.

C1.00099 Afterglow Study of ZnS:Cu,Co Water-soluble Nanoparticles and Potential Applications

, LUN MA, WEI CHEN — ZnS:Cu,Co water-soluble afterglow particles with average size of 4 nm have been prepared by using simple wet chemistry method. The X-ray diffraction pattern of the nanoparticles shows a cubic zinc blende structure as the synthesis temperature is low comparing with solid state reactions. The nanoparticles have two photoluminescence emission peaks. The blue emission is from sulfur defects (vacancies), while the green emission is from Cu^{2+} luminescent center which also contributes to the particle's afterglow. The presence of co-dopant Co^{2+} is critical to perform the afterglow of these nanoparticles. The afterglow intensity and decay vary on different $Cu^{2+}$and Co^{2+} doping levels. Further conjugation of ZnS:Cu,Co nanoparticles and photosensitizers presents a new method for deep cancer treatment in photodynamic therapy. The successful afterglow observation from water-soluble nanoparticles may find many new applications in biological imaging, detection and treatment.

C1.00100 Characterization of GaN grown on tilt-cut γ-$LiAlO_2$ by molecular beam epitaxy

, WEN-YUAN PANG, IKAI LO, YU-CHI HSU, CHENG-HUNG SHIH, CHIA-HO HSIEH, Department of Physics, National Sun Yat-Sen University, Kaohsiung, Taiwan, MING-CHI CHOU, Department of Materials and Optoelectronic Science, National Sun Yat-Sen University, Kaohsiung, Taiwan — The non-polar GaN film is a potential candidate for high-efficient optoelectronic devices. This study reports on the characterization of GaN grown on tilt-cut γ-$LiAlO_2$ by plasma-assisted molecular beam epitaxy. The (100) γ-$LiAlO_2$ substrate was tilt-cut about the angle of 11 degree to in-plane. It was found that the GaN thin film tilts to match the atoms of (100) γ-$LiAlO_2$. The basal plan stacking fault and the interface between substrate and thin film have been investigated by transmission electron microscopy. In addition, the characteristics of GaN films for different growth temperatures were studied by X-ray diffraction, scanning electron microscopy, and photoluminescence measurements. From the full width at half maximum of X-ray rocking curve, we found that the quality of GaN film can be improved by tuning the growth temperature. The crystal structure, film surface, and optical properties of the samples will be discussed, as well.

C1.00101 Characterization of M-plane GaN film grown on β-$LiGaO_2$ (100) by plasma-assisted molecular beam epitaxy

, CHIA-HSUAN HU, IKAI LO, CHENG-HUNG SHIH, WEN-YUAN PANG, YING-CHIEH WANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung, Taiwan, MITCH M.C. CHOU, Department of Materials and Optoelectronic Science, National Sun Yat-Sen University, Kaohsiung, Taiwan — Lithium gallate ($LiGaO_2$) has an orthorhombic crystal structure that can be described as a wurtzite-like structure. The **M**-plane basis of GaN wurtzite structure is nearly matched to the selected lattice axes of pseudo-hexagonal $LiGaO_2$. **M**-plane GaN thin films have been grown on β-$LiGaO_2$ (100) substrates by plasma-assisted molecular-beam epitaxy in our group. Pure **M**-plane GaN crystal films have been verified by the measurements of x-ray diffraction, micro-Raman scattering, polarization-dependent photoluminescence and atomic force microscopy. The measurements of x-ray diffraction and micro-Raman scattering exhibited the evidences of large compressive stress on the **M**-plane GaN thin films. Based on experimental results, we showed that the large compressive stress is the major source leading to the peeling of **M**-plane GaN thin film off substrate after thermal recycles.

C1.00102 Effect of substrate induced strains on the magnetic and ferroelectric properties of epitaxial bilayer thin films of lead zirconate titanate and cobalt ferrite[1]

, DEVAJYOTI MUKHERJEE, TARA DHAKAL, ROBERT HYDE, PRITISH MUKHERJEE, HARIHARAN SRIKANTH, SARATH WITANACHCHI, University of South Florida — Epitaxial bilayer thin films of cobalt ferrite (CFO) and lead zirconium titanate (PZT) were deposited on MgO (100) and $SrTiO_3$ (STO) (100) substrates by pulsed laser deposition. The structural properties were characterized using X-ray diffraction and atomic force microscopy. The magnetic properties were measured at 10 K and 300 K in both parallel and perpendicular magnetic fields. The CFO-PZT bilayers showed enhanced or reduced magnetization compared to the single layer CFO films depending on the substrate of deposition. The ferroelectric properties of the CFO-PZT bilayers showed enhanced polarization compared to PZT single layer films on both types of substrates. A strain compression-relaxation mechanism was proposed in order to explain the structure-property relationships in the CFO-PZT bilayers.

[1]This work was supported by NSF (Grant Nos. DMI-0217939 and DMI-0078917) and DOD (Grant No. W81XWH-07-1-0708).

C1.00103 Photochemical synthesis of porous silicon thin films[1]

, OLIVIA SKEEN, TONI SAUNCY, Angelo State University — Porous silicon thin films were produced by photochemical synthesis with a solution of hydrofluoric acid (HF) and the oxidizer cobalt nitrate ($Co[NO_3]_2$). An 11mW HeNe laser was used during synthesis to produce the local electric field necessary for the formation of the porous matrix on the surface of the crystalline silicon substrate. Substrates used were n-type (Antimony), and p-type (Boron). Samples prepared with variations in process time from 15 minutes to 5 hours were examined using photoluminescence, SEM and Raman spectroscopy. Results indicate that the presence of the oxidizer during synthesis enhances the intensity and persistence of p-Si photoluminescence when compared with samples prepared using only HF. In addition, post process analysis reveals that the porous layer on the samples is present only on samples processed for less than 4 hours.

[1]Angelo State Research Enhancement

C1.00104 Bipolar resistive switching in $Ba_{0.5}S_{r0.5}Co_{0.2}Fe_{0.8}O_3$ thin films

, ZHONGWEN XING, Dept. of Materials Science and Engineering, Nanjing University, NAIJUAN WU, ALEX IGNATIEV, Center for Advanced Materials and Department of Physics, University of Houston — Five-component perovskite Ba0.5Sr0.5Co0.2Fe0.8O3 (BSCFO) thin films are reported to have polarized electrical-pulse-induced resistance (EPIR) change at room temperature. Such an EPIR change is attributed to a combined effect of the resistance change of the Schottky barrier and the oxygen ion/vacancy movement near the interface. In the BSCFO, the lower threshold voltage of the electric pulse that leads to nonvolatile resistive changes is close related to its higher oxygen permeability.

C1.00105 Effect of spin-orbit interaction on the ballistic transport properties of nanowires

, SHEEHAN AHMED, RYAN BRENNAN, Fordham University, GODFREY GUMBS, Hunter College, CUNY, ANTONIOS BALASSIS, Fordham University, DANHONG HUANG, Air Force Research Laboratory, Kirtland Air Force Base — We calculated the effects of spin-orbit interaction (SOI) on the energy bands, ballistic conductance (G) and the electron-diffusion thermoelectric power ($S_{\rm d}$) of a nanowire by varying the temperature, electron density and width of the wire. We used the effective mass approximation in a model for the quasi-1D electron system that includes a Rashba potential lateral confinement of the 2DEG and a quasi-square potential well confinement transverse to the 2DEG. Both terms (α and β) give rise to SOI coupling which affects significantly the band structure obtained from numerical solutions of a pair of coupled equations. Comparing our model with the already published work where harmonic confinement was employed to describe the transverse confinement, we found that the energy bands are different and, in addition to crossing effect of the transverse energy bands, there is also anticrossing for specific values of the wavevector k_y along the wire. The β-term of the Hamiltonian causes a displacement and a deformation of the transverse energy band structure which is more pronounced for large values of the wave vector.

C1.00106 Investigation of first principle thermoelectric properties of compound semiconductor

, CEM SEVIK, ALPER KINACI, TAHIR CAGIN, Artie McFerrin Dept of Chemical Engineering, Laboratory of Computational Engineering of Nanomaterials Texas A&M University, College Station, TX, TEXAS A&M UNIVERSITY TEAM — We analyze relevant electronic and transport properties of several different compound semiconductors, Cu_2ZnSnX_4, (X = S, Se, Te), $Cu_2CdSnSe_4$, and Cu_3SbM_3, (M = Se, S) to assess their potential as thermoelectric materials. Using density functional theory and Boltzmann transport equations, we determine Seebeck coefficients, conductivities, and power factors for each compound. To assess their potential application as thermoelectrics, we calculated a simple measure: "maximum" thermoelectric figure of merit, ZT_{max} at experimentally amenable doping levels. We compared this with results for other well known bulk thermoelectrics (Bi_2Te_3 and $SrTiO_3$). However, our calculations indicate that it is not possible to reach ZT values higher than 1, so that these materials to be competitive with other materials for power generation and refrigeration applications.

C1.00107 Transport Anisotropy of Epitaxial VO_2 films grown on (100) TiO_2

, SALINPORN KITTIWATANAKUL, Department of Physics, University of Virginia, JIWEI LU, Department of Materials Science and Enginieering, University of Virginia, STUART WOLF, Department of Physics, University of Virginia — Vanadium dioxide (VO_2) exhibits a metal semiconductor transition (MST) at 340 K. This transition is accompanied by the abrupt change in the electrical conductivity, optical transmittance and reflectance in infrared region, which can be used in the electronic devices such as temperature sensors and electric switches. In this study, Reactive Bias Target Ion Beam Deposition was used for epitaxial VO_2 thin film growth on TiO_2 (100) substrates. The out-of-plane and the in-plane XRD scans have been performed to confirm the single phase VO_2 and the epitaxial relationship between the film and the substrate. The hall bars along the in-plane c-axis and b-axis of R-VO_2 were fabricated via the photolithographic process. It is found that the maximum conductivity was parallel to c-axis, while the minimum conductivity was parallel to b-axis. The conductivity anisotropy persisted through the metal semiconductor transition. The conductivity anisotropy ratio σ_c/σ_b was found to be $\sim$16.2 at 300 K, much larger than that of single crystal VO_2. The temperature dependent anisotropy of the carrier concentration and the mobility is to be discussed.

C1.00108 Transport Characteristics of Amorphous Borocarbides: A Variable Range Hopping Treatment

, NASEER DARI, DONALD PRIOUR, JR, University of Missouri, Kansas City — We calculate the temperature dependent conductivity of amorphous borocarbide materials within a variable range hopping framework. We study the impact of disorder on borocarbide transport characteristics by beginning with a regular rombahedral lattice of periodically placed icosahedral arrangements of boron and carbon atomic species. A self consistent numerical procedure is used to calculate the charge occupancy factors. Three dimensional lattices containing several hundred icosahedral clusters are considered; disorder is introduced in the form of random translational displacements of the icosahedral cages. In addition, we use stochastic rotations about three independent randomly selected axes to implement orientational disorder for each of the icosahedral clusters. We find the sensitivity to random lateral displacements of the boron-carbon icosahedra to be on the order of 5%, whereas the effects of even appreciable orientational disorder appears to be negligible within the assumptions of our model. In sum, we find temperature and the density of icosahedral clusters to have the strongest effect on the conductivity, while the transport characteristics are largely robust with respect to the introduction of disorder.

C1.00109 Temperature dependent adsorption and dissociation of water molecules on the Si(001)-(2×1) surface

, JA-YONG KOO, Korea Research Institute of Standards and Science, YONG-SUNG KIM, HANCHUL KIM, SANG-YONG YU — The dissociative adsorption of water molecules on the Si(001)- (2×1) surface was studied up to 850 K by scanning tunneling microscopy (STM). A water molecule is dissociated into on-dimer (OD) and inter-dimer (ID) configurations and the population ratio n_{ID}/n_{OD} changes from $\sim$5 at room temperature to $\sim$0.5 above 500 K. A quantitative analysis was made by considering the flipping motion of Si dimers to overcome the discrepancy between the experiment and theoretical estimations from the model of simple energy barrier. The flipping motion of Si dimers plays a dominant role in the dissociation of water molecules on the Si (001)-(2×1) surface.

C1.00110 Asymmetric Double Quantum Dot Energy States in a Quantizing Magnetic Field

, NORMAN HORING, SPENCER HORTON, SINA BAHRAMI, Stevens Inst. Tech. — This work is concerned with electron states and propagation in a two-dimensional asymmetric quantum double-dot system embedded in a two dimensional host sheet subject to Landau quantization. The two dots are represented by two Dirac delta function potential terms of differing depths each of which would support just one subband state if the other were absent, if there were no magnetic field. The integral equation for the Schrodinger Green's function for this double-dot system is solved exactly in closed form in terms of the infinite sheet Green's function for two dimensional electrons subject to Landau quantization with no quantum dots. The dispersion relation for the double dot subband energies is formulated and examined by analyzing the frequency poles of the Green's function with Landau-quantization-like splintering of the levels by the magnetic field. The effects of the asymmetry in regard to the potential well depths are analyzed as functions of the well-depth difference and dot-separation.

C1.00111 Core level XAS study on high pressure solids

, MIN WU, JIANZHONG JIANG, Zhejiang University, JOHN TSE[1], University of Saskatchewan — We investigated the K and L-edge core level X-ray absorption spectra of solid CO2 and Silica (SiO2) under high pressure, using methods based on pseudopotentials and all-electron Bethe-Salpeter Equation. A comparison of the calculated spectra with both methods is present. We found that the calculated Si K and L-edge spectra of quartz and stishovite are in good agreement with experiment. Particularly, the origin of the second peak in the O K-XAS observed in compressed silica which is often used as an indication of six-fold coordinate is explained. Preliminary calculations show both the full core hole and no core hole approximations failed to reproduce quantitatively the observed C and O K-edge XAS.

[1]corresponding author

C1.00112 An Ab Initio Study of Hydrogenation induced Metallization of SiC001 (3x2)

, JAMES WESTOVER, ABDELKADER KARA, University of Central Florida — We will present results for the band structure of hydrogenated Silicone Carbide (001) (3x2) surface with various levels of hydrogenation. These band structures were obtained using density functional theory with a generalized gradient exchange correlation function. Further, the calculations reveal the following scenario. Initially, Hydrogen atoms saturate all the dangling bonds of the surface dimers. This in turns allows for the subsequent H atoms to bind with Si atoms in the second layer. Those new bonds for the appropriately hydrogenated surface cause a "metallization" of the surface. Hydrogenation beyond that brings the system to its semiconducting state.

C1.00114 Electron affinities of d1 transition metal chloride clusters and onset of super halogen behavior

, SWAYAMPRABHA BEHERA, JORLY JOSEPH, PURUSOTTAM JENA, VCU — Geometry, electronic structure, and electron affinity of d1 transition metal chloride clusters (MCl_n, M = Sc,Y, La; n = 1–5) have been calculated using density functional theory. Chlorine atoms are chemically bound in all cases except for MCl_5. The electron affinities of MCl_n (n = 1–3) are small and increase only marginally as a function of n until the valence of the metal atom is consumed. Beyond this, they rise sharply and reach a value of 5.96, 6.03 and 5.90 eV for $ScCl_4$, YCl_4 and $LaCl_4$, respectively and remain high for n = 5. MCl_n, (n = 4,5) clusters, therefore, behave as superhalogens. Results are compared with available experimental data

C1.00115 Calculation of the Electronic Structure for the AlGaAs Quantum Well

, CHIN-SHENG WU, Yuan Ze University — Quantum wells are important in semiconductor lasers because they allow some degree of freedom in the design of the emitted wavelength through adjustment of the energy levels. We apply the various the well width w and barrier height V in order to match the device information made by Willander. Solving the Schrödinger equation with exchange- correlation energy and effective mass of electrons for a finite potential will produce values of the energy levels within the well. Alternating GaAs-AlGaAs layers produce high and low energy gaps. The result is the generation of quantum wells. The electrons in the donor section AlGaAs diffuse into the low band gap GaAs section, where is free of impurity atoms, therefore the effective mass of electrons reduces and the mobility increases. Dispersion relations in conduction band and valence band are applied for the effective mass approximation. Because of the presence of quantum wells the electrons have discrete energies and these appear as peak in the absorption measurements.

C1.00116 Carrier cooling and Auger heating in Si doped InN thin films

, Y.-G. ZENG, D. -J. JANG, C.-F. TZEN, Department of Physics, National Sun Yat-sen University, M.-E. LEE, Department of Physics, National Kaohsiung Normal University, L.-W. TU, Department of Physics, National Sun Yat-sen University — Silicon doped InN thin films grown on sapphire substrates by plasma-assisted molecular beam epitaxy have been studied using time-resolved photoluminescence (TRPL) upconversion technique. The back ground carrier densities vary from 6.2×10^{18} to 1.27×10^{20} cm^{-3}. The carrier temperature curves, derived from the TRPL at different time delay, indicate that the hot carriers lost most of their excess energy within the first 10 ps after photoexcitaiton. For low doping densities, the carrier cooling curves can be explained by carriers releasing excessive energy through the carrier–LO-phonon interaction. The extracted effective phonon emission times decreased as the photoexcited carrier concentration reduced. The radiative and nonradiative decay rates were obtained with the TRPL signals and the nonlinear dependence of the PL intensity on the carrier concentration. The derived radiative recombination rates were consistent with the theoretical predications. The Auger recombination was found to increase with the doping concentration. The reduced carrier cooling rates for large doping densities can be accounted for by the Auger heating occurred during carrier relaxation.

C1.00117 Radiative and nonradiative recombination rates of Si:InN thin films

, S.-F. WANG, D. -J. JANG, C.-F. TZEN, Department of Physics, National Sun Yat-sen University, M.-E. LEE, Department of Physics, National Kaohsiung Normal University, L.-W. TU, Department of Physics, National Sun Yat-sen University — Silicon doped InN thin films with background carrier densities vary from 6.2×10^{18} to 1.27×10^{20} cm^{-3} were investigated by time-resolved photoluminescence (TRPL) upconversion technique. The radiative and nonradiative decay rates as a function of carrier density were derived from the TRPL signals. The Shockley-Read-Hall, radiative recombination, and Auger recombination coefficients were obtained by fitting the derived decay rates with the rate equation. The defect density can be determined from the differences of doped and undoped carrier densities. We found that the SRH coefficient is proportional to the defect density. The capture cross sections, determined from the SRH coefficient, defect density, and thermal velocity, were $1.5\sim3.0\times10^{16}$ $cm.^2$ The radiative decay times determined from the rate equation were compared with those determined by a model developed by Gourdan and Lavallard, which is recently used to determine radiative lifetimes of InN by several reports. We found the discrepancy of radiative lifetimes determined by these two approaches is attributed to the large nonradiative recombination rates in these samples.

C1.00118 Differential reflectance study of InN

, M.-S. WANG, D. -J. JANG, Department of Physics, National Sun Yat-sen University, M.-E LEE, Department of Physics, National Kaohsiung Normal University, L.-W TU, Department of Physics, National Sun Yat-sen University — Time-resolved differential reflectance (TRDR) of Si:InN thin films grown on sapphire substrates by plasma-assisted molecular beam epitaxy were investigated. The background carrier densities of $4.4\times10^{18}\sim1.27\times10^{20}$ cm^{-3} were measured by van der Pauw Hall geometry for undoped and Si doped InN thin films. The energy of the degenerated pump and probe beams were tuned from 1.37 to 1.65 eV. All the signals were measured at room temperature. The intensity and the temporal position of the TRDR peak intensity increase with the pumping intensity and show trivial dependence on photoexcitation energy. The TRDR intensity exhibits single-exponentially decay for photogenerated carrier density up to 6×10^{18} cm^{-3}. For higher excited carrier density, two decay times must be employed to describe the decay behavior. The rate equation includes the Shockley-Read-Hall, radiative, and Auger recombination were used to fit the decay rate. While the Auger recombination is insignificant for low photoexcitation, it becomes the dominated recombination mechanism within 10 ps for high photoexcitaiton. The dominated recombination mechanism for different pumping energy will be discussed.

C1.00119 Precision Bandgap Control of Titanium Dioxide Nanoparticles by Ultrasonication

, ROBBY FLAIG[1], LESTER LAMPERT, JORGE CAMACHO, JAMES HAMILTON, University of Wisconsin-Platteville — TiO2 is a commonly used material in many areas of industry including photocatalysis and pigments. Band gap narrowing and particle size are engineered with a high level of control. We report precision bandgap control by ultrasonication in novel stable solvent systems in which unmodified TiO2 can be suspended. The effects of ultrasonication in these unique solvent systems are monitored by optical band gap (UV-Vis), scanning electron microscopy (SEM), atomic force microscopy (AFM), and x-ray diffraction (XRD).

[1]Nanotechnology Center for Collaborative Research & Development

C1.00120 Seung-Nelson representation for singular thin sheets[1]

, THOMAS WITTEN, JIN WANG, University of Chicago — We extend the popular Seung-Nelson model [1] to better study thin elastic sheets with singular or multi-scale structures, which are common phenomena in thin sheets [2]. Because it requires a uniform distribution of lattice points over the simulated sheets, the original model is ill-equipped to study these singular structures. Our extended model retains the essence of the original one, but it allows lattice points to be concentrated as needed in regions of large curvatures. We will compare the two methods by applying them to study the energy of the core region of a developable cone [3].

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[2] T. A. Witten, *Rev. Mod. Phys.* **79**, 643 (2007).
[3] E. Cerda, S. Chaieb, F. Melo, and L. Mahadevan, *Nature* **401**, 46 (1999).

[1]Supported by NSF award DMR 0820054.

C1.00121 Hamiltonian monodromy , CHEN CHEN, JOHN DELOS, MEGAN IVORY, SETH AUBIN, College of William and Mary — We say that a system exhibits monodromy if we take the system around a closed loop in its spectrum space, and we find that the system does not come back to its original state. We report a method for experimental realization of a newly discovered dynamical manifestation of monodromy by investigating the behavior of atoms in a trap. The trapping potential has long range attraction to and short range repulsion from the center. Calculations include two parts. First we consider atoms as classical particles for which we can choose any desired set of initial conditions. As was shown previously for different systems, when we take the system around a monodromy circuit, a loop of initial conditions evolves into a topologically different loop. Second, we incorporate the limitations that would appear in experimental implementation. The atoms have a range of initial angles, initial angular momenta, and initial energies. Our work shows how real atoms can be driven by real forces around a monodromy circuit, and thereby shows how one can observe dynamical monodromy in a laboratory. Finally, we extend classical dynamical monodromy to quantum dynamical monodromy by examining wave function evolution under comparable conditions.

C1.00122 The complete interpretation of the fractions in quantum Hall effect , KESHAV SHRIVASTAVA, University of Malaya — We propose that the modified cyclotron energy is given by $(h/2\pi)\omega_c(1/2)g(n+1/2)$ so that the fractional charge is given by the angular momentum with both signs of spin, $j = l \pm$ s. In addition to the (i) principal fractions given by (1/2)g our theory with effective charge e*=(1/2)ge, has (ii) resonances at $\nu_1 - \nu_2$ and (iii) two-particle states at $\nu_1 + \nu_2$ and there are (iv) clusters with spin >1/2, where ν is a filling factor. This theory explains all of the 101 fractions and full graphene series. The fractional charges of graphene [2] are also explained. The series also explains the even denominators for S=0,1,2, . . . , as in electron clusters. The S=0, L=0, corresponds to half filled Landau level. S=1/2, L=0 with negative sign before s in j gives the zero-energy state. All of the predicted fractions agree with the data.

[1] K. N. Shrivastava, AIP Conf. Proc. 1150, 59-67 (2009).
[2] K. I. Bolotin, et al, Nature 462, 196(2009).

C1.00123 Trial Wavefunctions and Ground State Energies of Some Non-Laughlin Correlated Quantum Hall Systems , JOHN QUINN, University of Tennessee — In the lowest Landau level (LL0), incompressible quantum liquid (IQL) states occur at the Laughlin-Jain sequence of filling factors $\nu = n(2pn \pm 1)^{-1}$, where n and p are positive integers. In all of these states, Laughlin correlations (avoidance of pair states with the largest repulsion) are the cause. In the first excited Landau level (LL1), IQL states occur at $\nu' = \nu - 2 = 1/2$. This state and daughter states of Laughlin quasiparticles with $\nu_{QE} = 1/3$ cannot be caused by Laughlin correlations. Paired states described by the Moore-Reed Pfaffian wavefunction and by a novel wavefunction with different pairing correlations are studied as candidate wavefunctions. The energy of each of these states is evaluated analytically for an arbitrary pair pseudopotential $V(L_2)$, where L_2 is the pair angular momentum. Explicit results are derived for a six particle system. The generalization to N particle systems is proposed and compared for both trial functions.

C1.00124 Density functional study of the effects of doping and stoichiometry on gallium diffusion in gallium arsenide , J.T. SCHICK, Villanova Univ., C.G. MORGAN, Wayne State Univ. — Previous experimental [1-4] and theoretical [5,6] work on the properties of diffusion of gallium within gallium arsenide has produced some results that are apparently at odds with each other. We present results of a wide theoretical survey of the point defects that form in this material with special attention paid to the formation and diffusion of excess-gallium-related point defects. In this study we applied density functional theory in the local density approximation [7]. Diffusion was examined through the use of the nudged elastic band method [8]. After considering the accuracy of the approximations used, the calculations yield information compatible with the experimental situation and capable of shedding light on areas of apparent disagreement.

[1] G Bösker *et al.*, Phys. Rev. B **52**, 11927 (1995). [2] G Bösker *et al.*, J. Appl. Phys. **86**, 791 (1999). [3] H Bracht and S Brotzmann, Phys. Rev. B **71**, 115216 (2005). [4] H Bracht *et al.*, Physica B **308-210**, 831 (2001). [5] K Levasseur-Smith and N. Mousseau, J. Appl. Phys. **103**, 113502 (2008). [6] PA Schultz *et al.*, Mod. and Sim. in Mat. Sci. and Engr. **17**, 084007 (2009). [7] G. Kresse and J. Hafner, Phys. Rev. B **47**, 558 (1993); *ibid.* **49**, 14251 (1994). [8] H. Jónsson *et al.*, "Classical and quantum dynamics in condensed phase systems," (World Scientific, 1998) Chap. 16, pp. 385-404.

C1.00125 Investigation of Mg- and Si- doped AlN epilayers by Transmission Electron Microscopy , BO CAI, Department of Physics, Brooklyn College of CUNY, NY 11210, M.L. NAKARMI — Aluminum nitride (AIN) has emerged as a promising deep ultraviolet (UV) material for the development of optoelectronic devices operating in deep UV region. Low dislocation density AIN on sapphire substrate has been achieved by metal organic chemical vapor deposition technique. Doping in AIN is very crucial in order to use it in active devices. Silicon and magnesium are usually used for n- and p- type doping in III-nitride materials. We report on microstructure analysis of Mg- and Si- doped AIN epilayers by transmission electron microscopy (TEM). The samples were grown on low dislocation density AIN/sapphire templates. Cross section and plan view TEM images were taken to characterize the threading dislocations in these samples during the growth process. High resolution TEM images are also taken to study the detailed nature of the dislocations, and their generation and propagation. The TEM images will be compared with the undoped AIN epilayers to investigate the effect of doping in the generation/annihilation of threading dislocations. Implications of our finding for the applications in deep UV optoelectronic devices will be discussed.

C1.00126 Spin transport and spin minibands in a magnetic superlattice: dependence on geometrical and physical parameters[1] , NAMMEE KIM, JINWOO KIM, HEESANG KIM, Soongsil University — We have studied the spin miniband structure and the ballistic spin-polarized transport through a magnetic superlattice, formed by inhomogeneous magnetic field in a semiconductor nanowire. Based on the transfer matrix theory and the Bloch's theorem, we calculate the energy dispersion having spin miniband and minigap due to Bloch periodicity and spin dependent ballistic conductance for various geometrical and physical parameters. It is shown that full spin polarization in the ballistic conductance of the system occurs clearly for each spin, and that the fully spin polarized range for each spin can be enhanced by modulation of geometrical and physical parameters.

[1]This work was supported by the Korea Research Foundation (NRF, grant No. 20100021328).

C1.00127 Magnetocurrent of a multiferroic resonant tunneling diode[1] , NAMMEE KIM, HEESANG KIM, Soongsil University — We study the resonant tunneling magnetoresistance of a multiferroic resonant tunneling diode, which is hybridized of ferroelectric double barriers and a ferromagnetic quantum well. Magneto-current is calculated, focusing on its dependence on ϕ, the angle between an external magnetic field and the spontaneous magnetic field in the diluted magnetic semiconductor quantum well, by using the non-equilibrium Green's function method. The magneto-current varies from zero to 440%, and the spin polarization of the current varies from zero to 1 by changing the angle ϕ. We also perform controlling of the transmission energy level by reversing the direction of dipole polarization in ferroelectric barriers. Therefore, the magneto-current and its current spin polarization through this multiferroic resonant tunneling diode can be manipulated either by the direction of the external magnetic field in the diluted magnetic semiconductor quantum well or by the direction of the dipole polarization in ferroelectric barriers. This study shows the possible application of this structure to a multiferroic spin device to control the amount of current and spin polarization of current through it.

[1]This work was supported by the Korea Research Foundation (NRF, grant No. 20100021328).

C1.00128 Effect of disorder on the Curie temperature of GaMnN and InMnN diluted magnetic semiconductors

, AHMAD ALSAAD, Department of Physical Sciences, Jordan University of Science and Technology, Irbid-Jordan — The critical Curie temperatures of GaN, InN, CrN, and MnN diluted magnetic semiconductors and those of ordered and disordered diluted (Ga,Mn)N and (In,Mn)N magnetic semiconductors are investigated by using the classical Heisenberg model within the mean field approximation with the structural parameters are obtained from first principles total energy calculations. We show that Curie temperature depends on the Mn and Cr concentrations. Our calculations on these systems have shown that above room-temperature can be observed. Ferromagnetic stability in GaN, InN, CrN, and MnN is systematically studied. Our results indicate that 3d Mn and Cr impurities in GaN and InN favor the ferromagnetic state rather than the spin-glass phase. The mechanism behind this behavior is discussed and explained in details.

C1.00129 Spin resolved transverse electron focusing in wide leads due to diffuse collimation in InSb/InAlSb two-dimensional electron gases

, L.F. COHEN, A.M. GILBERTSON, Imperial College, A. KORMÁNYOS, C.J. LAMBERT, Lancaster University, M. FEARN, T. ASHLEY, QinetiQ, S.A. SOLIN, Washington University in St. Louis — Using the transverse electron focusing geometry, we report spin-resolved cyclotron motion in an InSb two-dimensional electron gas (2DEG). A zero field spin spitting[1] causes electrons from different spin subbands to have slightly different cyclotron radii in external field which manifest as a splitting in the first focusing peak.[2] Traditionally in focusing experiments, electrons are emitted and collected via quantum point contacts that host only a few open channels. We show that spin resolved electron focusing is observable in $wide$ leads with many open channels due to diffuse collimation of ballistic electrons emitted into the bulk 2DEG region. The results are compared to a semiclassical model[3] from which a Rashba-type spin-orbit coupling parameter of $\alpha = 5x10^{-11}$ eVm is deduced at 2 K. We compare these results to values determined from the beating of Shubnikov-de Haas oscillations.[4] We also present ballistic transport results extending over 3 μm.
[1]A. M. Gilbertson, et al., Phys. Rev. B 77, 165335 (2008). [2]L. P. Rokhinson, et al., Phys. Rev. Letts. 93, 146601 (2004). [3]A. Kormanyos, Phys. Rev. B 82, 155316 (2010). [4]A. M. Gilbertson, et al., Phys. Rev. B 79, 235333 (2009).

C1.00130 Spin-orbit coupling in InAs-based wurtzite quantum wells[1]

, J.Y. FU, POLIANA H. PENTEADO, J. CARLOS EGUES, University of Sao Paulo — By folding down the 8×8 Kane model, accounting for the s-p_z orbital mixing, we derive an effective Hamiltonian for the conduction electrons. In this derivation, we consider the renormalization of the spinor component of the conduction band wave function. In addition to the Rashba-type term arising from the bulk inversion asymmetry of the wurtzite lattice, we obtain the usual linear in momentum Rashba term induced by the structural inversion asymmetry of the well. We also find a new Rashba-like contribution, proportional to the well profile only and not to its derivative. We self-consistently calculate the spin-orbit coupling parameters for single and double wurtzite InAs-based wells with two subbands. By gating the structures, we find that the new Rashba term shows a distinctive voltage dependence as compared to that of the usual Rashba coupling. Finally, for the double-well case, we find that both the intersubband spin-orbit coupling and the Dresselhaus term for each subband show a resonant behavior for the symmetric configuration of the well.

[1]This work was supported by FAPESP and CNPq. One of the authors (J.Y.F) thanks Gerson J. Ferreira, Marco O. Hachiya and E. Bernardes for valuable discussions.

C1.00131 2D Waveguides as spin devices: spin-orbit and lead effects[1]

, LILIA MEZA-MONTES, Instituto de Fisica BUAP — Straight waveguides with different shapes have been proposed as devices to control the spin polarized transport, with Rahsba spin-orbit interaction as the mechanism to induce spin mixing. Several theoretical approaches have been applied, mostly based on transfer-matrix method. Here, the Schroedinger equation is solved by means of the Finite-Element Method,finding good agreement with previous calculations. It is known that positions of the leads influence the ballistic transport in this sort of cavities due to changes in the spatial symmetry. The role of the lead positions on the transmission and, in turn on the spin polarization, will be discussed for several geometries. The linear Dresselhaus interaction is taken into account to consider zincblende structure. Implications for quantum dots is also addresed.

[1]Partially supported by VIEP-BUAP.

C1.00132 First principles calculations of magnetic properties of Gd-doped ZnSiN[1]

, J. RUFINUS, Science Division, Widener University, Chester, PA 19013 — Diluted metal-doped chalcopyrite compounds have recently attracted a great attention due to some experimental confirmations on their ability to achieve high temperature ferromagnetism. Such a material would likely play a role in building future spintronic devices. First principles calculations of the magnetic properties of Gd-doped $ZnSiN_2$, a semiconductor chalcopyrite, have been performed using the density functional theory within generalized gradient approximation. Our results show, independent of the substitutional sites, the lowest energy structure is ferromagnetic.

[1]Computational time provided by the NSF through Teragrid resources provided by Pittsburgh Supercomputing Center.

C1.00133 Zitterbewegung-induced Spin Resonance in Quantum Wires[1]

, MARCO O. HACHIYA, Instituto de Fisica de Sao Carlos, Universidade de Sao Paulo, 13560-970 Sao Carlos, SP, Brazil, GONZALO USAJ, Instituto Balseiro and Centro Atomico Bariloche, Comision Nacional de Energia Atomica, 8400 San Carlos de Bariloche, Argentina, J. CARLOS EGUES, Instituto de Fisica de Sao Carlos, Universidade de Sao Paulo, 13560-970 Sao Carlos, SP, Brazil — Recently, the *Zitterbewegung* in quantum wires was proposed theoretically by Schliemann *et al.* [1]. This effect is characterized by an oscillatory motion in the position and spin components of an electron wave packet injected along the quantum wire with spin-orbit coupling. We investigate the *Zitterbewegung* evaluating time dependent expectation value for the spin operators. Here we consider the *Zitterbewegung* in a multi-band quantum wire with both the Rashba and Dresselhaus spin-orbit interactions. We find that an external magnetic field perpendicular to the quantum wire can be used to tune the probability of spin flip, i.e., the resonance condition. A possible experimental scenario to observe this effect is proposed using injection via a quantum point contact.

[1] J. Schliemann, D. Loss, and R.M. Westervelt, Phys. Rev. Lett. **94**, 206801 (2005).

[1]This work is supported by the CIAM program (NSERC-CNPq-CONICET) and FAPESP.

C1.00134 Deep level transient spectroscopic study of oxygen-implanted ZnO single crystal[1] , ZIRAN YE, GUANGWEI DING, JINCHENG FAN, CHI CHUNG LING, The University of Hong Kong — ZnO single crystal samples were implanted by oxygen with the energy of 150keV. After the pretreatment of hydrogen peroxide [1], Schottky contacts were fabricated with Au film deposited by thermal evaporation. Deep level defects were studied by deep level transient spectroscopy (DLTS). The activation energy of the 0.29eV deep trap was observed in the as-implanted sample and samples anneal at 350 °C , 650 °C and 750 °C. Three peaks were identified in the DLTS spectra of the 900 °C sample, with the activation energies of 0.11eV, 0.25eV and 0.37eV respectively. The thermal evolutions of the deep levels up to the temperature of 1200 °C were also investigated.

[1] Q. L. Gu, C. C. Ling, X. D. Chen, C. K. Cheng, A. M. C. Ng, C. D. Beling, S. Fung, A. B. Djurišić, L. W. Lu, G. Brauer and H. C. Ong, Appl. Phys. Lett. 90, 122101, (2007).

[1]This work was supported by the RGC HKSAR under the GRF scheme (No. 703108P).

C1.00135 ABSTRACT WITHDRAWN –

C1.00136 Observation of defects in $CuInSe_2$ by 300kV aberration corrected scanning transmission electron microscope , AKANE TAKESHITA, TAKAYUKI TANAKA, Tokyo Institute of Technology, TADAHIRO KUBOTA, Honda R&D Co., Ltd., HIDETO MIYAKE, Mie University, HIDETAKA SAWADA, YUKIHITO KONDO, Japan Electron Optics Laboratory, YOSHIFUMI OSHIMA, Osaka University, YASUMASA TANISHIRO, KUNIO TAKAYANAGI, Tokyo Institute of Technology — Vacancies (V_{Cu}, V_{In}) and substitutional atoms (In_{Cu}, Cu_{In}) in $CuInSe_2$ crystal, which is the key semiconductor material for thin film solar cell applications, were directly observed by 300kV aberration-corrected high angle annular dark field scanning transmission electron microscope (HAADF-STEM). The atomic columns of Cu, In and Se were independently observed from $CuInSe_2$ [100] crystal zone axis by HAADF-STEM. Some In and Cu columns showed reduced and increased intensities from that of column without defect, respectively. On the other hand, no defects in Se columns were observed. The intensity analysis suggests In substitution of Cu site (In_{Cu}) and Cu substitution of In site (Cu_{In}). The concentrations of Cu and In substitutions were evaluated based on comparison with the multi-slice calculation.

C1.00137 LaF3:Ce/CdTe nanocomposites for radiation detection application , MINGZHEN YAO, UT Arlington, PACIFIC NORTHWEST NATIONAL LABORATORY TEAM — Radiation detection demands new scintillators with high quantum efficiency, high energy resolution, and short luminescence lifetimes. Nanocomposites consisting of quantum dots and Ce^{3+} doped nanophosphors may be able to meet these requirements. Here, we report the luminescence enhancement of LaF_3:Ce/CdTe nanocomposites which were synthesized by a wet chemistry method. The results show that CdTe luminescence in LaF_3:Ce/CdTe nanocomposites is enhanced about five times. Energy transfer, light reabsorption, and defect passivation are the likely reasons for the luminescence enhancement

C1.00138 Determination of property in semiconductors , CARLOS FIGUEROA, Depto de IIS Unison, RAÚL RIERA, DIFUS Unison, MARTÍN MOLINAR — In this work it is doing a comparative study of the most conventional semiconductors in electronics, such as silicon (Si), germanium (Ge) and gallium arsenide (GaAs). We present the mathematical development of the magnitude that determines the intrinsic semiconductor property, which is the concentration of charge carriers, and is discussed in each case with respect to temperature variation. On the other hand, in the case of extrinsic semiconductors is calculated potential barrier of a pn junction. The task to make in this work is to use the intrinsic concentration of each material and their respective potential barrier to verify their behavior in relation to temperature. In the case of reverse bias generates a graphical output capacitance associated with these quantities. It is also used matlab to solve the transcendental equation that defines the relationship between voltage, resistance and current of a semiconductor diode bias. These demonstrations and concepts are important because they govern the operation of basic electronic devices and can characterize the differences between the Si, Ge and GaAs.

C1.00139 SURFACES, INTERFACES AND THIN FILMS –

C1.00140 Modeling the Self- and Directed-assembly of Viruses on Surfaces , DANIEL SULLIVAN, Colorado School of Mines, GEORGE GILMER, Lawrence Livermore National Laboratory, CRISTIAN CIOBANU, Colorado School of Mines — The exploitation of naturally self-assembling viruses has received much attention recently in regards to fabrication of nanomaterials and devices. Formation of dense viral mono- and multilayers as well as viral immobilization via chemospecific surface functionalization can be studied by modeling viruses as colloidal particles. We use a modified Lennard-Jones (LJ) potential, characterizing each colloid as an integrated collection of LJ particles, to describe intercolloidal and colloid-surface interactions. By carefully selecting the LJ interaction parameters and performing molecular dynamics simulations, we are able to replicate experimentally observed behavior of viruses on both strongly and weakly interacting surfaces in our surrogate colloidal system. Kinetic properties of the computational system are monitored and we find them to be in good agreement with predictions based on experimental data. We provide a basis for further investigation into the capabilities and limitations of modeling self-assembly of viral systems of technical interest using classical molecular dynamics.

C1.00141 Silicon Nanoparticle Formation Analysis and Optical Properties[1] , DANIEL FRASIER, GREG SPENCER, ANUP BANDYOPADHYAY, WIM GEERTS, Texas State University-San Marcos — In this study, the formation of silicon nanoparticles by thermal annealing of an initial silicon-on-insulator (SOI) structure is being performed. The SOI samples are synthesized by thermal oxidation of Si (100) wafers followed by magnetron and ion beam sputtering of a thin Si top layer. The thermal anneals are performed in a rapid thermal anneal system at temperatures ranging from 600 °C to 900 °C under atmospheric pressure of Ar gas. The nanoparticle formation process is being studied as a function of the thermal anneal maximum temperature, anneal time, and Si layer thickness. The annealed samples are measured by atomic force microscopy to determine the resulting nanoparticle size distributions and synthesis details. Electron microscopy is also being used for physical analysis in addition optical properties being studied through Effective Medium Approximations (EMA) proposed in the Lorentz-Lorenz (LL), Maxwell-Garnett (MG), and Bruggeman methods. Results for these experiments as well as comparisons with the work of others will be presented.

[1]Supported in part by NSF IGERT.

C1.00142 A study of the structure and dynamics of the interface between a nanoparticle and a surface: the case of Cu and Ag , JAMES BORRELLI, JAMES WESTOVER, ABDELKADER KARA, University of Central Florida — We performed a Molecular Dynamics study using the Embedded Atom Method for interatomic potentials for silver and/or copper nanoparticles projectiles incident on Ag and/or Cu (100) surfaces. Nanoparticles in the range of 1 to 2 nm in diameter were used with incident energies ranging from 50 to 500 meV/atom; while the surface temperature is kept at a temperature ranging between 300 and 700K. After collision and thermalization, distributions of nearest neighbor distances show a variety of values that reflect the strength of the local bonding. Using a Real Space Green's Function approach, we have determined the vibrational densities of states and the corresponding thermodynamical functions for a limited number of cases. Results for the vibrational dynamics show a strong effect at the high frequency end of the densities reflecting the stiffness of the bond at the interface. Results for the vibrational enery, entropy, lattice heat capacity as well as Debye temperatures will be presented.

C1.00143 Cluster growth driven by long range de-wetting interactions in thin films , ADI CONSTANTINESCU, LEONARDO GOLUBOVIC, West Virginia University, ARTEM LEVANDOVSKY, University of California Riverside — Long range de-wetting inteactions acting across thin films, such as the van der Waals forces, may drive the formation of large clusters (tall multi-layer islands). We study, by analytic arguments and simulations, the growth of these clusters within a unified model explicitly incorporating de-wetting interactions. The ultimate cluster growth scaling laws at long times are universal: Short and long range de-wetting interactions yield the same coarsening exponents. However, long range de-wetting interactions introduce a long lasting early-time scaling behavior characterized by a slow growth of the cluster height/lateral size aspect ratio (i.e., a time-dependent Young angle). This stage of cluster evolution is characterized by effective coarsening exponents that we calculate from our simulations and from an analytic approach.

C1.00144 Insights in to hetero diffusion and growth: A DFT Study , H. YILDIRIM, SUBRAMANIAN SANKARANARAYANAN, JEFF GREELEY, Argonne National Laboratory — We report the results of first principles calculations performed to study heteroatom diffusion on the terraces and step edges of fcc(001) surfaces on a series of 3d, 4d and 5d transition metals. For each adsorbate-substrate pair, we report the most stable adsorption sites and the corresponding adsorption energies. The corresponding terrace diffusion barriers are also reported, and periodic trends in the barrier heights are related to differences in adsorbate adsorption energies, cohesive energies of both adsorbate and substrate, and the differences in bond length/strength. Diffusion barriers and mechanisms at the step edges are also reported. Finally, insights into the possibility of 2D vs. 3D growth for each studied system are discussed via the calculated Ehrlich-Schwoebel barriers.

C1.00145 Initial growth of CrAs on GaAs(001)-c(4×4)α[1] , KAZUMA YAGYU, SHIGERU KAKU, JUNJI YOSHINO — CrAs is a ferromagnetic material which has a hexagonal structure. It is, however, predicted by first-principles calculation that zincblende (ZB) CrAs shows ferromagnetism and has a halfmetaric electronic structure [1-3]. Although ferromagnetism of a CrAs epitaxial film was confirmed so far, its crystal structure is still unclear. It turned out that ferromagnetism originated at the interface. In this study, initial growth of CrAs film has been investigated with scanning tunneling microscopy at 80 K. CrAs was grown on a GaAs(001)-c(4×4)α surface by means of exposing Cr as well as As_4 atoms at 250° C, followed by annealing at the same temperature. Randomly grown CrAs islands were observed form larger islands in proportion to the annealing time. Dimer structure which is similar to that of the substrate was confirmed on the surface of CrAs islands. This means that a CrAs island may have a ZB structure. The detailed structure and electric state of CrAs islands are discussed in the presentation.

[1] H. Akinaga et al., Jpn. J. Appl. Phys. 39 (2000) L1118
[2] M. Shirai, Physica E 10 (2001) 143
[3] A. Sakuma, J. Phys. Soc. Jpn. 71 (2002) 2534

[1]Global Center of Excellence Program "Nanoscience and Quantum Physics" of Tokyo Institute of Technology

C1.00146 Effect of deposition temperature on the properties of ZnO thin films , ALI ER, ASHRAF FARHA, Old Dominion University, YUKSEL UFUKTEPE, Cukurova University — The effect of deposition temperature on the surface morphology of zinc oxide thin films prepared by spray pyrolysis has been studied. The surface morphology of the films was studied by using X-ray diffraction (XRD), scanning electron microscopy (SEM) and atomic force microscopy (AFM). The effects of substrate temperature during deposition on the structure with optical properties of ZnO thin films were determined. Surface parameters were calculated and compared for different thin films. It showed that the films were polycrystalline with hexagonal wurtzite structure and c-axis was perpendicular to the substrate. The grain size of the films changed from 240 to 440 nm with different substrate deposition temperatures. It was found that growth temperature has significantly affected the morphological (grains size, surface roughness) as well as optical properties of ZnO films.

C1.00147 ABSTRACT WITHDRAWN –

C1.00148 Investigation of Chemical Reactivity at the Co/CuO interface by X-ray Photoelectron Spectroscopy[1] , J. EDMONDSON, Y. JUDIE, A. CHOURASIA, TAMU-Commerce — The technique of x-ray photoelectron spectroscopy has been utilized to investigate the chemical reactivity between cobalt and copper oxide at the Co/CuO interface. Thin films of copper (about 15 nm) were deposited on silicon substrates by the e-beam method. Such samples were oxidized in an oxygen environment in a quartz tube furnace at 400 ° C. The formation of CuO was checked by the XPS spectral data. Thin films of cobalt were then deposited on these CuO samples. The cobalt 2p, oxygen 1s and copper 2p regions were investigated by XPS. The magnesium anode (energy = 1253.6 eV) has been used for this purpose. The spectral data show chemical reactivity at the Co/CuO interface. The samples were annealed afterwards in air at 400 ° C. The spectral data were recorded at different take-off angles. Diffusion of copper through the cobalt overlayer with the formation of CuO is observed in the annealed samples.

[1]Supported by Organized Research, TAMU-Commerce

C1.00149 High resolution scanning tunneling microscope (STM) image of $SrTiO_3$(100)-$\sqrt{5} \times \sqrt{5} - R26.6°$ surface , ICHIRO SHIRAKI, Interdisciplinary Graduate School of Medical and Engineering, University of Yamanashi, Japan, KAZUSHI MIKI, National Institute for Materials Science (NIMS), Japan, SHUHENG PAN, Department of Physics, University of Houston, Houston, Texas — $SrTiO_3$(100)-$\sqrt{5} \times \sqrt{5} - R26.6°$ surfaces were studied by scanning tunneling microscope (STM) in ultra-high vacuum conditions at room temperatures. STM images with truly atomic resolution in filled states, which have never been reported, were successfully obtained. The atomic arrangement in $\sqrt{5} \times \sqrt{5}$ unit cell is clearly seen. It is currently assumed that Ti and its fourfold site O atoms were separately imaged with varying bias voltages, which indicates that TiO_2 plane is a basic plane of $\sqrt{5} \times \sqrt{5}$ surface superstructures. The dI/dV images simultaneously taken with topographic images were also obtained in filled states. Comparing our experimental results with the previous works, especially a theoretical study of O-vacancy model [1] and an experimental and theoretical study of Sr adatom model [2], possible structures on $\sqrt{5} \times \sqrt{5}$ surfaces will be discussed.

[1] Z. Fang and K Terakura, Surf. Sci. 470, L75(2000)
[2] T. Kubo and H. Nozoye, Phys. Rev. Lett. 86, 1801(2001)

C1.00150 Molecular-scale Structure of Pentacene at Functionalized Electronic Interfaces , SOON-JOO SEO, Chungbuk National University, GUOWEN PENG, MANOS MAVRIKAKIS, ROSE RUTHER, ROBERT HAMERS, PAUL EVANS, University of Wisconsin-Madison, HEE JAE KANG, Chungbuk National University, GUOWEN PENG AND MANOS MAVRIKAKIS COLLABORATION, ROSE RUTHER AND ROBERT J. HAMERS COLLABORATION, PAUL G. EVANS TEAM, HEE JAE KANG TEAM — A dipolar interlayer can cause dramatic changes in the device characteristics of organic field-effect transistors or photovoltaics. We have conducted a series of experiments in which different molecular linkages are placed between a pentacene thin film and a silicon substrate. Interface modifications with different linkages allow us to predict the nature of tunneling through pentacene on modified Si surfaces with different dipole moment. The molecular-scale structure and the tunneling properties of pentacene thin films on modified Si (001) with nitrobenzene and styrene were examined using scanning tunneling spectroscopy. Electronic interfaces using organic surface dipoles can be used to control the band lineups of a semiconductor at organic/inorganic interfaces. Our results can provide insights into the charge transport characteristics of organic thin films at electronic interfaces.

C1.00151 Chemisorption of Anthracene on Cu(110) , JERONIMO MATOS, ABDELKADER KARA, University of Central Florida — We use density functional theory (PBE) to calculate the adsorption of an Anthracene molecule on Cu(110). Anthracene adsorbs at a height of 2 Å above the surface and has a binding energy of 562 meV/molecule. We also found noticeable changes in the atomic and electronic structures of both the molecule and the substrate. The molecule is bent while the surface atoms experience a buckling. The dz^2 state of the copper atoms that are directly under carbon atoms presents new states near the Fermi level. These effects, in addition to a change in the work function, classify this system as chemisorption. We also determined the barrier for diffusion along the Cu(110) channel to be 77 meV.

C1.00152 A low friction coefficient between graphane coated surfaces , CAN ATACA, Department of Physics, Bilkent University, Ankara, Turkey, 06800, HASAN SAHIN, UNAM-Material Science and Nanotechnology, Bilkent University, Ankara, Turkey, 06800, SALIM CIRACI, Department of Physics, Bilkent University, Ankara, Turkey, 06800; UNAM-Material Science and Nanotechnology, Bilkent University, Ankara, Turkey, 06800 — Using first-principles calculations, we investigate the electronic properties and stability of recently synthesized 2D hydrocarbon in honeycomb structure, namely graphane. Varios charge analysis result that in graphane geometry negatively charged carbon atoms are sandwiched between positively charged hydrogen atoms bound from both sites. In addition high frequency vibration modes associated with C-H bonds are well separated from the rest of the spectrum. The repulsive interaction between two graphane layers due to mainly strong Coulomb interaction serves as if a boundary lubricant and prevents the sliding graphane surfaces from being closer to each other even under high normal forces. As a result, calculated lateral force variation generated during sliding has small magnitude under high constant loading forces. Superlow friction observed earlier between diamondlike carbon-coated surfaces can be understood strong and stiff carbon-carbon and carbon-hydrogen bonds which do not favor energy dissipation.

C1.00153 Tribological Properties of Atmospheric Pressure Plasma Polymerized Silica-like Films , BING HAN, JAMES BOERIO, University of Cincinnati — Thin silica-like films were deposited on ferrotype plate and polycarbonate (PC) substrates with an atmospheric pressure plasma jet using hexamethyldisiloxane (HMDSO) as the precursor. It was found that the thickness and properties of the film were sensitive to the flow rate of the precursor, the deposition distance, and the radio frequency power Residual methyl groups were incorporated into the film when the distance between the nozzle of the plasma jet and the substrate was increased, or when the RF power used in deposition was decreased. This was confirmed by an increase in Si-CH_3 peak intensity in the Fourier transform infrared spectroscopy spectra of the films. The atomic compositions and chemical bonding of HMDSO-air plasma-polymerized SiO_xC_y were analyzed by X-ray photoelectron spectroscopy. Low precursor flow rates produced smoother, more continuous, and more uniform films than high precursor flow rates. Low precursor flow rates produced films with atomic composition of Si:O:C=1:2.37:0.2. The deposited films presented mainly inorganic characteristics without adding oxygen or argon gas to the ionization gas mixture, as is common in the literature. Scratch resistance of the films was measured using a scratch tester with a diamond indenter under progressive load. Post scratch image and surface morphology of the substrate and the film was obtained by scanning electron microscopy and atomic force microscopy.

C1.00154 Diamagnetic Levitation Cantilever System for the Calibration of Normal Force Atomic Force Microscopy Measurements[1] , JAHN TORRES, Brown University/ Naval Undersea Warfare Center, JIN-WOO YI, Korean Institute of Science and Technology, COLIN MURPHY, Naval Undersea Warfare Center, KYUNG-SUK KIM, Brown University — In this presentation we report a novel technique for normal force calibration for Atomic Force Microcopy (AFM) adhesion measurements known as the diamagnetic normal force calibration (D-NFC) system. The levitation produced by the repulsion between a diamagnetic graphite sheet and a set of rare-earth magnets is used in order to produce an oscillation due to an unstable mechanical moment produced by a silicon cantilever supported on the graphite. The measurement of the natural frequency of this oscillation allows for the calculation of the stiffness of the system to three-digit accuracy. The D-NFC response was proven to have a high sensitivity for the structure of water molecules collected on its surface. This in turns allows for the study of the effects of coatings on the structure of surface water.

[1]This work was supported by the Coatings/Biofouling Program and the Maritime Sensing Program of the Office of Naval Research as well as the ILIR Program of the Naval Undersea Warfare Center DIVNPT.

C1.00155 Modeling of charged particles trajectories in order to optimize the design of a new, higher resolution, Time of flight- Positron Annihilation Induced Auger Electron Spectroscopy (TOF PAES) System[1] , PRASAD JOGLEKAR, L. LIM, SUMAN SATYAL, SUSHANT KALASKAR, K. SHASTRY, ALEX WEISS[2], U T Arlington — Time of Flight Positron Annihilation Induced Auger Electron Spectroscopy (TOF PAES) is a surface analytical technique with high surface selectivity. TOF PAES is used to study elemental composition, surface defects, and various energy loss mechanisms. Positrons incident on the sample surface at low energies can be trapped in an image-potential well just above the surface Prior to annihilation. Consequently it is possible to use positron annihilation related signals to selectively probe the top-most atomic layer. This poster presents the results of modeling of the charge particle beam transport system performed in connection with the optimization of the the design of the new TOF-PAES system currently under construction at U T Arlington. The system will incorporate a 2 m long drift tube in order to achieve better energy resolution than our previous TOF-PAES system design which used a 1 m long drift tube

[1]NSF DMR 0907679, Welch Foundation Y 1100

[2]Advisor

C1.00156 Coherent x-ray surface scattering applied to Pt (001)[1]

, MICHAEL S. PIERCE, DANIEL HENNESSY, KEE-CHUL CHANG, Materials Science Division, Argonne National Laboratory, VLADIMIR KOMANICKY, Faculty of Science, Safarik University, ALEC SANDY, JOSEPH STRZALKA, Advanced Photon Source, Argonne National Laboratory, HOYDOO YOU, Materials Science Division, Argonne National Laboratory — Scattering using highly coherent light provides information about the very small scale, but over a very large area suitable for an ensemble measurement. We have used coherent x-ray diffraction to study the surfaces Pt (001) single crystal surfaces at high temperature in vacuum and compare them with earlier measurements of Au (001) in similar conditions. Both metals possess a temperature dependent quasi-hexagonal surface reconstruction. The speckled scattering patterns can be quantitatively compared against each other to determine how quickly configuration is changing, even when the macroscopically the system appears in equilibrium. We have been able to obtain measurements of the dynamic temperature dependent surface processes for these two different systems. For Pt (001) we have also directly observed step-flow motion of the terraces, obtaining step-edge velocity as a function of temperature. Our results point to two very different mechanisms at work in lifting the surface reconstruction at high temperature in vacuum.

[1]Work at ANL is supported by DOE-BES and work at SU by VEGA.

C1.00157 Ion neutralization as a probe to study electronic dynamics on clean and nanostructured surfaces[1]

, HEE SUK LEE, RYAN O'CONNELL, ANDREW SCHMITZ, JOHN SHAW, HIMADRI CHAKRABORTY, Northwest Missouri State University — Resonant charge transfer in ion-surface collisions is a classic tool to explore the surface electronic structure. Using the Crank-Nicholson propagation [1] we solve the time-dependent Schroedinger equation to simulate electrons' motion during the interaction of a H^- anion with clean, nanostepped, and nanolayered metal surfaces. Ion survival from a clean surface is found to depend adiabatically on the metal band gap, but for the fast (diabatic) ion-speed perpendicular to the surface interactions with image states dominate [2]. For larger distance of ion's closest approach, however, the image interaction intrudes the adiabatic region. For the stepped surfaces, conversely, the survival is found to depend on the ion speed parallel to the surface from super-lattice sub-band effects, resulting in rich structures in the survival probability. Electrons that populate a nanolayered surface, in contrast, are found to modify the Shockley surface state and image states by inducing standing waves in the direction perpendicular to the surface.

[1] Chakraborty et al., *Phys. Rev.* A **70**, 052903 (2004);
[2] Schmitz et al., *Phys. Rev.* A **81**, 042901 (2010).

[1]Supported by NSF and Applied Research NWMSU.

C1.00158 Electronic structure of oxygen di-vacancies on the (110) surface of rutile

, WILLIE MADDOX, BRANDEN KAPPES, CHRISTIAN CIOBANU, Department of Engineering, Colorado School of Mines — We report the results of electronic structure calculations for the reduced surface of rutile (110). We have performed density functional theory calculations in the framework Hubbard-corrected generalized gradient approximation (GGA+U) to investigate the electronic signatures of single and di-vacancies on rutile (110) slabs, both neutral and positively charged. We have also carried out Bader charge analysis to evaluate the charge transfer that occurs upon the reduction of the rutile surface. We observe n-type character for the neutral systems and p-type character for the positive slabs. For U=3 eV, we observe mid-gap states for the neutral system, while for U=6 eV, we observe mid-gap states for the positively charged system as well. Bader analysis shows that the atoms associated with mid-gap states are those that experience a larger charge transfer. The dependence of the band gap on the U parameter was also investigated, and the results were compared with experimental observations in the literature for both electronic properties and for structural atomic relaxations.

C1.00159 ABSTRACT WITHDRAWN –

C1.00160 Electronic structure of alkali/Si(111):B semiconducting interfaces

, LAURENT CHAPUT, ANTONIO TEJEDA, CEDRIC TOURNIER-COLLETTA, YANNICK FAGOT-REVURAT, LUIS CARDENAS, BERTRAND KIERREN, DANIEL MALTERRE, IJL, UMR CNRS 7198, Nancy Universite, France, PATRICK LEFEVRE, FRANCOIS BERTRAN, AMINA TALEB-IBRAHIMI, Synchrotron-SOLEIL, Cassiopee Beamline, France — We have evidenced by LEED and STM a novel $2\sqrt{3} \times 2\sqrt{3}$ surface reconstruction for K, Rb and Cs on Si(111):B.[1] The $2\sqrt{3}$ charge ordering occurring mainly in Si dangling bonds has been evidenced by high resolution photoemission measurements on core levels whereas the k-dependent photoemission spectral function agrees with the $2\sqrt{3}$ symmetry establishing a full gap higher than 1 eV.[2] These results will be discussed in the light of ab initio calculations giving evidence for strong atomic distortions associated with a possible full charge ordering in dangling bonds, in connection to a large energy gap,[3] which is compatible with a bi-polaronic scenario.

[1]L. A. Cardenas et al, Phys. Rev. lett. 103, 046804 (2009)
[2]C. Tournier-Colletta et al., Phys. Rev. B 82, 165429 (2010)
[3] L. Chaput et al., to be published

C1.00161 Scanning Tunneling Spectroscopy Observation of New Type of Resonances on the Dense Pb Overlayer on the Si(111)

, SHIN-MING LU, H.Y. CHOU, Institute of Physics, Academia Sinica, Nankang, Taipei 115, Taiwan, Y.P. CHIU, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan, W.B. SU, P.H. CHU, C.L. JIANG, C.S. CHANG, Institute of Physics, Academia Sinica, Nankang, Taipei 115, Taiwan, H.L. HSIAO, Department of Physics, Tunghai University, Taichung 407, Taiwan, TIEN T. TSONG, Institute of Physics, Academia Sinica, Nankang, Taipei 115, Taiwan — We use scanning tunneling spectroscopy (STS) to investigate the electronic structures of the dense Pb overlayers of 1×1, $\sqrt{7}\times\sqrt{3}$ and stripe incommensurate (SIC) phases grown on the Si(111) surface. Although their atomic structures are all very different, very surprisingly the STS spectra of these three phases show a nearly identical oscillatory feature with two resonance peaks. These resonances are not the common quantum-well states but the energy bands originating from the dominant 1×1 potential in these phases. However, the local electronic states found by STS on the $\sqrt{7}\times\sqrt{3}$ and SIC phase exhibit that the resonances can be affected locally by the superstructures of two phases. It reflects that there exists a weak additional one-dimensional periodic potential on the $\sqrt{7}\times\sqrt{3}$ phase and the SIC phase is of the local variation of the work function.

C1.00162 Effect of substrate strain on the charge dynamics of $Nd_{0.5}Sr_{0.5}MnO_3$ investigated by pump-probe technique , MUNKHBAATAR PUREVDORJ, J.S. KIM, Institute of Photonics and Information Technology, Chonbuk National University, Korea, H.Y. HWANG, Department of Advanced Material Science, University of Tokyo, Japan, K. MYUNG-WHUN, Institute of Photonics and Information Technology, Chonbuk National University, Korea — We present the polarization and time dependent transmittance of $Nd_{0.5}Sr_{0.5}MnO_3$ (NSMO) thin films grown on $SrTiO_3$ (STO) (100) and STO (110) substrates. We used the normal transmission technique and the pump-probe technique for the measurement. While the transmittance of NSMO film on STO (100) is isotropic, the transmittance of NSMO on STO (110) measured with the electric field parallel to [-110] direction (E//[-110]) is larger than that of E//[100]. The time dependent transmittance change of NSMO film on STO (100) shows a sharp increase near the zero time delay and exponential decreases as the time delay between the pump and the probe pulse increases. The transmittance change of NSMO film on STO (110) shows almost the same time dependence. The time dependent transmittance change of NSMO film on STO (100) shows no significant polarization direction dependence, however the magnitude of time dependent transmittance change of NSMO on STO (110) is different depending on the polarization direction. The mechanism of the polarization dependence of transmittance change and the polarization direction independent relaxation will be discussed in terms of the substrate strain and its effect on the charge dynamics.

C1.00163 Angular Distributions and Total Yields of Bi Sputtered by 20 keV He^+, Ne^+ and Ar^+ , NARESH DEOLI, LUCAS PHINNEY, JOSE PACHECO, DUNCAN WEATHERS, University of North Texas, IBMAL TEAM — The angular distributions of neutral atoms sputtered from the surface of solid Bi by normally incident 20 keV He^+, Ne^+ and Ar^+ ions have been measured. The sputtered atoms were collected on pure aluminum foils under ultrahigh vacuum conditions, and the collector foils were subsequently analyzed using heavy ion Rutherford backscattering spectroscopy. The angular distributions obtained were integrated to determine the total sputtering yields of Bi for the different incident ions. Details of the measurements and data analysis are presented.

C1.00164 Segregation of impurities at γ' (L12) / γ (fcc) interfaces in a Ni-based superalloy , DE NYAGO TAFEN, MICHAEL GAO, National Energy Technology Laboratory, 1450 Queen Ave SW, Albany, OR 97321, USA; URS Corporation, P.O. Box 1959, Albany, OR 97321, USA — One of the most technologically advanced energy conversion devices is the gas turbine used in aerospace jet engines and gas- fired land-based turbines for electricity generation, fabricated from Ni-based superalloys. However, these materials lack of long- term mechanical and microstructure stability, which is largely due to an excessive coarsening of γ' that can cause substantial loss of creep resistance and mechanical instability at high temperatures. Theoretical prediction of the creep rate of these important compounds is very imperative, but yet is extremely challenging. Interfacial energy is one of the most important factors that control the coarsening kinetics of these important phases. It indirectly determines the creep resistance of the alloy through the coarsening rate of the strengthening precipitate phase. In this talk, we will present the results of various γ'/γ interfaces of a Ni-based superalloy obtained using DFT calculations. Then, we will discuss the segregation of impurities at these interfaces. Minor alloying elements in superalloys can alter the interfacial energy between γ and γ', and change the strength behavior of the alloy. Alloying elements or impurity species can segregate to interfaces. A favorable segregation would result in enhancing the interfacial cohesion and thus lower the energy.

C1.00165 METALS —

C1.00166 Structural properties of nanometric HfN/VN superlattices[1] , P. PRIETO, Excellence Center for Novel Materials, M. VILLAREAL, C. ESCOBAR, J.C. CAICEDO, G. CABRERA, Thin Film Group, Universidad del Valle, L. YATE, J. ESTEVE, A. LOUSA, Department de Fisica Aplicada i optica, Universitat de Barcelona — HfN and VN systems have broadly been used as protective hard and anticorrosive coatings. [HfN/VN]n multilayered were deposited on silicon substrates by two target-r.f. magnetron sputtering with alternatively changing the sputtering plasma composition between pure Hf and V elements under a reactive mixture Ar/N_2. HfN/VN bilayer period varied from nanometric range (15 nm) to higher nanometric range (600 nm) values. Structural, morphological and stoichiometric of the coatings were analyzed by high angle and low-angle X-ray diffraction, X-ray photo electron spectroscopy (XPS), secondary ion mass spectrometry (SIMS), atomic force microscopy (AFM) and cross sectional transmission electron microscopy (TEM). We determined multilayer period, Λ, and individual layer thicknesses. We found a cube-on-cube epitaxial growth structure with an epitaxial relationship between layers inside each columnar crystallite given by $(111)[100]_{HfN}//(200)[100]_{VN}$.

[1]This work was supported by the Center of Excellence for Novel Materials (CENM) under Colciencias-CENM contract # RC-043-2005. Colciencias-Univalle.

C1.00167 Synthesis and Characterization of Multifunctional Epitaxial Metal-oxide Films[1] , JIE XIONG, JUNYI ZHAI, GUIFU ZOU, Los Alamos National Laboratory, HAIYAN WANG, Texas A&M University, LI YAN, MUJIN ZHUO, YINGYING ZHANG, Los Alamos National Laboratory, BOWAN TAO, YANRONG LI, University of Electronic Science and Technology of China, J.L. MACMANUS-DRISCOLL, University of Cambridge, QUANXI JIA, Los Alamos National Laboratory — Transition metal-oxides have attracted great attention due to their versatile properties. Multilayers, and/or artificial superlattices, are especially interesting since these architectures usually exhibit unique physical properties in comparison with single phase thin films. Furthermore, the lattice strains and the coupling in the multilayered systems can strongly affect the films' growth and their physical properties. We have grown and characterized different multilayered metal-oxide thin films using laser molecular beam epitaxy (MBE). Specifically, we have prepared $[(BiFeO_3)_n/(La_{0.7}Sr_{0.3}MnO_3)_n]_m$ and $[(BiFeO_3)_n/(BiMnO_3)_n]_m$ superlattices and strained $BiFeO_3$ $(BFO)_{0.5}$: $BiMnO_3$ $(BMO)_{0.5}$ films. We have systematically investigated the strain states on the magnetic properties of these multilayer films.

[1]This work was supported by the U.S. Department of Energy and the Center for Integrated Nanotechnologies. J. X. acknowledges the support from National Science Foundation of China under Grant Nos. 50902017.

C1.00168 Origin of interfacial gap states in Ga_2O_3 layer grown on GaAs surface and interface passivation by F and Gd , WEICHAO WANG, K. XIONG, Department of Materials Science & Engineering, The University of Texas at Dallas, ROBERT M. WALLACE, KYEONGJAE CHO, Department of Materials Science & Engineering and Department of Physics, The University of Texas at Dallas — III-V compound semiconductors are potential candidates to replace Si as the channel of future high performance n-MOSFETs. However, the poor III-V/dielectric interface quality leads to low performance of device operations. Prior to any high-k deposition on III-V, a passivated III-V surface could help to obtain a high quality high-k/III-V interface. We examine the native oxides of Ga_2O_3 on GaAs with density functional theory to determine the origin of gap states and propose possible ways to passivate the interface. Ga_2O_3 molecular species is gradually added in first principles molecular dynamics until one monolayer formed on the top of GaAs at 700 K within 3 ps. During the growth process, O atoms tend to diffuse into GaAs, and Ga-Ga dimer forms as well. The interface states originate from the Ga dangling bonds, Ga-Ga dimers and under-coordinated Ga suboxides Based on the understanding of the origin of the gap states, F and Gd are proposed to remove the gap states.

C1.00169 Crystal Growth of MoO_2 and $K_xMoO_{2-\delta}$[1] , B.S. DE LIMA, C.A.M. DOS SANTOS, L.M.S. ALVES, S.S. BENAION, A.D. BORTOLOZO, Departamento de Engenharia de Materiais - Escola de Engenharia de Lorena - USP, M.R. ANDREETA, Instituto de Fisica de São Carlos - USP, J.J. NEUMEIER, Department of Physics - Montana State University — During the last years our group has searched for new quasi-one- dimensional (1D) conductors, which led to the discovery of $K_xMoO_{2-\delta}$. The electrical resistivity of this compound is well described by a power law in temperature [1]. In this presentation, progress on the crystal growth of $K_xMoO_{2-\delta}$ will be discussed. Crystal growth of the parent compound MoO_2 utilizes chemical vapor transport (CVT) with iodine as transport agent. Crystal growth of $K_xMoO_{2-\delta}$ by CVT was carried out using high purity K_2MoO_4, MoO_3, and Mo powders which were mixed in appropriate amounts ($0 \leq x \leq 0.25$) and sealed with I_2 in quartz tubes, followed by heat treatment in temperature gradients from 750 to 950^{o}C for 100 h. The crystals were characterized by X-ray diffraction, scanning electron microscope (SEM), Raman spectroscopy, electrical resistance and magnetization measurements.

[1] L. M. S. Alves *et al.*; Phys. Rev. B 81, 174532 (2010) and references therein.

[1]This material is based upon support by FAPESP (2008/10574-6, 2009/14524-6, and 2010/06637-2) and CNPq (301334/2007-2, 490182/2009-7).

C1.00170 Induced Magnetic Behavior and Anomalous X-ray Fluorescence Spectra of Thermally Tailored Copper , PATRICK BRADLEY, CLAIRE CHANENCHUK, CHRIS NAGEL, Continuum Energy Technologies — When a high purity (>99.98 wt%) copper ingot was melted, subjected to high temperature thermal cycling including rapid electromagnetic field oscillation (thermally tailored), the resultant solidified metal exhibited unexpected magnetic regions with unique spectroscopic behavior. A high-resolution magnetic microscope was used to provide current density imaging with resultant surface mapping of magnetic fields of the magnetically active regions on the copper ingot. Energy-dispersive, X-ray fluorescence (XRF) analysis of the magnetic regions exhibited energy emissions inconsistent with the known starting composition of the material. An analysis of the magnetic field and XRF data shows them both to be a result of the tailoring process and eliminates the possibility of causation by impurities accumulated during the process.

C1.00171 Crystal structure and electrical properties of the $Bi_{2-y}Sr_yIr_2O_7$ α-pyrochlore solid solution , CARLOS COSIO-CASTANEDA, GUSTAVO TAVIZON, Facultad de Quimica, PABLO DE LA MORA, Facultad de Ciencias, UNAM, FRANCISCO MORALES, Instituto de Materiales — In this work we report the synthesis and crystal structure of the $Bi_{2-y}Sr_yIr_2O_7$. From structural Rietveld refinements we show that in this system the local geometry of the IrO_6 passes from a trigonal antiprism (y<0.4); a regular octahedron (y=0.5), reaching a new trigonal antiprism at the end compositions (y>0.5). Experimentally, this is a metallic system with a conductivity that decreases as a function of the Sr content in the (10-300 K) low temperature range. By means of electronic structure calculations, using WIEN2k to study $Bi_2Ir_2O_7$ and two hypothetical compounds, $BiSrIr_2O_7$ and h-$BiSrIr_2O_7$, we show that a) the main contribution to conductivity come from the shift of the oxygen towards the Ir atoms; b) the lattice imperfections (random occupation of Sr) and lattice vibrations are responsible for the drop of the electrical conductivity, and c) the IrO_6 local geometry (and crystal field configuration, t_{2g}^5 $e_g^0/e_g^4a_{1g}^1b_{2g}b_{1g}$ change), this last one does not seem to affect the electrical conductivity.

C1.00172 Effect of Temperature, Pressure and Precursor flux ratios on InSb Thin film Growth: Morphology and Properties , SAMUEL MENSAH, ALEXANDER VOGEL, JOERG WITTEMANN, JOHANNES DE BOOR, VOLKER SCMHIDT, Max-Planck Institute of Microstructure Physics — We have investigated the growth of InSb thin films on InAs and GaAs substrates by Chemical Beam Epitaxy (CBE). Raman spectroscopy measurements show that the optical properties of the grown layers is not greatly affected even when varying the growth conditions over a wide range (varying the V/III flux ration between 1 and 10, growth temperature between 390-480°C). The lattice mismatch between the layers and substrates, results in regions of no growth during the deposition of InSb layers. To circumvent this problem, the growth process is preceded by a 10 mins exposure of the substrates to TMIn. This step eliminates the regions of no growth. Our results show that at constant pressure, the growth rate decreases with increasing temperature and with increasing V/III flux ratio. A much slower response was observed for increasing antimony partial pressure. The lattice mismatch between the layer and substrate give rise to stacking fault and twins. A decrease in particle size from 34.89 to 9.95nm was observed for increasing flux ratio and an increase from11.31 to 32.68nm for increasing temperature. Evidence of Raman spectroscopy results confirms the crystalline nature of the deposited films. Details of our results will be presented at the meeting.

C1.00173 Growth of thin, transparent and high quality phase pure hBN films , MUHAMMAD SAJJAD, XIOAN ZHANG, PETER FENG, University of Puerto Rico — A simple approach using pulse laser deposition technique was made in order to obtain multi layers transparent hexagonal boron nitride films at low substrate temperature (700 °C) with iron nano-particles as catalyst. The catalyst helped in creating reactive species of boron and nitrogen to react quickly and formed h-BN base layer. The formation of film layers were studied systematically with increasing amount of catalyst keeping same experimental conditions and steps. Transparent and ultra thin base layer was obtained using small amount of catalyst. However, with increasing amount of catalyst, few more layers were formed on the base layer which affected the transparency of the films. Therefore, it was revealed that with optimized amount of catalyst helped in nucleating ultra thin transparent layers of BN with clear variation in atomic wall layers, sharp edge of the film, shape and surface smoothness. Scanning Electron Microscopy was used to analyze the surface images of hBN thin films whereas Energy Dispersive X-Ray spectroscopy (EDS) verified dominance of boron and nitrogen in the structure. The crystalline structure of the films was analyzed with Raman spectroscopy and XRD technique.

C1.00174 Magnetic and thermodynamic properties of Americium-II: An *Ab Initio* Study[1] , JIANGUANG WANG, LI MA, ASOK RAY, University of Texas at Arlington — Hybrid density functional theory based method has been used to study the structural, magnetic, electronic, and thermodynamic properties of Americium-II. Non-magnetic, ferromagnetic (FM), and anti-ferromagnetic (AFM) configurations without and with spin-orbit coupling (SOC) have been considered. The experimental NM ground state configuration is indeed obtained for Am-II at a level of 40% HF exchange with SOC and the computed structural properties and electronic density of states are in good agreement with experimental observations. The importance of SOC is found to be significant. The phonon related properties of Am-II are presented for the NM ground state configuration and the computed heat capacity and entropy are in good agreement with the experimental measurements. The lattice constant, bulk modulus, heat capacity, and entropy of Am-II are predicted to be 9.44 a.u., 21.7 GPa, 24.3 $JK^{-1}mol^{-1}$, and 55.7 $JK^{-1}mol^{-1}$, respectively.

[1]This work is partially supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525) and by the Department of Energy.

C1.00175 Characterization of Doped $CeCoIn_5$, A.R. TREAT, Boston College, J.C. COOLEY, Los Alamos National Laboratory, C.P. OPEIL, Boston College — Department of Physics, Boston College, Chestnut Hill, Massachusetts 02467. Los Alamos National Laboratory, Los Alamos, New Mexico 87545. $CeCoIn_5$ is an unconventional, d-wave, heavy fermion superconductor with a critical temperature of ∼2.3K. The physical properties of doped samples of $CeCo_{1-x}M_xIn_5$, where M is Fe, Cr, Rh, Ru, Ir, Mn, Ni, V, or Cu for $x \leq 0.03$, are characterized. Resistivity, magnetoresistance, and magnetization are measured in a temperature range 5 - 300K and magnetic field up to 9 Tesla; the magnetization is measured using a capacitive cantilever magnetometer. The effect of the dopants on resistivity and magnetization, with regard to percentage x present in the sample, provides valuable insight into the character of the parent material $CeCoIn_5$. Implications of magnetic, diamagnetic, and non-magnetic doping of $CeCoIn_5$ will be discussed.

C1.00176 A Universal Relation between Heat Conduction and Diffusion[1]

, SHA LIU, BAOWEN LI, National University of Singapore — We rigorously prove a useful equality relating the heat current autocorrelation function and the mean square displacement of the energy diffusion. From this equality, we are able to recover the existing theories for normal diffusion and normal heat conduction. Moreover, we are also able to obtain a connection between anomalous diffusion and anomalous heat conduction. We are results are applicable to all isotropic systems with any dimension.

[1]This work is supported by the Grants No. W-144-000-222-646 of NUS

C1.00177 Study of the angular-dependence of the L-alpha and L-beta radiation produced by 0-15 kev photons incident on Au targets of various thicknesses

, SEBASTIAN REQUENA, SCOTT WILLIAMS, Angelo State University — We report the results of experiments involving the L-alpha and L-beta x-ray lines produced by 0-15 keV bremsstrahlung incident on gold targets of various thicknesses at forward-scattered angles ranging from 20 to 160 degrees. Previous reports [1, 2] have shown the L-beta peaks to be isotropic and the L-alpha peaks to be anisotropic due to the symmetry/asymmetry associated with the orbital being filled during the transition. The relative intensities are compared to the predictions of the Monte Carlo code, PENELOPE.

[1] K. S. Kahlon, et al., Phys. Rev. A 44, 7 (1991)
[2] L. Demir, et al., Radiat. Phys. And Chem., 59, 355-359 (2000)

C1.00178 Hexagonal motifs on the Ir(100) surface reconstructions from a first-principles study

, WAN-SHENG SU, National Center for High-Performance Computing, Tainan 741, Taiwan, FENG-CHUAN CHUANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan, KEN-MING LIN, TSAN-CHUEN LEUNG, Department of Physics, National Chung Cheng University, Chia-Yi 621, Taiwan — The hexagonal motifs of the Ir(100) surface overlayer are examined by using first-principles calculations. The studied hexagonal motifs are formed on the Ir(100) surface overlayer with (5x1), (8x1), (12x1), and (14x1) periodicities. Our results showed that the unstrained (5x1) phase is the most stable phase, which is consistent with not only previous theoretical calculations but also experimental findings. Further analysis on the strain-induced phase transition among various hexagonal reconstructions is presented. Such a phenomenon can be further qualitatively elucidated by analyzing the computed average standard deviation of angles.

C1.00179 An *Ab Initio* Study of FCC $Pu_{1-x}Ga_x$[1]

, KINJAL GANDHA, ASOK RAY, Department of Physics, University of Texas at Arlington — As is known, the addition of a few atomic percent of Ga stabilizes the fcc δ – phase of Pu at room temperature. In this work, conventional and hybrid density functional theory have been used to study the electronic, geometric, and magnetic structure properties of $Pu_{1-X}Ga_x$with varying Ga concentrations in the fcc δ phase. The calculations have been performed using the all-electron full-potential linearized augmented plane wave plus local orbitals basis method and the *WIEN2k* software. Each compound has been studied at the non-magnetic, ferromagnetic, and anti-ferromagnetic configurations with and without spin-orbit coupling (SOC) and full geometry optimizations. The ground state structures are found to be anti-ferromagnetic with a contraction of the lattice constants from pure δ-Pu. The obtained lattice parameters are in satisfactory agreement with experimental data.

[1]Work supported, in part, by the Welch Foundation (Grant No. Y-1525) and Department of Energy.

C1.00180 Spectroscopic ellipsometry of NTO/ultrathin Cu/NTO films

, JUN WOO PARK, HYUNG KEUN JANG, HOSUK LEE, HOSUN LEE, JUN-HYUK PARK, HAN-KI KIM, Kyung Hee University, BO HYUN KONG, HYUNG KOUN CHO, Sungkyunkwan University — NTO/Cu/NTO/glass thin films were grown using sputtering deposition. The thickness of the Cu film (t) varied between 1.5 nm and 50 nm. The ellipsometric angles (Ψ, Δ) of the NTO/Cu/NTO/glass thin films were measured by using spectroscopic ellipsometry. The thicknesses and dielectric functions of the Cu films in the NTO/Cu/NTO/glass were estimated by using a multi-layer model analysis with the parametric optical constant and Drude models. Transmission electron microscopy measurements showed that the Cu layers evolved from aggregates of Cu nanoparticles to coalesced Cu thin films as the Cu film thickness increased. According to sheet resistance data, the Cu films thinner than 8 nm were aggregations of Cu nanoparticles that were not well-connected and the Cu films thicker than 8 nm were above the percolation threshold. From the Drude model, the plasmon frequency (ω_p) and the electron relaxation time (τ) were estimated and were found to increase with increasing film thickness. We obtained the second derivatives of the dielectric function spectra that were composed of several peaks near 1.5, 2.1, 2.5, 3.5, and 4.3 eV, and attributed to interband transitions. The peak energies (except 1.5 eV) matched to the band structure calculations found in the literature.

C1.00181 Magnetic properties of $Mn_{11}Si_{19}$ and Mn_4Si_7 in their bulk and powdery states

, KIYOTAKA HAMMURA, Hitachi Cambridge Laboratory, HARUHIKO UDONO, TOMOSUKE AONO, Ibaraki University, ISAO OHSUGI, Salesio Polytechnic, ELISA DE RANIERI, Hitachi Cambridge Laboratory, KEN-ICHI YAJIMA, YUSUKE UJIIE, Ibaraki University — The purpose of this paper is to determine by experiment whether $Mn_{11}Si_{19}$ and Mn_4Si_7 in their bulk and powdery states have a finite magnetic moment or not. High quality bulk samples for both were prepared using the temperature gradient solution growth method. Powery samples for both were prepared by pounding bulk crystals in a mortar. Magnetisation measurements were carried out using both SQUID system and Kerr rotation system. SQUID measurements revealed that $Mn_{11}Si_{19}$ has finite magnetism while Mn_4Si_7 does not in their bulk states. It was also confirmed that Mn_4Si_7 became magnetic and $Mn_{11}Si_{19}$ exhibited a distinctive hysteresis, in their powdery state. The enhancement of magnetism in their powery states implied that the surface of the samples was to a great extent linked to its magnetism.

C1.00182 Polarization-dependent optical excitations in AB-stacked graphite

, CHIH-WEI CHIU, YUAN-CHENG HUANG, FENG-LIN SHYU, MING-FA LIN — The band structure of AB-stacked graphite exhibits two pairs of parabolic bands, where the band-edge states induce the peaks and shoulders in the density of states and in the joint density of states (JDOS). The dipole matrix element M^{cv} plays an important role in the relationship between the spectral function A(ω) and JDOS. It is strongly dependent on the polarization directions $\hat{\mathbf{E}}$ of the laser beams, showing a anisotropic property. The optical excitations do not fully reflect the special structures of JDOS. For $\hat{\mathbf{E}}$ on the graphene plane, A(ω)$'$s are isotropic and include one sharp peak and some shoulders. As for $\hat{\mathbf{E}}$ along the stacking direction, A(ω) is much weaker, and only shows a broadened peak. The spectra contrast sharply with those of AA-stacked graphite.

C1.00183 Correlation effect investigations on the Magneto-optical Kerr Spectra of Co-based Heusler alloys from first principles[1]

, MIYOUNG KIM, Division of Energy System Research, Ajou University, HANJO LIM, JAE IL LEE, Dept of Physics, Inha University — Here, we report our *ab-initio* calculational results on the electronic structures and magneto-optical (MO) properties of the ferromagnetic Co_2MnX full Heusler alloys. Employing the +U corrections for the transition metal $3d$ bands in addition to the local density approximation (LDA), we investigate the correlation effect on the MO spectra in polar geometry as well as the detailed electronic structures using FLAPW [1] method. Results show that the correlation effect results in a blue-shift of the peak positions and large enhancement of the low energy MO spectra, which are attributed to the increased t_{2g}-e_g splitting of spin minority Co and Mn $d-$bands indicating the suppression of diagonal elements of optical conductivity at energy region of 1$\sim$2 eV where the interband transitions are forbidden.

[1] E. Wimmer, K. Krakauer, M. Wienert, and A.J. Freeman, Phys.Rev B 24, 864 (1981).

[1]This work is supported by Korean Research Foundation Grant by MOEHRD (KRF 2007-412-J04001) and also by Basic Science Research Program through the National Research Foundation of Korea (NRF-2010-0005387).

C1.00184 Theoretical Study of tip apex electronic structure in Scanning Tunneling Microscope[1]

, HEESUNG CHOI, MIN HUANG, Department of Materials Science & Engineering and Department of Physics, The University of Texas at Dallas, JOHN RANDALL, Zyvex Lab, KYEONGJAE CHO, Department of Materials Science & Engineering and Department of Physics, The University of Texas at Dallas — Scanning Tunneling Microscope (STM) has been widely used to explore diverse surface properties with an atomic resolution, and STM tip has played a critical role in controlling surface structures. However, detailed information of atomic and electronic structure of STM tip and the fundamental understanding of STM images are still incomplete. Therefore, it is important to develop a comprehensive understanding of the electronic structure of STM tip. We have studied the atomic and electronic structures of STM tip with various transition metals (TMs) by DFT method. The d-electrons of TM tip apex atoms show different orbital states near the Fermi level. We will present comprehensive data of STM tips from our DFT calculation. Verified quantification of the tip electronic structures will lead to fundamental understanding of STM tip structure-property relationship. This work is supported by the DARPA TBN Program and the Texas ETF.

[1]DARPA Tip Based Nanofabrication Program and the Emerging Technology Fund of the State of Texas

C1.00185 Exchange constants and spin waves of MnV_2O_4 from first principles DFT calculations

, RAVINDRA NANGUNERI, SERGEY SAVRASOV, University of California, Davis — We present results of DFT calculations of exchange constants of the magnetic spinel MnV_2O_4. The starting point is the one-particle eigenfunctions of the Kohn-Sham auxiliary Hamiltonian as a function of the self-consistent, converged charge density. Using linear response and perturbation theory, the exchange constants between the magnetic ions Mn and V are calculated in both the collinear and non-collinear, orbital-ordered phases of the spinel. The collinear exchanges have exchange constants proportional to the unit matrix, which means they are isotropic. On the other hand, the non-collinear exchanges have unequal diagonal elements and in addition have off-diagonal elements, revealing anisotropic magnetic interactions. The anisotropy is traced to the orbital-order and non-collinear spin structure of the low-temperature ground-state. We find that the interactions between the V atoms can sometimes be anti-ferromagnetic. The V atoms are located at the vertices of a corner-sharing tetrahedral lattice, commonly known as a pyrochlore lattice. AFM interactions on such a lattice are geometrically frustrated because all pair-wise bond energies cannot be simultaneously minimized with a classical spin configuration. It has been experimentally found that as the temperature is lowered, MnV_2O_4 undergoes a transition from a paramagnet with a cubic symmetry structure phase to a ferrimagnetic with cubic symmetry phase at 56 K.

C1.00186 Comparative Studies of Constitutive properties of Nanocrystalline and Bulk Iron During Compressive Deformation

, XIAOHUI YU, JIANZHONG ZHANG, LIPING WANG, YUSHENG ZHAO — We present a comparative study of mechanical properties of bcc nano-crystalline iron and microncrystalline iron by in-situ high-pressure synchrotron x-ray diffraction under tri-axial compression. For nano-Fe with a starting high dislocation density of 10^{16} m^{-2}, the peak broadening is almost reversible upon unloading from 8.6 GPa to ambient pressure, indicating that no additional dislocations are built up during compressive deformation inside grains, at grain boundaries or twin boundaries. Furthermore, an orientation dependent surface strain is found to be stored in the surface layer of the bcc nano Fe, which is in agreement with the core-shell model of the nano crystals. For micron-Fe, a significant and continuous peak sharpening and the associated work softening were observed after the sample is yielded at pressures above 2.0 GPa, which can be presumably attributed to a pressure-induced dislocation annihilation. This finding/interpretation supports the hypothesis that the annihilation of dislocations is one of the dominant mechanisms underlying the plastic energy dissipation. The determined yield strength of 2.0 GPa for nano-Fe is more than 15 times higher than that for micron-Fe (0.13 GPa), indicating that the nano scale grain-size reduction is a substantially more effective strengthening mechanism than the conventional carbon infusion in iron.

C1.00187 Density functional study of the mechanical properties in single-layered graphene sheet[1]

, JORGE TAPIA, FRANCIS AVILES, RICARDO PEON, FI-UADY, GABRIEL CANTO, CICORR-UAC, MMS-NM TEAM — By means of the density functional theory, we studied the structural and mechanical properties (the Young's modulus, shear modulus and Poisson's ratio) of single-layered graphene sheets (SLGS). The calculations were performed with a linear combination of atomic orbitals method using pseudopotentials and the generalized gradient approximation for the exchange-correlation potential. The uniaxial stress is applied along the one preferential direction for the range of $\pm$10% in the unitary deformation. We found that the bond lengths between carbon atoms in SLGS are larger than the experimental value of graphite and the mechanical properties showed good agreements with the data available in the literature.

[1]This research was supported by SEP under Grants: PROMEP/103.5/07/2595, PROMEP/103.5/08/2971 and CONACYT under Grants: No. 82497 and No. 60534.

C1.00188 The morphological evolution and migration of inclusions in thin-film interconnects under electric loading

, YINFENG LI, Department of Engineering Mechanics, Shanghai Jiaotong University and Division of Engineering, Brown University, XI WANG, ZHONGHUA LI, Department of Engineering Mechanics, Shanghai Jiaotong University — The paper reports the result of an investigation into electromigration-driven morphological evolution of inclusions in finite scale thin-film interconnects using a phase field method. In examples, two types of inclusion defect are simulated and discussed. The results show that the morphological evolution and migration of inclusion is proportional to the electric field strength applied on thin-film interconnects. It is also seen from the result that the inclusion with anisotropic diffusion interface will move faster than one with isotropic interface under the identical electric field, and the one with anisotropic diffusion interface may evolves into an irregular shape with protuberance.

C1.00189 Calculation of the Peierls barrier of screw dislocations in bcc metals and its dependence on stress

, ROMAN GROGER, Institute of Physics of Materials, Academy of Sciences of the Czech Republic, VACLAV VITEK, Department of Materials Science and Engineering, University of Pennsylvania — Plastic deformation of bcc metals at low temperatures is governed by thermally activated glide of $1/2\langle 111\rangle$ screw dislocations over Peierls barriers. Thermodynamic models of the dislocation glide depend on the shape of the Peierls barrier and its changes under stress. Atomistic simulations provide only the maximum slope of the Peierls barrier and, therefore, its overall shape as well as the path of the dislocation are generally unknown. We introduce a new approach by which the Peierls barrier and its changes under stress can be calculated if a suitable set of constraints is imposed to prevent the dislocation from falling into the nearest potential minima. The state of the system at any point along the path is described by the position of the intersection of the dislocation with the perpendicular $\{111\}$ plane. Hence, both the Peierls barrier and the transition path are obtained directly. This is a clear advantage over the currently used approach, where one calculates the path of the system of N atoms through the space of $3N$ degrees of freedom. We compare the results of these two approaches by employing the Finnis-Sinclair potential for tantalum.

C1.00190 Hydrogen Segregation in Crystalline Palladium and Effects on Mechanical Properties

, HIEU PHAM, AMINE BENZERGA, TAHIR CAGIN, Texas A&M University — Calculations of tensile strength and tensile modulus were carried out to investigate the effects of hydrogen interactions, diffusion and segregations in palladium single crystal, high-vacancy crystal and bicrystal, by using the embedded atom method. Elevated temperature, hydrogen absorption and defects such as vacancy and grain boundary (GB) individually induce a loss in mechanical strength of palladium in a monotonous manner. The hydrogen-induced mechanical degradation was noticed at the grain boundary, as well as in bulk. The failure induced by hydrogen in palladium up to x_H=0.1 is plastic rather than brittle, even around grain boundary region, by formation of dislocations. At high H absorption, the global hydrogen concentration is a dominant factor over crystal defects. However, a high-angle grain boundary such as $\sum$5 (2 1 0) provides a great driving force for diffusion and tendency for physical trapping of hydrogen. Therefore, the existence of grain boundary makes materials more susceptible and easily exposed to high hydrogen absorption and segregation. Also, our simulation shows that hydrogen maintains the highest localization at GB in the vicinity of ambient temperatures; and this finding coordinates with experimental observation that hydrogen embrittlement are generally observed at room temperatures.

C1.00191 Atomic analyzis and photocurrent studies of isolated sub-100 nm diameter silicon nanowires

, DIDIER STIEVENARD, CNRS - ISEN, TAO XU, ISEN, BRUNO GRANDIDIER, CNRS - ISEN, YANNICK LAMBERT, ISEN, CHRISTOPHE KREMINSKY, CNRS - ISEN, ABDELLATIF AKJOUJ, YAN PENNEC, BAHRAM DJAFARI-ROUHANI, Universite de Lille 1, WANGHUA CHEN, RODRIGUE LARDE, EMMANUEL CADEL, PHILIPPE PAREIGE, CNRS INSA Universite de Rouen, PHYSICS GROUP TEAM, PHYSICS OF MATERIALS GROUP TEAM — n-doped Si NWs were synthesized by the vapor-liquid-solid mechanism using the chemical vapor deposition (CVD) technique.The nanowires were grown to a nominal length of 10 μm with a diameter ranging typically from 60 to 110 nm. Atom Probe Tomography analyzes evidence a gradient of concentration of the phosphorous atom dopants, inducing a built-in potential accros the nanowires. Photocurrent on isolated nanowires was performed with a monochromator source. Depending on the light energy and on the nanowire diameters, we measure various absorption thresholds. Calculations have been performed on a periodic array of wires of varying diameters and with different periodicity by using a Finite Difference Time Domain (FDTD) method. The results evidence a clear dependence of the optical absorption with the nanowire diameters. This work was supported by DGA REI contract N°2008.34.0031.

C1.00192 Raman Study of the Verwey Transition in Magnetite (Fe_3O_4) at High Pressure and Low Temperature: Effect of Aluminum Doping

, Z. SHIRSHIKOVA, L. GASPAROV, Department of Physics, University of North Florida, V. STRUZHKIN, A. GAVRILIUK, Geophysical Laboratory, Carnegie Institution of Washington, H. BERGER, EPFL, CH-1015 Lausanne, Switzerland — Raman spectra of pure and doped magnetite provide a set of markers allowing one to study how the Verwey transition in magnetite changes with the change of pressure. At ambient pressure Verwey transition temperature, Tv, of the single crystals of magnetite, Fe3O4, is determined to be 123K. High-pressure experiment indicates strong dependence of the change of pressure vs. change in the Verwey transition temperature on the amount of impurities: for pure Fe_3O_4 the change is -0.2 GPa/K; for doped iron, $Fe_{2.98}Al_{0.02}O_4$, the change is -0.09 GPa/K. Aluminum-doped magnetite ($Fe_{2.98}Al_{0.02}O_4$) where Al substitutes Fe^{+2} and Fe^{+3} atoms, represents a 2% aluminum doping, which shifts the Verwey transition temperature to T_v=118.5K. The rate with which the Verwey temperature decreases with pressure is further discussed based on the molar specific heat measurements.

C1.00193 INSTRUMENTATION AND MEASUREMENTS –

C1.00194 Design and Construction of a Radio Telescope for Undergraduate Research[1]

, CHRISTOPHER STATHIS, Ithaca College — Radio telescopes provide a practical and economical alternative to optical observatories for astrophysics research and education at primarily undergraduate physics and astronomy institutions. Ithaca College is in the testing phase of development for a low cost, flexible frequency band radio telescope which I have developed as the research component of my undergraduate thesis. I have constructed a three-stage low noise superheterodyne radiometer on custom printed circuit boards for signal detection, which is mounted on a 3 meter parabolic antenna. Data collection and signal processing is achieved using custom software written in MATLAB. We are currently performing preliminary drift continuum observations of the Sun and Milky Way at Ku band frequencies. We expect that the receiver can also be easily adapted to measure spectral emission of neutral hydrogen and OH masers at L band. I present my design methods for the radiometer and printed circuit boards, including measured noise characteristics and SPICE simulations, as well as an overview of applied signal processing methods and a discussion of observable celestial sources.

[1]Dr. Bruce G. Thompson and Dr. Matthew Price, Research Advisors, Ithaca College

C1.00195 Synthesis and characterization of ZnO nanostructures for sensor application[1]

, XIAOYAN PENG, JIN CHU, University of Puerto Rico, BOQIAN YANG, University of Massachusettes, PETER FENG, University of Puerto Rico, FENG TEAM — ZnO nanostructures including nanoparticles (diameter about 50nm), nanorods (diameter about 150 nm and length about 1-1.5μm) and nanoparticles (diameter $\sim$ 20 nm) were prepared onto Si (100) substrates using both r.f sputtering and PLD technique, respectively. Thermal annealing was performed at 800 ^{o}C in atmosphere for 2 hours to improve the qualities of ZnO crystalline structures. X-ray diffraction, electron scanning microscope and Raman scattering have been used to characterize all these nanostructured samples After synthesis and initial characterizations, the ZnO nanostructure-based field effect transistor sensors have been designed, fabricated, and tested. High sensitivity (few PPM), quick time response (less than 1 second) of the newly designed sensors have been achieved. Experimental data indicate that the sensitivity of the sensor highly relies on the operating temperature.

[1]This work is partially supported by NSF-DMR (0706147)

C1.00196 Doped and functionalized ZnO nano films and their applications for gas sensors[1]

JIN CHU, XIAOYAN PENG, PETER FENG, University of Puerto Rico, FENG TEAM — We demonstrate efficient gas sensors using Cu-doped ZnO nanowires and Li atoms-modification of ZnO nanorods. Various Cu-doped ZnO nanowires were synthesized on Si substrates by plasma sputtering at 300 °C with deposition duration of 30 minutes, while Li-coated ZnO nanorods were prepared by coating Li on the surface of the as-grown nanorods. Raman and EDX data indicated that the obtained ZnO nanowires and nanorods have wurtzite structure with Cu-doping concentration of 1 wt.% and ZnO nanorods with Li-coated concentration of 3 wt.%, respectively The sensing properties were examined by being exposed to H_2, N_2 and CH_4 gases with a home-made system that can facilitate the detection of the resistance change and the control of gas flow as well as temperature. The sensitivities of both samples increased with the operating temperature from RT to 200 °C and signal intensity of the sensor increased with gas concentration at each type of gas. Experimental data indicates that both types of samples-sensors showed highly sensitive to H_2 and selectivity against N_2 and CH_4. However, the response time for Li-coated ZnO nanorods-based sensor is less than 1 second, much quicker than that for Cu-doped ZnO nanowires-based sensors.

[1]This work is partially supported by NSF-DMR(0706147)

C1.00197 First-principles study of γ-ray detector materials : heavy alkali metal compounds[1]

HOSUB JIN, JUNG-HWAN SONG, ARTHUR J. FREEMAN, BRUCE W. WESSELS, MERCOURI G. KANATZIDIS, Northwestern University — In an effort to find good candidate materials for γ-ray detectors, alkali metal based chalcogenide semiconductors containing heavy elements were investigated. We performed ab- initio density functional theory calculations using the highly precise full-potential linearized augmented plane wave (FLAPW) method[2] to estimate their electronic characteristics. The state-of-the-art screened-exchange LDA scheme was adopted to correct the underestimation of the band gap in the LDA method. Several candidate materials for γ- ray detectors such as $Cs_2Cd_3Te_4$ and $Cs_2Hg_6S_7$ were suggested based on the electronic properties like band gaps, effective masses, absorption coefficients, and work functions. Lattice degrees of freedom such as static dielectric constants and bulk modulus were also calculated, and are reported.

[1]Supported by DTRA (Grant No. HDTRA1-09-1-0044)
[2]Wimmer, Krakauer, Weinert, Freeman, Phys. Rev. B, **24**, 864 (1981)

C1.00198 ZSM-5, Y, and Mordenite Zeolites as Sensing Materials for Ethanol Vapor

ANUVAT SIRIVAT, INTIRA YIMLAMAI, The Petroleum and Petrochemical College, Chulalongkorn University — The effects of the framework type, the charge balancing cation type, and the Si/Al ratio of ZSM-5, Y, and Mordenite zeolites on the electrical conductivity responses towards ethanol vapor have been investigated. All zeolites were characterized using XRD, FT-IR, SEM, TGA, BET, and NH_3-TPD techniques. For the effect of the framework type, H^+Y has a higher electrical conductivity sensitivity value than that of H^+MOR because of a greater pore volume and available surface area. For the effect of the charge balancing cation, all NH_4^+ZSM-5 zeolites (Si/Al = 23, 50, 80, 280) show negative responses, whereas the H^+Y zeolites (Si/Al = 30, 60, 80) and the H^+MOR zeolites (Si/Al = 30, 200) show positive responses. These differing behaviors can be traced to the interactions between ethanol molecules and the reactive sites of the zeolites. For the effect of Si/Al ratio, the electrical conductivity sensitivity towards the ethanol decreases with increasing Si/Al ratio or decreasing Al content, and there is a lesser degree of interaction between ethanol molecules and the active sites of the zeolites. The interactions between the ethanol molecules and the zeolites were investigated through infrared spectroscopy.

C1.00199 Apparatus for the analysis of surfaces in gas environments using Positron Spectroscopy[1]

SUMAN SATYAL, LAWRENCE LIM, PRASAD JOGLEKAR, SUSHANT KALASKAR, KARTHIK SHASTRY, ALEXANDER WEISS — Positron spectroscopy performed with low energy beams can provide highly surface specific information due to the trapping of positrons in an image potential surface state at the time of annihilation. Here we present design details of a new positron beam system for the analysis of surfaces gas environments. The new system will employ differential pumping to transport the positrons most of the way from the source to the sample under high vacuum. The positrons will then be transported through a thin gas layer surrounding the sample. The positrons will be implanted into the sample at energies less than ∼10 keV ensuring that a large fraction will diffuse back to the surface before annihilation. The Elemental content of the surface interacting with the gas environment will then be determined from the Doppler broadened gamma spectra.

[1]Welch Y1100, NSF DMR 0907679

C1.00200 High-resolution X-ray Emission Spectroscopy as a Microprobe Imaging Modality[1]

JOSEPH PACOLD, GERALD SEIDLER, BRIAN MATTERN, MATTHEW HAAVE, University of Washington, ROBERT GORDON, Simon Fraser University, University of Washington — Hard x-ray microprobe beamlines at third generation light sources have made significant impacts in several fields of science and technology. Such facilities permit rapid 2-dimensional studies of multiphase materials on submicron length scales using a variety of pixel-by-pixel imaging modalities (e.g., x-ray diffraction, x-ray absorption near edge fine structure, or x-ray fluorescence). Here, we aim to expand hard x-ray microprobe imaging modalities to include high-resolution x-ray emission spectroscopy (XES). When performed at 1-eV resolution, such measurements can provide quite direct atomic-level information on ionic valence, spin, and local electronic and chemical environment. Ongoing work in our research group has improved the efficiency of XES via the development of a new type of compact and inexpensive x-ray spectrometer design, the "miniature x-ray spectrometer" or "miniXS" paradigm. We will report preliminary 2-dimensional XES studies of planar multiphase materials, with specific applications to samples of interest for geophysics and catalysis science.

[1]Supported by the U.S. Department of Energy Office of Basic Energy Sciences

C1.00201 Measurements of chemical bonds using diffraction of electronic waves traveling through crystals[1]

ROBERT LANNING, CRISTIAN BAHRIM, Department of Physics, Lamar University — We propose a simple and intuitive procedure for discovering the atomic arrangement and the chemical bonds in transparent crystals using the diffraction of light or electronic waves by crystals. This study can help to improve methods of optical imaging, electronic microscopy, microbiology, and crystallography. Using fundamental principles of quantum mechanics, we also explain the formation of electronic wave packets when a free electronic beam passes through the atoms of a solid target. The atoms in solids act as the narrow slits of a diffraction grating producing a Fourier transform of the sinusoidal waves associated to free electrons incident on the solid target. Such a model allows measuring the chemical bonds within 1% precision. This research project was done under a NSF-DUE-sponsored program, called STAIRSTEP [1], which was designed to engage STEM undergraduate students in high-quality research in several fields of science including physics, at Lamar University.

[1] Doerschuk P, Bahrim C, Daniel J, Kruger J, Mann J, and Martin Ch, *39th ASEE/IEEE Frontiers in Education Conference,* San Antonio 2009, M3F-1-2.

[1]Project sponsored by the NSF-STEP program, award #DUE 0757057.

C1.00202 Negative thermal expansion in Prussian Blue analogs , S. ADAK, H. NAKOTTE, L. DAEMEN, LANSCE (Lujan Center), LANL — While many Prussian Blue (PB) analogs are known to display negative thermal expansion (NTE), few have been studied in detail. Not all compounds in this family exhibit NTE. Because it is possible to systematically vary ion size and charge in these materials, they represent an interesting playground to study NTE and possible correlations with electronic and crystal structures. By contrast with many silicates displaying NTE and in which tetrahedral units are linked with apical oxygens, the octahedral units in PB compounds are linked with a linear cyanide ligand. This introduces more degrees of freedom in the (mostly) cubic PB structures compared to the silicates. Polycrystalline samples of PB analogs, $M_2^{II}[Fe^{II}(CN)_6]$ and $M_2^{III}[A^{III}(CN)_6]_2$*(M = Mn, Co, Ni, Cu, Zn; A = Cr, Fe, Co)* were synthesized via standard chemical precipitation. Variable temperature X-ray powder diffraction patterns were collected *in-situ* in the range 300-123 K to study the T-dependence of the lattice parameter and to obtain an average coefficient of thermal expansion (CTE). Lattice parameters were extracted using the Rietveld refinement technique with the General Structure Analysis System (GSAS) software. The determined average CTEs, for the compounds showing NTE behavior, are in the range -4.9 x $10^{-6}K^{-1}$ to -39.5 x 10^{-6} K^{-1} while the CTEs for the other materials showing positive TE behavior are in the range 5.9 x $10^{-6}K^{-1}$ – 59.2 x 10^{-6} K^{-1}.

C1.00203 New Approach to Image Aerogels by Scanning Electron Microscopy , FRANCISCO SOLÁ, FRANCES HURWITZ, NASA Glenn Research Center, JIJING YANG, Carl Zeiss SMT Inc. — A new scanning electron microscopy (SEM) technique to image poor electrically conductive aerogels is presented. The process can be performed by non-expert SEM users. We showed that negative charging effects on aerogels can be minimized significantly by inserting dry nitrogen gas close to the region of interest. The process involves the local recombination of accumulated negative charges with positive ions generated from ionization processes. This new technique made possible the acquisition of images of aerogels with pores down to approximately 3nm in diameter using a positively biased Everhart-Thornley (E-T) detector. Well-founded concepts based on known models will also be presented with the aim to explain the results qualitatively.

C1.00204 Three-axis positional drift correction in scanning probe microscopy[1] , NATHAN D. FOLLIN, CHRISTOPHER J. MUSALO, MATTHEW L. TRAWICK, Department of Physics, University of Richmond, Richmond, VA — Positional drift in scanning probe microscopy can cause image distortion and metrological errors of tens of nanometers or more. It can arise from thermal drift, due to thermal expansion of materials in the sample and microscope while scanning, or from piezo creep, particularly along the z axis. We present a technique for correcting positional drift errors in all three axes. Our method works by comparing each scanned topographical image to a second, partial scan, taken immediately afterwards, on which the fast and slow scan axes have been reversed. We model the positional distortion as a low-order polynomial function in three dimensions, searching for the set of correctional coefficients that minimizes the difference between the two scans. Using this technique we have successfully reduced positional errors from 50 nm to 0.5 nm in the z axis, and from 40 nm to 2 nm (about half of a single pixel) in the xy plane.

[1]Supported by an award from Research Corporation for Science Advancement, and by the American Chemical Society Petroleum Research Fund through Grant number 46380-GB7

C1.00205 Three Electrode Control of the NanoDeposition of Gold Nanoparticles With Atomic Force Controlled Capillary Electrophoresis , AARON LEWIS, TALIA YESHUA, MILA PALCHAN, Hebrew University of Jerusalem, YULIA LOVSKY, HESHAM TAHA, Nanonics Imaging Ltd. — Controlled deposition of the metallic features such as nanoparticles with high spatial accuracy has a great interest in different applications such as surface plasmons, surface enhanced Raman scattering (SERS), nanophotonics and nano biophysics. Lithography based scanning probe microscopy techniques have been shown as a potential methodology for accurate and localized deposition of material in the nanometer scale. Here we report an accurate deposition of high resolution features of single gold nanoparticles using Three Electrodes and atomic force microscopy (AFM) controlled capillary based fountain pen nanolithography. In this methodology three electrodes are attahced one on the outside of the metal coated glass probe, one on the inside of the hollow probe in the solution contained in the capillary and a third electrode on the surface on which the writing is to take place. The three electrodes provide electrical pulses for accurate control of the deposition and retraction of the liquid from the surface. We will demonstrate depositing of single gold nanoparticle with size of 1.2nm onto surfaces such as semiconductors.

C1.00206 Have some large structures? Try small-angle neutron scattering (SANS) , LISA DEBEER-SCHMITT, KATHY BAILEY, NSSD, ORNL, LILIN HE, GEORGE WIGNALL, YURI MELNICHENKOV, NSSD,ORNL, KEN LITTRELL, NSSD, ORNL — The small-angle neutron scattering (SANS) beam line, CG-2, has been in operation since 2007. CG-2 has been optimized so that structures from 0.5 to 200 nm can be thoroughly investigated. HFIR's cold source places the flux at CG-2 among the best in the world. Along with high flux, many varied sample environments can easily be integrated into the beam line which gives the user a versatile temperature range from 1.5 K to 1000 K. In addition there are two cryomagnets (horizontal 4.5 T and vertical 7 T), pressure cells and load frames available to users allowing for the availability of multiple configurations of experimental setups. Due to all the above equipment and the flux at CG-2, there have been many diverse and intriguing scientific developments. One such outcome is the study of flux-line lattices found in Type-II superconductors including the highly touted iron pnictides. Besides superconductors, other science studied on CG-2 ranges from molecular self-assembly and interactions in complex fluids to phase separation to grain growth and orientation in metallurgical alloys.

C1.00207 Characterization and Modeling of Off-Specular Neutron Scattering for Analysis of Two Dimensional Ordered Structures , CHRISTOPHER METTING, University of Maryland, BRIAN MARANVILLE, PAUL KIENZLE, NIST Center for Neutron Research, ROBERT BRIBER, University of Maryland, JOSEPH DURA, CHUCK MAJKRZAK, NIST Center for Neutron Research — The University of Maryland along with NIST Center for Neutron Research (NCNR) and the NSF funded DANSE project are currently developing off-specular neutron reflectometry modeling software for fitting scattering data from multilayer samples. The software includes a robust sample representation scheme for easy development of various models. Theory functions are being calculated using a variety of approximations. The suite of approximations allows for the evaluation of each calculation's usefulness in representing the scattering data. In this presentation we describe corrections made to a purely Born approximation that capture dynamical scattering and resolution effects seen in measured data. We then show modeled data taken on the Advanced Neutron Diffractometer/Reflectometer (AND/R) at the NIST Center for Neutron Research (NCNR) from a sample of gold pillars using a substrate modified Born approximation, and compare it to a model which uses a purely Born approximation.

C1.00208 On-demand Control of Micro Quartz Resonator in Scanning Probe Microscopy[1] , JUNGHOON JAHNG, WONHO JHE, BONGSU KIM, Physics and Astronomy, Seoul National University — We demonstrate generalized theoretical analysis and experimental realization of active feedback control for the self-oscillating quartz tuning-fork (QTF) which is a widely used probe for sensing applications in scanning probe microscopy. In this work, we present the damping control, feedback cooling, resonance control and nonlinear dynamics for the QTF by implementing active feedback control scheme. Finally, we suggest the prospect of several novel applications in scanning probe microscopy by using the active feedback control of QTF such as increasing the force sensitivity, reducing the thermal noise and modulating the resonance of the sensor.

[1]This work supported by Korean Ministry of Science and Technology.

C1.00209 Low Temperature Scanning Probe Microscope(LT-SPM) operating in a Cryogen-Free Cryostat, 1.5-300K , OZGUR KARCI, NanoMagnetics Instruments Ltd, MUNIR DEDE, NanoMagnetics Instruments Ltd., YURY BUGOSLAVSKY, RENNY HALL, Cryogenic Limited, AHMET ORAL, Sabanci University, NANOMAGNETICS INSTRUMENTS LTD. TEAM, CRYOGENIC LIMITED TEAM, SABANCI UNIVERSITY TEAM — We present the design of a Low Temperature Scanning Probe Microscope(LT-SFM) operating in a vibration-free cryogen-free cryostat. A 0.5W ultra now noise Pulse Tube cryocooler is integrated into the cryostat with a 9T magnet. Stick slip coarse approach mechanism is used to bring the sample in to close proximity of the sample. The sample can be moved in XY directions within 3 mm range, while the position is measured with capacitive encoder with 3μm accuracy. An improved fiber interferometer with $\sim$12fm/$\sqrt{}$Hz noise level is used to detect cantilever deflection. The resonance of the cantilever controlled by a digital Phase Locked Loop (PLL) integrated in our Control Electronics with 5mHz frequency resolution. We can achieve $\sim$1nm resolution in AFM mode & $<$10nm resolution in MFM mode. Results from different imaging modes; non-contact AFM, MFM, Piezoresponse, Conductive AFM etc. will be presented.

C1.00210 A 129 GHz dynamic nuclear polarizer in a wide-bore superconducting magnet[1] , LLOYD LUMATA, RICHARD MARTIN, ASHISH JINDAL, CRAIG MALLOY, A. DEAN SHERRY, UT Southwestern Medical Center, MARK S. CONRADI, Washington University in St. Louis, MATTHEW MERRITT, UT Southwestern Medical Center — Dynamic nuclear polarization via fast dissolution method has allowed production of solutions containing highly-polarized nuclei (>10,000-fold enhancement of the room-temperature liquid-state NMR signal) of bio-molecules for *in vitro* and *in vivo* metabolic nuclear magnetic resonance spectroscopy (MRS) and imaging (MRI). Here we present the construction and use of a 129 GHz dynamic nuclear polarizer in a 4.6 T wide-bore superconducting magnet. The relatively large bore (150 mm) of the superconducting magnet allows the use of a cryostat separate from the magnet and routing of the microwaves such that the waveguide does not have to be removed before dissolution. A 100 mW microwave source operating at 129 GHz was used to irradiate the samples. The cryostat has a 10-liter liquid Helium capacity which lasts for 10-12 hrs of continuous operation. Base temperature of 1.15 K is achieved with a 450 m^3/hr roots blower pump. Preliminary results will be discussed.

[1]This work is supported in part by the National Institutes of Health grant numbers 1R21EB009147-01 and RR02584.

C1.00211 Diffuse Reflectance Spectroscopy and Colorimetry as a Diagnostic Tool for Acanthosis Nigricans , BENSACHEE PATTAMADILOK, Henry Ford Health System, SUNEETHA DEVPURA, Wayne State University, ZAIN U. SYED, PRANITA VEMULAPALLI, MARSHA HENDERSON, Henry Ford Health System, STEVEN J. REHSE, Wayne State University, ILTEFAT HAMZAVI, BASSEL H. MAHMOUD, HENRY W. LIM, Henry Ford Health System, RATNA NAIK, Wayne State University — The purpose of this study was to quantify skin color changes due to Acanthosis Nigricans, a disorder common among prediabetic and obese individuals. The non-invasive optical technique diffuse reflectance spectroscopy (DRS) was used to determine skin melanin, oxyhemoglobin and deoxyhemoglobin content through the measured absorption spectrum. Colorimetery was used to measure skin color based on the standard Tristimulus values (L*, a*, and b*). Data was obtained from eight patients, spanning eight months of treatment. Measurements were obtained from lesion tissue on the neck and healthy skin was used as a control. L*, a* and b* values showed significant differences between lesion and normal controls, whereas melanin was the only parameter which showed statistical significant differences in DRS measurements. Future work will use more sensitive chemometric methods to increase diagnostic accuracy based on the raw spectra of the DRS.

C1.00212 Toward contrast-enhanced, optically-detected NMR spectroscopy[1] , CARLOS MERILES, DANIELA PAGLIERO, Department of Physics, City College of New York - CUNY — Optical detection of Nuclear Magnetic Resonance (NMR) takes place via a two-step process that relies on the interaction between optical photons and electrons on the one hand, and the hyperfine coupling between electrons and nuclear spins on the other. The latter depends on the material system under consideration while the former is dominated by the difference between the illumination and optical transition wavelengths. Here we use optical Faraday rotation to monitor nuclear spins in real time after resonant radio-frequency excitation at high-magnetic field. Comparison between inductively and optically detected NMR spectra in model sample fluids indicates that each of these mechanisms can lead to alternate forms of spectral contrast. Extension of these findings may find application in solvent suppression protocols, sensitivity-enhanced NMR of metalloproteins, or the characterization of molecular orbitals in diamagnetic systems.

[1]We acknowledge support from the National Science Foundation.

C1.00213 STATISTICAL AND NONLINEAR PHYSICS –

C1.00214 DEFINITION of (so MIScalled) "Complexity" as UTTER-SIMPLICITY!!! VERSUS DEVIATIONS From It As COMPLICATEDNESS-MEASURE(S) , F. YOUNG, EDWARD CARL-LUDWIG SIEGEL, FUZZYICS=CATEGORYICS(SON OF TRIZ)/CATEGORY-SEMANTICS — (so MIScalled) "complexity" with INHERENT BOTH SCALE-Invariance Symmetry-RESTORING, AND 1/w^(1.000..) "pink" Zipf-law Archimedes-HYPERBOLICITY INEVITABILITY power-spectrum power-law decay algebraicity. Their CONNECTION is via simple-calculus SCALE-Invariance Symmetry-RESTORING logarithm-function derivative: (d/dω) ln(ω) = 1/ω , i.e. (d/dω) [SCALE-Invariance Symmetry-RESTORING](ω) =1/ω . Via Noether-theorem continuous-symmetries relation to conservation-laws: (d/dω) [{inter-scale 4-current 4-div-ergence} = 0](ω) = 1/ω. Hence (so MIScalled) "complexity" is information inter-scale conservation, in agreement with Anderson-Mandell [Fractals of Brain/Mind, G. Stamov ed.(1994)] experimental-psychology!!!], i.e. (so MIScalled) "complexity" is UTTER-SIMPLICITY!!! Versus COMPLICATEDNESS either PLUS (Additive) VS. TIMES (Multiplicative) COMPLICATIONS of various system-specifics. COMPLICATEDNESS-MEASURE DEVIATIONS FROM complexity's UTTER-SIMPLICITY!!!: EITHER [SCALE-Invariance Symmetry-BREAKING] MINUS [SCALE-Invariance Symmetry-RESTORING] via power-spectrum power-law algebraicity decays DIFFERENCES: ["red"-Pareto] MINUS ["pink"-Zipf Archimedes-HYPERBOLICITY INEVITABILITY]!!!

C1.00215 A Revelation: Quantum-Statistics and Classical-Statistics are Analytic-Geometry Conic-Sections and Numbers/Functions: Euler, Riemann, Bernoulli Generating-Functions: Conics to Numbers/Functions Deep Subtle Connections , R. DESCARTES, G.-C. ROTA, L. EULER, J. D. BERNOULLI, EDWARD CARL-LUDWIG SIEGEL, FUZZYICS=CATEGORYICS(SON OF TRIZ)/CATEGORY-SEMANTICS — Quantum-statistics Dichotomy: Fermi-Dirac(FDQS) Versus Bose-Einstein(BEQS), respectively with contact-repulsion/non-condensation(FDCR) versus attraction/ condensationBEC are manifestly-demonstrated by Taylor-expansion ONLY of their denominator exponential, identified BOTH as Descartes analytic-geometry conic-sections, FDQS as Elllipse (homotopy to rectangle FDQS distribution-function), VIA Maxwell-Boltzmann classical-statistics(MBCS) to Parabola MORPHISM, VS. BEQS to Hyperbola, Archimedes' HYPERBOLICITY INEVITABILITY, and as well generating-functions[Abramowitz-Stegun, Handbook Math.-Functions–p. 804!!!], respectively of Euler-numbers/functions, (via Riemann zeta-function(domination of quantum-statistics: [Pathria, Statistical-Mechanics; Huang, Statistical-Mechanics]) VS. Bernoulli-numbers/ functions. Much can be learned about statistical-physics from Euler-numbers/functions via Riemann zeta-function(s) VS. Bernoulli-numbers/functions [Conway-Guy, Book of Numbers] and about Euler-numbers/functions, via Riemann zeta-function(s) MORPHISM, VS. Bernoulli-numbers/ functions, visa versa!!! Ex.: Riemann-hypothesis PHYSICS proof PARTLY as BEQS BEC/BEA!!!

C1.00216 RANDOMNESS of Numbers DEFINITION(QUERY:WHAT? V HOW?) ONLY Via MAXWELL-BOLTZMANN CLASSICAL-Statistics(MBCS) Hot-Plasma VS. Digits-Clumping Log-Law NON-Randomness Inversion ONLY BOSE-EINSTEIN QUANTUM-Statistics(BEQS) .

, Z. SIEGEL, EDWARD CARL-LUDWIG SIEGEL, FUZZYICS=CATEGORYICS(SON OF TRIZ) — RANDOMNESS of Numbers cognitive-semantics DEFINITION VIA Cognition QUERY: WHAT???, NOT HOW?) VS. computer-"science" mindLESS number-crunching (Harrel-Sipser-...) algorithmics Goldreich "PSEUDO-randomness"[Not.AMS(02)] mea-culpa is ONLY via MAXWELL-BOLTZMANN CLASSICAL-STATISTICS(NOT FDQS!!!) "hot-plasma" REPULSION VERSUS Newcomb(1881)-Weyl(1914;1916)-Benford(1938) "NeWBe" logarithmic-law digit-CLUMPING/ CLUSTERING NON-Randomness simple Siegel[AMS Joint.Mtg.(02)-Abs. # 973-60-124] algebraic-inversion to THE QUANTUM and ONLY BEQS preferentially SEQUENTIALLY lower-DIGITS CLUMPING/CLUSTERING with d = 0 BEC, is ONLY VIA Siegel-Baez FUZZYICS=CATEGORYICS (SON OF TRIZ)/"Category-Semantics"(C-S), latter intersection/union of Lawvere(1964)-Siegel(1964)] category-theory (matrix: MORPHISMS V FUNCTORS) "+" cognitive-semantics" (matrix: ANTONYMS V SYNONYMS) yields Siegel-Baez FUZZYICS=CATEGORYICS/C-S tabular list-format matrix truth-table analytics: MBCS RANDOMNESS TRUTH/EMET!!!

C1.00217 Collective states of interacting Yang-Lee anyons in 1D: the golden chain's twin

, EDDY ARDONNE, Nordita, JAN GUKELBERGER, ETH Zurich, ANDREAS LUDWIG, UCSB, SIMON TREBST, Microsoft Station Q, MATTHIAS TROYER, ETH Zurich — Collective states of interacting non-Abelian anyons have recently been studied mostly in the context of exotic quantum Hall states. In this talk we will further expand this line of research and present certain non-unitary generalizations of the original golden chain model. In particular, we introduce the notion of Yang-Lee anyons, discuss their relation to the 'Gaffnian' quantum Hall wave function, and describe an elementary model for their interactions. A one-dimensional version of this model can be fully understood in terms of an exact algebraic solution and numerical diagonalization. We discuss the gapless phases of these models, and comment on the physical implications of the non-unitarity of their underlying critical theories.

C1.00218 Long-range in a system of thermal brownian particles[1]

, ALEXANDRO HEIBLUM, Posgrado Ciencias Fisicas, Universidad Nacional Autonoma de Mexico, FRANCISCO SEVILLA, Instituto de Fisica, Universidad Nacional Autonoma de Mexico, VICTOR DOSSETTI, Instituto de Fisica, Benemerita Universidad Autonoma de Puebla — We present a model that exhibits an order-disorder phase transition in two spatial-dimensions. The model considers a collection of N thermal Brownian particles moving in a square of length L subjected to periodic boundary conditions and to velocity-alignment forces. The alignment force affects only the velocity direction in a way that it makes it equal to the velocity direction of the nearby group. Our results contrast with those obtained from the well known model of Vicsek *et al.* [Phys. Rev. Lett. **75**, 1226 (1995)] where such a transition occurs out of equilibrium.

[1]We acknowledge support from PCF-PAEP and PAPIIT-IN117010

C1.00219 Long-range order in a system of thermal Brownian particles[1]

, ALEXANDRO HEIBLUM, Posgrado en Ciencias Fisicas, Universidad Nacional Autonoma de Mexico, FRANCISCO J. SEVILLA, Instituto de Fisica, Universidad Nacional Autonoma de Mexico, VICTOR DOSSETTI, Instituto de Fisica, Benemerita Universidad Autonoma de Puebla — We present a model that exhibits an order-disorder phase transition in two spatial-dimensions. The model considers a collection of N thermal Brownian particles moving in a square of length L subjected to periodic boundary conditions and to velocity-alignment forces. The alignment force affects only the velocity direction in a way that it makes it equal to the velocity direction of the nearby group. Our results contrast with those obtained from the well known model of Vicsek *et al.* [Phys. Rev. Lett. **75**, 1226 (1995)] where such a transition occurs out of equilibrium.

[1]We acknowledge support from PCF-UNAM-PAEP, PAPIIT-IN117010

C1.00220 Investigating Low Dimensional Chaos with Nearly Elastic Spheres

, ALEX SABEY, COREY LAFONTAINE, JEFFREY OLAFSEN, Department of Physics, Baylor University — An experimental and numerical study of the dynamics in a system which is prone to chaotic motion is implemented via a shaking plate and two nearly elastic particles. Confined to move in the vertical direction, one spherical particle is driven by the shaking plate while the other sphere is driven by collisions with the first. The motion of the two particles and the plate were captured with a relatively high speed ($\sim$340 fps) CCD camera via image analysis algorithms written in IDL. Measurements of position, velocity, acceleration, and energy and are used to formulate a thorough description of the system. The experimental results are compared to those of a numerical simulation to explore phase space for chaotic orbits of the two trajectories as well as phase synchronization between the particles and the plate. A thorough investigation of the phase space to describe the low dimensional system as well as to examine the dynamics for phase synchronization between the two particles will be presented.

C1.00221 Simulation studies of diffusion limited ballistic growth of particles from a surface[1]

, STEPHEN M. KUEBLER, Department of Chemistry & The College of Optics and Photonics, University of Central Florida, Orlando, ANIKET BHATTACHARYA, Department of Physics, University of Central Florida, Orlando — Motivated by electroless deposition of metals on polymeric surfaces we plan to study evolving morphologies of deposited particles from a surface using Monte Carlo simulation in continuum which shares characteristics of both diffusive and ballistic behavior. In the proposed model we assume that the particles residing at the surface of a growing pattern are capable of attracting particles those are within a certain range. Once one of these seed particles attracts a particle it transfers its attractive characteristics to the newly adsorbed particle which then acquires this characteristics for further growth. The motion of the particles in the bulk is diffusive. However, once they are within the range of an "active" particle they move ballistically along a straight line and gets adsorbed to a cluster unless hindered by other particles on its way. We plan to report the characteristics of the evolving patterns as a function of density of the diffusive particles, the range of the attractive particles, and the speed of ballistic moves.

[1]Supported by NSF-CHEM

C1.00222 Intermittency and ergodicity breaking in a system of interacting self-propelled particles[1]

, FRANCISCO J. SEVILLA, Instituto de Fisica, Universidad Nacional Autonoma de Mexico, VICTOR DOSSETTI, Instituto de Fisica, Benemerita Universidad Autonoma de Puebla — A comprehensive dynamical model for cooperative motion of self-propelled particles [Dossetti et al. Phys. Rev. E 79, 051115 (2009)], that combines velocity alignment interactions, spatial interactions, and angular noise, is studied. The noise considered in this model comes about nonlinear with correlations that decay in time, leading to a unique collective behavior. In particular, for a certain arrangement of the parameters, the system develops intermittent behavior and some sort of ergodicity breaking. In this work, we characterize these phenomena by studying the distributions of time intervals between turbulent bursts and changes between metastable states, respectively.

[1]FJS Acknowledge support from PAPIIT-IN117010.

C1.00223 Non-Equilibrium Statistical Dynamics of River Network Evolution[1] , XU-MING WANG, School of Physics and Electric Informantion, Ningxia University, PING ZHANG, JIE HUO, RUI HAO, School of Physics and Electric Informantion, Ningxia University — According to the erosion rule in a natural process, a Langevin Equation describing the prolongation of river channel is defined. The determinate prolongation is given by consideration of the characteristics of the early stage in the development of a river channel. The random growth (diffusion) is expressed by the fluctuations of the related stochastic variables or factors. A Fokker-Planck equation that describes the evolution of the distribution of the channel length is derived from this Langevin Equation. The solution presents the transition probability and exceedence probability with a Power-Exponent function which indicates that the channel length distributes in a complicated way. The details show that there exists a critical time, before which river network is developing and marked by exponent distribution., and beyond which river network is developed and marked by power distribution. On the basis of Hack's law, the transition probability of river's area and the corresponding exceedence probability are obtained. They are in excellent agreement with them obtained by field observations.

[1]NNSF Nos:10965004 and 10565002, NCET-06-0914, NXNSF:NZ0944

C1.00224 Introduction to the Mu-bit , FLORENTIN SMARANDACHE, University of New Mexico, Gallup Campus, V. CHRISTIANTO, Sciprint.org — Mu-bit is defined here as 'multi-space bit'. It is different from the standard meaning of bit in conventional computation, because in Smarandache's multispace theory (also spelt multi-space) the bit is created simultaneously in many subspaces (that form together a multi-space). This new 'bit' term is different from multi-valued-bit already known in computer technology, for example as MVLong. This new concept is also different from qu-bit from quantum computation terminology. We know that using quantum mechanics logic we could introduce new way of computation with 'qubit' (quantum bit), but the logic remains Neumann. Now, from the viewpoint of m-valued multi-space logic, we introduce a new term: 'mu-bit' (from 'multi-space bit).

C1.00225 Stochastic Phase Decoupling in Dynamical Networks , WILLIAM SULIS, McMaster University — Network models and their theories play a central role in the understanding of complex systems, in particular complex social systems such as societies and organizations. An important problem is to understand how agent attributes become organized within the connectivity structure of a network. The effective matching of agent attributes is important for the expression of functionality by a network. The creation of static networks relative to some control parameter has been extensively studied and gives rise to order-disorder phase transitions. This paper extends this work to dynamic networks. Several models of dynamic networks are created relative to two control parameters and their associated stochastic phase transitions are examined. Under conditions of weak coupling between the control parameters, it is shown that the relevant stochastic phase transitions become decoupled from one another, each qualitatively distinct and dependent on a single (distinct) control parameter.

C1.00226 Range of spectral exponents in rigor-state muscle fibers – a 1/f noise family affair? , CAROLINE RITZ-GOLD, Center for Biomolecular Studies, Fremont CA 94536 — Using EPR spectroscopy, we have followed changes in crossbridge state in rigor-state muscle fibers as a function of time. These observed changes were of two types – erratic fluctuations taking place on multiple time scales, and slowly-relaxing transients in response to substrate analog. For both types of change, the resulting power spectra had a 1/f-like power-law form with spectral exponents ranging from near 0 (white noise) to around 2 (brown noise). The average exponent was around 1 (pink noise). This observed broad range of spectral exponents is similar to that seen in the extended-family model of 1/f noise processes – a model that includes members ranging from white noise to pink to brown (JM Halley, Trends. Ecol. Evoln. 11, 33, 1996). Properties of this extended family model include self-affinity, long correlation times (memory), and non-stationarity (JM Halley & P Inchausti, Fluct. Noise. Lett 4, R1, 2004). We conclude that the broad range of spectral exponents observed in rigor-state muscle fibers reflects a type of underlying 1/f process. However, this particular type of process is unusual in that, although produced by a single biological source (rigor muscle fibers), it appears to include not just one but all of the members of the extended 1/f noise family – from white to pink to brown.

C1.00227 Self organization of social hierarchy in competitive societies , TAKASHI ODAGAKI, Tokyo Denki University, RYO FUJIE, Kyushu University — We investigate self organization of social hierarchy in a competitive society where all individuals have rights to participate in fighting. The winning probability of an individual against an opponent depends on the difference of their wealth. We introduce cost to participate in the fighting and show that the emergence of the hierarchical society depends strongly on the ratio of the cost to the reward for the winner. We show numerically and analytically that the phase transition occurs in two steps for most values of the ratio. Furthermore, we determine the phase diagram as a function of the ratio and the probability of participating in fighting. We show that there are four different phases in the parameter space, one egalitarian phase and three distinct hierarchical phases

C1.00228 Fermi Acceleration in a Periodically Driven Fermi-Ulam Model , O.F. DE ALCANTARA BONFIM, University of Portland — The dynamics of a particle bouncing between two harmonically vibrating walls is analyzed in the context of the static wall approximation. Fermi acceleration is observed for a wide range of the ratio between the frequencies of the oscillating walls and their relative phases. However, no acceleration is observed if the frequency ratio is an integer. In the phase versus frequency-ratio diagram, the region in which Fermi acceleration is observed is separated by an upper and lower boundary. At the lower boundary, after a large number of collisions the particle average velocity increases with the square-root of the number of collisions (n) with the walls. Between the lower and upper boundaries, the particle average velocity behaves as $V(n) \sim n^{\beta}$, with β in the interval [0.5, 1.0]. Below and near the lower boundary, the average particle velocity initially grows with the number of collisions until it eventually reaches a plateau. In this region, for a fixed frequency ratio, the velocity of the particle exhibits scaling properties over a range of the relative phases of the vibrating walls. Inelastic collisions with the walls cause suppression of the Fermi acceleration inside the previously accelerating region and lead to the particle velocity exhibiting scaling properties with respect to changes in the coefficient of restitution.

C1.00229 Moment ratios and dynamic critical behavior of a reactive system with several absorbing configurations[1] , WAGNER FIGUEIREDO, MARCELO FREITAS DE ANDRADE, Departamento de Física - UFSC - Brazil — We determine the critical behavior of a reactive model with many absorbing configurations. Monomers A and B land on the sites of a linear lattice and can react depending on the state of their nearest-neighbor sites and temperature of the catalyst. We consider that monomers of the type A are allowed to react with nearest-neighbor monomers A or B, but reactions between monomers B are forbidden. Besides the temperature of the catalyst, we also include lateral interactions between pairs of nearest-neighbor monomers. We employ Monte Carlo simulations and finite-size scaling arguments to calculate the moments of the order parameter of the model as a function temperature. Some ratios between pairs of moments are independent of temperature and are in the same universality class of the Contact Process. We also find the dynamical critical exponents of the model and we show that they are in the direct percolation universality class whatever the values of temperature.

[1]The authors would like to acknowledge the Brazilian agencies CAPES (PROBRAL program) and CNPq for the financial support.

C1.00230 Simulating Electroweak Baryogenesis in the Standard Model , ANDREW BLAIKIE, R. MIKE WINTERS, The College of Wooster, DEVA O'NEIL, Bridgewater College — One explanation for the abundance of matter over anti-matter in the universe is Electroweak Baryogenesis, which proposes that an excess of baryons was created during the electroweak phase transition, when particles first acquired mass. This transition, which occurred about one-tenth of a nanosecond after the Big Bang, proceeded through bubble nucleation, with the walls of the "bubbles" expanding until the electroweak symmetry was broken everywhere in space. We modeled this process in Mathematica using the Standard Model. Although current mass limits for the Higgs boson rule out Electroweak Baryogenesis in the Standard Model, our simulation can provide the basis for modeling more sophisticated scenarios. We used the sonification software SuperCollider to create an audio representation of the growth of the bubbles.

C1.00231 Shannon's entropy decreases spontaneously in certain isolated systems , SATORU SATO, Dept. of Network and Multi-Media Engineering, Kanto Gakuin University — In this study, we present an isolated system in which the Shannon's entropy decreases spontaneously. Of course physical entropy must increase in an isolated system according to the second law of thermodynamics. But Shannon's entropy which depends on the view point of an observer can decrease in certain isolated systems entailed by the increase of the physical entropy. As Shrödinger said in his famous book "entropy, taken with the negative sign, is itself a measure of order"[1]. However, the order of living organisms is not just the decrease of the physical entropy itself, but something in larger scale, for example proteins. This fact suggests that the formation of order does not necessarily involve the emission of physical entropy from the view point of information theory.

[1] E. Shrödinger, WHAT IS LIFE?, first published 1944

C1.00232 Trajectory Analysis for Inelastic Gravitational Billiards , ANDY YOST, JEFFREY OLAFSEN, Department of Physics, Baylor University — We present an analysis for an experiment [1] involving the motion of a gravitational billiard undergoing inelastic collisions with a sloped boundary. The inelastic particle is set into ballistic motion within three types of boundary shapes: parabolic, hyperbolic, and wedge geometries. The two-dimensional experimental cell is oriented vertically with respect to gravity and motion is maintained by horizontal shaking. Trajectories for various boundary shapes, shaking frequencies, and amplitudes are analyzed to determine regions of periodic and chaotic behavior. The shaking is provided by a DC-motor and armature that allows for control of both the shaking amplitude and frequency. Comparison of the experimental results to numerical methods provides a sensitive test of the velocity dependence of the coefficient of restitution. The trajectories may also be examined to extract a Lyapunov exponent for the motion.

[1] S. Feldt and J. S. Olafsen, Phys. Rev. Lett. **94**, 224102 (2005).

C1.00233 Nonlinear dynamics of an electronic model of one-way coupling in one and two dimensions , AARON DOUD, BARBARA BREEN, JAMIE GRIMM, ANDREW TANASSE, STUART TANASSE, University of Portland, JOHN LINDNER, KATSUO MAXTED, The College of Wooster — One-way or unidirectional coupling is a striking example of how topological considerations – the parity of an array of multistable elements combined with periodic boundary conditions – can qualitatively influence dynamics. Here we introduce a simple electronic model of one-way coupling in one and two dimensions and experimentally compare it to an improved mechanical model and an ideal mathematical model. In two dimensions, computation and experiment reveal richer one-way coupling phenomenology: in media where two-way coupling would dissipate all excitations, one-way coupling enables soliton-like waves to propagate in different directions with different speeds.

C1.00234 Gauss Modular-Arithmetic Congruence = Signal X Noise PRODUCT: Clock-model Archimedes HYPERBOLICITY Centrality INEVITABILITY: Definition: Complexity= UTTER-SIMPLICITY: Natural-Philosophy UNITY SIMPLICITY Redux!!! , E. E. KUMMER, EDWARD CARL-LUDWIG SIEGEL, FUZZYICS=CATEGORYICS(SON OF TRIZ) — Clock-model Archimedes [http://linkage.rockeller.edu/wli/moved.8.04/ 1fnoise/ index. ru.html] HYPERBOLICITY inevitability throughout physics/pure-maths: Newton-law F=ma, Heisenberg and classical uncertainty-principle=Parseval/Plancherel-theorems causes FUZZYICS definition: (so miscalled) "complexity" = UTTER-SIMPLICITY!!! Watkins[www.secamlocal.ex.ac.uk/people/staff/mrwatkin/]-Hubbard[World According to Wavelets (96)-p.14!]-Franklin[1795]-Fourier[1795;1822]-Brillouin[1922] dual/inverse-space(k,w) analysis key to Fourier-unification in Archimedes hyperbolicity inevitability progress up Siegel cognition hierarchy-of-thinking (HoT): data-info.-know.-understand.-meaning-...-unity-simplicity = FUZZYICS!!! Frohlich-Mossbauer-Goldanskii-del Guidice [Nucl.Phys.B:251,375(85);275,185 (86)]-Young [arXiv-0705.4678y2, (5/31/07] theory of health/life=aqueous-electret/ ferroelectric protoplasm BEC = Archimedes-Siegel [Schrodinger Cent.Symp.(87); Symp.Fractals, MRS Fall Mtg.(89)-5-pprs] 1/w-"noise" Zipf-law power-spectrum hyperbolicity INEVITABILITY= Chi; Dirac delta-function limit w=0 concentration= BEC = Chi-Quong.

C1.00235 Network-Physics(NP) BEC DIGITAL(#)-VULNERABILITY VERSUS FAULT-TOLERANT ANALOG , G. K. ALEXANDER, M. HATHAWAY, H. E. SCHMIDT, E. SIEGEL, FUZZYICS=CATEGORYICS(SON OF TRIZ) — Siegel[AMS Joint Mtg.(2002)-Abs.973-60-124] digits logarithmic-(Newcomb(1881)-Weyl(1914; 1916)-Benford(1938)-"NeWBe"/"OLDbe")-law algebraic-inversion to ONLY BEQS BEC:Quanta/Bosons= digits: Synthesis reveals EMP-like SEVERE VULNERABILITY of ONLY DIGITAL-networks(VS. FAULT-TOLERANT ANALOG INvulnerability) via Barabasi "Network-Physics" relative-"statics"(VS.dynamics-[Willinger-Alderson-Doyle(Not.AMS(5/09)]-]critique); (so called)"Quantum-computing is simple-arithmetic(sans division/ factorization); algorithmic-complexities: INtractibility/ UNdecidability/ INefficiency/NONcomputability / HARDNESS(so MIScalled) "noise"-induced-phase-transitions(NITS) ACCELERATION: Cook-Levin theorem Reducibility is Renormalization-(Semi)-Group fixed-points; number-Randomness DEFINITION via WHAT? Query(VS. Goldreich[Not.AMS(02)] How? mea culpa)can ONLY be MBCS "hot-plasma" versus digit-clumping NON-random BEC; Modular-arithmetic Congruences= Signal X Noise PRODUCTS = clock-model; NON-Shor[Physica A,341,586(04)] BEC logarithmic-law inversion factorization:Watkins number-thy. U stat.-phys.); P=/=NP TRIVIAL Proof: Euclid!!! [(So Miscalled) computational-complexity J-O obviation via geometry.

C1.00236 Finite-Size-Scaling at the Jamming Transition: Corrections to Scaling and the Correlation Length Critical Exponent[1] , STEPHEN TEITEL, University of Rochester, DANIEL VÅGBERG, Umeå University, DANIEL VALDEZ-BALDERAS, MICHAEL MOORE, University of Manchester, PETER OLSSON, Umeå University — We carry out a finite size scaling analysis of the jamming transition in frictionless bi-disperse soft core disks in two dimensions. We consider two different jamming protocols: (i) quench from random initial positions, and (ii) quasistatic shearing. By considering the fraction of jammed states as a function of packing fraction for systems with different numbers of particles, we determine the spatial correlation length critical exponent $\nu \approx 1$, and show that *corrections to scaling* are crucial for analyzing the data. We show that earlier numerical results yielding $\nu < 1$ are due to the improper neglect of these corrections.

[1]Supported by DOE Grant No. DE-FG02-06ER46298, Swedish Research Council Grant No. 2007-5234, a grant from the Swedish National Infrastructure for Computing (SNIC) for computations at HPC2N and the University of Rochester Center for Research Computing.

C1.00237 Response of Jammed Ellipsoid Packings , ZORANA ZERAVCIC, Lorentz Institute, Leiden University and James Franck Institute and Department of Physics, University of Chicago, ANDREA LIU, Department of Physics and Astronomy, University of Pennsylvania, SIDNEY NAGEL, James Franck Institute and Department of Physics, University of Chicago — We investigate the nature of the jamming transition for packings of spheroids by examining the elastic moduli as a function of the aspect ratio of the particles ε and the compression. Irrespective of the particle aspect ratio, both shear modulus G and bulk modulus B show the same scaling as a function of compression as is found for packings of spheres. Moreover, for any value of ε, G is proportional to the excess of the coordination number above that found at the jamming threshold; this recovers the result for frictionless spheres at $\varepsilon = 1$. Our results imply a new diverging length scale associated with the loss of rigidity of these spheroid packings. The critical behavior of ellipsoid packings is an extension of that found for spheres.

C1.00238 A new solution to the statistics of hard elongated objects , MOHAMMAD H. ANSARI, Institute for Quantum Computing, IQC and University of Waterloo — We propose a formalism that helps to study elasticity of hard elongated objects (e.g. needles, rectangles, ellipses, etc) analytically. For this aim, we introduce an approximation to the exact model that simplifies the Gibbs free energy to be solved analytically and then extract some formulations for a collective number of Gibbs related physical quantities. Interestingly, this formalism reproduces the numerical results of the exact model. The simplicity and the accuracy of this formalism allows to study some previously unknown properties of of elongated objects in different compressions, such as the elasticity coefficients of objects with curved boundary shapes. Moreover we introduce a new quantity, i.e. the mean inverse distance, and investigate how it behaves under different compressions.

C1.00239 Multiscale Modeling of Biomimetic Self-Healing Materials , GERMAN KOLMAKOV, AMY SCARBROUGH, CHET GNEGY, ISAAC SALIB, Chemical Engineering Department, University of Pittsburgh, KRZYSZTOF MATYJASZEWSKI, Department of Chemistry, Carnegie Mellon University, ANNA BALAZS, Chemical Engineering Department, University of Pittsburgh — We use a hybrid computational approach to examine the self-healing behavior of polymeric materials composed of soft nanogel particles crosslinked by a network of both stable and labile bonds. The latter are highly reactive and therefore, can break and readily reform. To capture the multiscale structure of the material, we take advantage of the multi-level Hierarchical Bell Model (mHBM) where the labile crosslinks are organized into M levels of interconnected elements, each of them represents a number of bonds that lie in parallel and is described by a single-level HBM. We vary the number of hierarchical levels M and the number of labile bonds in each element to determine optimal conditions for improving strength and toughness of the material. We also compare the properties of the multiscale material with those for the gel, in which only single-level interconnections are presented. This study takes its inspiration from biological systems that show remarkable resilience in response to mechanical deformation.

C1.00240 (BNL/DoE-hyped) "Self-Organized-Criticality"(SOC) is Merely Newton's(1687) Third Law of Motion F = ma REdiscovery: LONG PRE-"Bak"!!! , P.R.E. BAK, I. NEWTON, EDWARD CARL-LUDWIG SIEGEL, FUZZYICS=CATEGORYICS(SON OF TRIZ)/CATEGORY-SEMANTICS — "Bak"/BNL/DoE "self-organized-criticality"(SOC) usual BNL/DoE media-hype P.R spin-doctoring "show-biz" "Bush-waaa-...-aaah!!!" is manifestly-demonstrated in two distinct ways to be nothing but Newton's Third Law of Motion F = ma REdiscovery!!! PHYSICS: (1687) cross-multiplied F = ma rewritten as 1/m = a/F = OUTPUT/INPUT = EFFECT/ CAUSE = inverse-mass mechanical-susceptibility = X ("w "); X ("w ") ∼(F.-D. theorem-equivalence /proportionality)∼ P("w ") "noise" power-spectrum; E ∼ w ; and E ∼(any/all media upper-limiting-speeds)∼ m. Thus: w ∼ E ∼ m; inversion yields: 1/w ∼ 1/E ∼ 1/m ∼ a/F = X ("w ") ∼ P("w "); hence: F = ma dual/inverse-integral-transform is "'SOC"'s" P(w) ∼ 1/wˆ(1) !!! ; "PURE"-MATHS: F = ma double-integral time-series s(t) = [vot + (1/2) atˆ(2)] inverse/dual-integral-transform formally defines power-spectrum: P(w) = S {s(t) eˆ[-(i OR no i)w t]} dt = S {[vot + (1/2) atˆ2)] eˆ[-(i OR no i)w t]} dt = vo S {t eˆ[-(i OR no i)wt]} dt + (1/2) S {[a =/= a(t)] eˆ[-(i OR no i)wt)} dt = vo (d/dw) Delta (w) +(1/2) [a =/= a(t)] (d/dw)ˆ(2) Delta (w) = vo/w ˆ(0) +(1/2) [a=/=a(t)] /w ˆ1: if a = 0, then P(w) ∼ 1/w ˆ0, VS. if a =/= a(t) =/= 0, then P(w) ∼ 1/w; = by physics: "SOC" RE-expresses F = ma!!!: "just 'a tad' late/tardy" REdiscovery of F=ma: LONG PRE-"Bak"!!!

C1.00241 Deformation of Entangled Random Fiber Networks , CATALIN PICU, GOPINATH SUBRAMANIAN, Rensselaer Polytechnic Institute — The mechanics of random fiber networks which are not bonded or cross-linked but are subjected to topological constrains imposed by the excluded volume of the fibers is studied by means of a computational model. The fibers do not cross, have linear constitutive behavior in the axial and bending deformation modes and interact with each other frictionally. The system-scale response is highly-non-linear (power law) and hysteretic. The system exhibits a rich dynamics in response to imposed deformation, characterized by intermittency and spatial and temporal correlations of localized deformation (fiber-fiber sliding events). The role of friction in defining the overall system response is discussed.

C1.00242 Study of Transient Nuclei near Freezing , MASAHARU ISOBE, Nagoya Institute of Technology, BERNI ALDER, Lawrence Livermore National Laboratory — The molasses tail in dense hard core fluids is investigated by extensive event-driven molecular dynamics simulation through the orientational autocorrelation functions. Near the fluid- solid phase transition, there exist three regimes in the relaxation of the pair orientational autocorrelation function, namely the kinetic, molasses (stretched exponential), and diffusional power decay. The density dependence of both the molasses and diffusional power regimes are evaluated and the latter compares with theoretical predictions in three dimensions. The largest cluster at the freezing density of only a few sphere diameter in size persist for only about 30 picoseconds ($\sim 2.8 \times 10^{-11}$[s]). The most striking observation through the bond orientatinal order parameter is the dramatic increase of the cluster size as the freezing density is approached.

C1.00243 COMPLEX STRUCTURED MATERIALS I —

C1.00244 From 2D graphene to 1D graphene nanoribbons: dimensional crossover signals in the structural thermal fluctuations , ARIEL DOBRY, Instituto de Física Rosario (Argentine), SEBASTIÁN COSTAMAGNA, International School for Advanced Studies (Italy) and tituto de Física Rosario (Argentine) — I this work, by analyzing the thermal excited rippling in the graphene honeycomb lattice, we find clear signals of an existing dimensional crossover from 2D to 1D while reducing one of the dimensions of the graphene layer. Trough a joint study, using montecarlo atomistic simulations and analytical calculation based, we find that the normal-normal correlation function $G(q)$ does not change the power law behavior valid on the long wavelength limit, however the system size dependency of the quadratic out of plane displacement h^2 shows a breakdown of its corresponding scaling law. In this case we show that a new scaling law appear which correspond to a truly 1D system. On the basis of these results, and having explored a wide number of realistic systems size, we conclude that narrow nanoribbons presents strongest corrugations than the square graphene sheets. This result could have important consequences on the electron transport properties of freestanding graphene systems.

C1.00245 Properties of anisotropically etched graphene devices , C.M. REYNOLDS, A. ROBERTS, A.S. SANDHU, B.J. LEROY, University of Arizona — Mechanically exfoliated graphene on a SiO2 substrate was etched using a solution of nickel nanoparticles. Using an atomic force microscope, etch lines 10 nm in width were observed. In addition, etch lines made angles of only 60 and 120 degrees and did not cross one another indicating that the etching occurs along a crystallographic edge. This resulted in structures such as equilateral triangles and nanoribbons as narrow as 35 nm wide. We have investigated these devices using Raman spectroscopy and scanning tunneling spectroscopy to determine the quality of the crystallographic edges and the local electronic properties.

C1.00246 Anisotropy and edge roughness scattering in the thermal conductivity of graphene nanoribbons[1] , ZLATAN AKSAMIJA, IRENA KNEZEVIC, University of Wisconsin-Madison — We present a calculation of the thermal conductivity of graphene nanoribbons, based on solving the Boltzmann transport equation with the full phonon dispersions, a momentum-dependent model for edge roughness scattering, as well as three-phonon and isotope scattering. The interplay between strong edge roughness scattering and the anisotropy of the phonon dispersions results in thermal conduction that strongly depends on the chiral angle of the nanoribbon. A minimum occurs in the armchair direction and a maximum is attained in zig-zag nanoribbons. We also show that both the thermal conductivity and the amount of armchair/zig-zag anisotropy depend strongly on the width of the nanoribbon and the rms height of the edge roughness, with smallest and most anisotropic thermal conductivities occuring in narrow GNRs with rough edges. We conclude that physical width of the nanoribbon and the rms roughness of its line edges can be used along with angular direction as parameters to tailor the value of the thermal conductivity.

[1]This work has been supported by the Computing Innovation Fellows Project (NSF award No. 0937060 to the Computing Research Association, sub-award CIF-146 to the University of Wisconsin) and by the AFOSR YIP program (award No. FA9550-09-1-0230).

C1.00247 Electro-Mechanical Actuation of Carbon Nanotube Yarns, Sheets, Composites , JIYOUNG OH, MIKHAIL KOZLOV, The Alan G. MacDiarmid NanoTech Institute, University of Texas at Dallas, MEI ZHANG, Florida State University, SHAOLI FANG, RAY BAUGHMAN, The Alan G. MacDiarmid NanoTech Institute, University of Texas at Dallas — We report preparation of highly conductive carbon nanotube yarns and sheets. The materials aim at such applications as electronic textiles, electro-mechanical actuators, and conductive coatings. The electro-mechanical response of the specimens was measured using custom made force transducer operating in an isometric mode. The measurements were carried out at room temperature in aqueous and organic electrolytes; square-wave potential of variable amplitude was applied with a potentiostat. It was found that the maximum isometric stress generated by nanotube actuators could be as large as 12 MPa. This approaches the stress generation capability of commercial ferroelectrics and is significantly larger than that of natural muscles. A variety of applications of the materials is discussed.

C1.00248 Convenient growth of millimeter-long, few-walled carbon nanotube forests , RAQUEL OVALLE-ROBLES, XAVIER LEPRO, MARCIO LIMA, RAY BAUGHMAN, NanoTech Institute University of Texas at Dallas, NANOTECH INSTITUTE TEAM — We report the efficient growth of 3 mm long, few-walled carbon nanotube (FW-CNT) forests by chemical vapor deposition on Si substrates. High yields (nearly 90%) of FW-CNTs were grown in a continuous and controlled way in 3 hours without resorting to water-assisted growth. TEM and SEM images of 1 and 3 mm long FW-CNTs show that the forests are comprised of mostly carbon double walled nanotubes and single walled nanotubes having large diameters. The number of walls was controlled by the catalyst thickness (ranging from 0.2 to 0.6 nm) and nanotube length was controlled by adjustment of gas pressures (ethylene, hydrogen and argon), temperature and residence time. The Al_2O_3 buffer layer was critically important for this controlled synthesis.

C1.00249 Super acid processing of Single walled carbon nanotube (SWNT): effect of SWNT aspect Ratio on Macroscopic properties , NATNAEL BEHABTU, ANSON MA, DMITRI TSENTALOVICH, COLIN YOUNG, MATTEO PASQULI, Rice University — Single walled carbon nanotubes are exceptional building blocks that combine great mechanical, electrical and thermal properties with low density. A number of processing techniques have been proposed to manufacture macroscopic articles made purely of carbon nanotubes. Superacid processing is the most flexible and promising of all since it allows dissolution of a wide range of carbon nanotube materials, including hundreds of micron long carpets. Here we show how SWNT aspect ratio influences the rheology (both shear and extensional) of SWNT/super acid solution. The longest SWNT ($\sim$10 microns as measured by cryo-TEM) are able to form stable, highly aligned fibrils under elongational flow. Fibrils thus made can be recovered and further characterized. These fibrils have some of the lowest resistivity of SWNT based material to date (160 μm-cm). These materials can also be processed into conducting and transparent films via dip coating and vacuum filtration. Films made with the longest SWNT gave a sheet resistance of 150 Ohm/sq at 90% transparency. We have also mixed long SWNT at high concentration (10 wt%) and, as expected, they form liquid crystalline solution. Surprisingly, we find that the viscosity of highly concentrated solution is not a function of the aspect ratio of the constitutive molecules (unlike dilute solutions). This allows for the high concentration solutions to be successfully spun into neat SWNT fibers.

C1.00250 Development of Side-gated Carbon Nanotubes for Terahertz Studies[1] , CHRIS MCKITTERICK, JOEL CHUDOW, DANIEL SANTAVICCA, DANIEL PROBER, Yale, PHILIP KIM, Columbia — The single-walled carbon nanotube is a truly one-dimensional conductor. The currently accepted theory describing propagation of electrons in the nanotube is Luttinger liquid theory, which predicts collective charge modes moving at a velocity greater than the Fermi velocity. By modeling the carbon nanotube as a transmission line, this propagation velocity can be determined from the standing wave resonances in the system. Due to the high resistance of carbon nanotubes, a length on the order of one micron must be used, resulting in resonances which occur at terahertz (THz) frequencies. These resonances can be measured using the heating of the nanotube electron system [1]. To avoid the use of a conducting substrate that absorbs THz, we use a side gate. We describe the development of nanotube samples with side gates for the proposed THz experiment.
[1] D.F. Santavicca, J.D. Chudow, D.E. Prober, M.S. Purewal and P. Kim, Nano Lett. 10, 4538 (2010).

[1]Supported by NSF-DMR

C1.00251 Understanding the emission current limiting step in the carbon nanotube based polymer composite cathodes , DAVID CAREY, THOMAS CONNOLLY, RICHARD SMITH, University of Surrey — Carbon nanotube (CNT) based electronic applications often make use of the intrinsically high electrical conductivity of the nanotubes for charge transport. One attractive area for the exploitation of nanotubes is to combine their high electrical conductivity with their high aspect ratio leading to the development CNT based cathodes. In the presence of an electric field the field lines concentrate on the tip of nanotube and the resultant high local electric field (few V/nm) can result in electron tunneling (Fowler – Nordheim tunneling) from the tip and emission. Embedding a nanotube in a polymer matrix opens up the possibility of a large area and a solution processable way to produce cathodes [1]. We have studied the factors that control the rate limiting step for electron transport in functionalized CNTs in polyvinyl alcohol composites. We demonstrate excellent emission and current transport for nanotube volume fractions down to as low as 1 vol.% and that in the range from 1 vol.% to 7 vol.% the threshold field for emission does not significantly depend on nanotube content. Key to good emission is the ability to disperse the nanotubes efficiently.

[1] T. Connolly, R. C. Smith, Y. Hernandez, Y. Gun'ko, J. N. Coleman and J. D. Carey, Small **5**, 826 (2009).

C1.00252 In-Air Growth of Carbon Nanotubes[1] , CHRISTOPHER HUYNH, RYAN LU, AYAX RAMIREZ, SPAWAR SYS CEN PAC, DEBJYOTI BANERJEE, Texas A&M University, SSCPAC/TAMU COLLABORATION — Carbon nanotubes were fabricated using catalytic metal growth methods in air. Their microstructures were characterized using scanning electron microscopy and micro Raman spectroscopy. The results indicate non-aligned carbon nanotubes. In-air growth would facilitate implementation of wide-area growth of carbon nanotubes in a variety of DoD and commercial applications.

[1]Supported by ONR.

C1.00253 Molecular dynamics simulations of oxide memory resistors (memristors) , ALEXANDER BRATKOVSKY, Hewlett-Packard Laboratories, Palo Alto, S.E. SAVELIEV, A.S. ALEXANDROV, Loughborough U, UK, R.S. WILLIAMS, Hewlett-Packard Laboratories, Palo Alto — Reversible bipolar nano-switches that can be set and read electronically in a solid-state two-terminal device are very promising for applications. We have performed molecular- dynamics simulations that mimic systems with oxygen vacancies interacting via realistic potentials and driven by an external bias voltage. The competing short- and long-range interactions among charged mobile vacancies lead to density fluctuations and short-range ordering, while illustrating some aspects of observed experimental behavior, such as memristor polarity inversion. The simulations show that the "localized conductive filaments" and "uniform push/pull" models for memristive switching are actually two extremes of one stochastic mechanism [1].

[1] S. E. Savel'ev, A. S. Alexandrov, A. M. Bratkovsky, R. Stanley Williams, arXiv:1010.5656v1

C1.00254 The electrical and magnetic properties of C-doped ZnO film , DONG HAK KIM, JOON WON PARK, DAEYOUNG LIM, Kyung Hee University — The theoretical explanation on the room temperature ferromagnetism (RTF) in ZnO:C is based on the C incorporation at the O-site and the consequent exchange interaction between the localized C2p spins and valence-band holes. Here, we investigated the C incorporation site and the electrical properties of C-doped ZnO films grown by pulsed laser deposition (PLD) at both an oxygen rich and a poor conditions. Contrary to the theoretical explanations, all the C-doped ZnO films exhibited n-type conductivity. Furthermore, most of the carbons were not incorporated at the O-site, but rather at the interstitial or Zn site, or formed C clusters. Our experimental results indicate that the defect-induced ferromagnetism mechanism can better explain most of the observed RTF in the PLD grown ZnO:C films.

C1.00255 Molecular Simulations of Graphene-Based Electric Double-Layer Capacitors[1] , RAJA K. KALLURI, DEEPTHI KONATHAM, ALBERTO STRIOLO, The University of Oklahoma, School of Chemical, Biological and Materials Engineering — Towards deploying renewable energy sources it is crucial to develop efficient and cost-effective technologies to store electricity. Traditional batteries are plagued by a number of practical problems that at present limit their widespread applicability. One possible solution is represented by electric double-layer capacitors (EDLCs). To deploy EDLCs at the large scale it is necessary to better understand how electrolytes pack and diffuse within narrow charged pores. We present here simulation results for the concentrated aqueous solutions of NaCl, CsCl, and NaI confined within charged graphene-based porous materials. We discuss how the structure of confined water, the salt concentration, the ions size, and the surface charge density determine the accumulation of electrolytes within the porous network. Our results, compared to data available for bulk systems, are critical for relating macroscopic observations to molecular-level properties of the confined working fluids.

[1]Research supported by the Department of Energy.

C1.00256 Capture and release of carbon dioxide by carbon nanotubes via temperature cycling[1] , DENIZ RENDE[2], NIHAT BAYSAL[2], Yeditepe University, RAHMI OZISIK, Rensselaer Polytechnic Institute — Carbon nanotubes (CNTs) received remarkable attention since they were shown to possess many unique properties as well as being effective and stable adsorbent materials that make them potentially useful for gas storage and separation of various gas mixtures. In this study, the effect of temperature variations on carbon dioxide (CO_2) capture via single walled carbon nanotubes (SWNTs) and multi walled carbon nanotubes (MWNTs) were investigated with molecular dynamics simulations. SWNTs of type (10,10), (15,15), and (20,20) and MWNTs formed from the combination of these were simulated. The temperature was varied between 300 and 360 K. The results suggest that absorption of CO_2 into the CNTs were directly related to the internal volume of the nanotube, but the cross-sectional area of the tube entrance had a significant effect on the number of CO_2 molecules retained. The number of CO_2 molecules collected in CNTs gradually decreases with increasing temperature. Separate simulations were performed to understand the potential use of CNTs as thermal pumps to collect/discharge CO_2 molecules via temperature cycling.

[1]Supported by the NSF (CMMI-0500324 and DMR-0117792).
[2]Currently at Rensselaer Polytechnic Institute

C1.00257 Half-Metallic Sandwich Molecular Wires with Negative Differential Resistance and Sign-Reversible High Spin-filter Efficiency , LU WANG, XIN YAN, JING ZHOU, JING LU, ZHENGXIANG GAO, State Key Laboratory for Mesoscopic Physics and Department of Physics, Peking University, Beijing 100871, P. R. China, XINGFA GAO, SHIGERU NAGASE, Department of Theoretical and Computational Molecular Science, Institute for Molecular Science, Okazaki 444-8585, Japan, STEFANO SANVITO, School of Physics and CRANND, Trinity College, Dublin 2, Ireland, YUTAKA MAEDA, Department of Chemistry, Tokyo Gakugei University, Tokyo 184-8501, Japan, TAKESHI AKASAKA, Center for Tsukuba Advanced Research Alliance, University of Tsukuba, Ibaraki 305-8577, Japan, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, Nebraska 68182-0266 — Using density functional theory and non-equilibrium Green's function method, we construct organometallic nanowires that consist of Fe or V atoms sandwiched between composite molecules (Cp*FeCp*, where Cp* is $C_5(CH_3)_5$). For the first time, we demonstrate that half-metallicity, negative differential resistance, and sign-reversible high spin-filter capability can coexist remarkably in one organometallic nanowire (FeCp* wire). This renders FeCp* wire promising in electronics and spintronics.

C1.00258 An investigation on work-function enhancement in multilayer graphene , ABBAS EBNONASIR, BRANDEN B. KAPPES, CRISTIAN V. CIOBANU — Using density functional theory calculations, we perform a detailed analysis of the electronic properties of multilayer graphene on a generic substrate. A range of the possible substrate effects is simulated by systematically changing the interlayer distance between the first two graphene layers and leaving the other layers at the nominal graphite spacing. We find that the work function on the graphite-like side varies with the number of layers and with the distance between the first two layers, and we analyze the charge transfer distribution and the surface dipole moment as a function of the distance between the first two graphene layers. We correlate our results with reported experimental observations and provide possible explanations of pronounced work-function variations.

C1.00259 Scanning Tunneling Microscopy Study of Grain Boundaries in Graphene Grown by Chemical Vapor Deposition on Copper Foil , JUSTIN KOEPKE, DAVID ESTRADA, JOSHUA WOOD, ERIC POP, JOSEPH LYDING, University of Illinois at Urbana-Champaign — There have been few scanning tunneling microscopy studies of graphene grown by CVD on Cu [1] and no atomic scale studies of the electronic properties of the films' grain boundaries. We present the electronic nature of grain boundaries in polycrystalline graphene grown by CVD on Cu foil and transferred to SiO2 substrates. These grain boundaries are continuous across large protrusions and wrinkles in the graphene and other surface topography. We observe misorientation angles of approximately 7°, 23°, and 30° across the grain boundaries and standing wave patterns adjacent to the grain boundaries with a decay length on the order of 1 nm. The spectroscopy shows enhanced conduction in empty states at the grain boundaries. The graphene is grown on 1.4 mil copper foil by CVD. After growth the graphene was transferred onto a SiO_2/Si substrate using PMMA and $FeCl_3$. Raman spectroscopy and atomic force microscopy are used to characterize the roughness and quality of the graphene. The sample was degassed in the UHV-STM system at 600 – 700 °C for 24 hours.

[1] X. Li et al., Science 324, 1312 (2009)

C1.00260 CVD graphene growth on different substrates[1] , P. HÄBERLE[2], A. CORTES, C. CELEDON, V. DEL CAMPO, UTFSM — Graphene growth on solid substrates have the advantage of growing high quality epitaxial graphene. In this sence it is important to choose substrates and precursors having in mind the final application and an efficiency if the process. In this work we grow graphene by CVD on three different substrates, changing temperatures and precursor concentration. For graphene growth on copper foil we heat the sample up to 1000 ° C in the presence of a hydrogen and acethylene flux. The same process is performed for graphene growth on copper oxide thin films. These thin films (∼400 nm) are prepared by conventional sputtering on SiO_2 substrates and the reduced inside the preparation chamber. The advantage of this process is that copper undergoes a dewetting process during graphene growth, so at the end we have graphene suported on the SiO_2 substrate. To monitor graphene growth we use Raman spectrometer. For graphene growth on Ru(0001) we heat the substrate, temperature between 840°C and 1000°C in ultra high vacuum (UHV). We introduce ethylene in the vacuum chamber and cool down the sample. To monitor graphene growth we use Low Energy Electron Diffraction.

[1]FONDECYT & CENAVA
[2]CENAVA

C1.00261 Controlling the Thermal Decomposition of Silicon Carbide into Graphene[1] , DAVID TORRANCE, TIEN HOANG, DAVID MILLER, BAIQIAN ZHANG, WALT DE HEER, PHILLIP FIRST, Georgia Institute of Technology — The quality of epitaxial graphene films grown by thermal decomposition of silicon carbide depends on experimental control of the net silicon desorption rate. Such control has been previously demonstrated by three techniques: tight confinement within an induction furnace, growth in 1-atm Ar buffer gas, or introduction of a silane overpressure. Our goal is to study the physics of these methods. We have constructed an all-graphite UHV induction furnace with maximum temperature over 1700° C and gas handling that allows process gas pressures from UHV to 1 atm. Sample holders with different orifices are used to vary the furnace confinement. Our initial systematic measurements of the effect of Ar buffer gas pressure establish that the silicon sublimation rate is adequately described by a 1D diffusion model with geometry-dependent parameters.

[1]Supported in part by the NSF, and the NRI-INDEX

C1.00262 Large area growth of single layer graphene on the C-face SiC , BAIQIAN ZHANG, MING RUAN, MICHAEL SPRINKLE, YIKE HU, JOHN HANKINSON, School of Physics, Georgia Institute of Technology, CLAIRE BERGER, School of Physics, Georgia Institute of Technology; Institut Néel, CNRS, Grenoble, France, WALT A. DE HEER, School of Physics, Georgia Institute of Technology — High quality graphene, from monolayer to many layers are consistently grown on the carbon terminated face of 4H-SiC, using the confinement controlled sublimation growth method in an induction furnace. Here we show large area monolayer graphene grown on silicon carbide substrates with this method. C-face 1cmx1cm SiC samples were graphitized by carefully controlling silicon sublimation. Ellipsometry measurements demonstrate an essentially uniform high quality graphene layer over the entire surface. The SiC chip is entirely covered by monolayer graphene, with less that 5% of bi-layer region. The thickness homogeneity is confirmed by photoemission electron microscopy, Raman spectroscopy, Atomic force microscopy (AFM). We also present transport measurements on single graphene layer C-face sample.

C1.00263 Micellization and phase transitions in a triblock copolymer-D_2O system[1] , HOSANNA ODHNER, Bryn Mawr, ALISON HUFF, KELLY PATTON, D.T. JACOBS, The College of Wooster, BRYNA CLOVER, University of Maryland, College Park, SANDRA GREER[2], University of Maryland and Mills College — The triblock copolymer ("unimer") of PPO-PEO-PPO (commercially known as 17R4) has hydrophobic ends and a hydrophilic center. When placed in D_2O at lower concentrations and temperatures, only a network of unimers exists. However, at higher concentrations or temperatures, micelles of different geometries can form. We have measured the micellization line marking the transition from only unimers to some micelles, as well as a one- to two-phase transition at higher temperatures. This second transition is an Ising-like, LCST critical point, based on the shape of the coexistence curve. We find the LCST to not correspond to the minimum of the cloud point curve, which indicates polydispersity as described by Sollich.

[1]We acknowledge the support from Research Corporation, NSF-REU grant DMR 0649112, The College of Wooster, and (for BC and SG) to the donors of the Petroleum Research Fund, administered by the American Chemical Society
[2]currently Provost at Mills College

C1.00264 INSULATORS AND DIELECTRICS —

C1.00265 The T_g of polycyanurate in cylindrical nanoporous confinement , SIYANG GAO, SINDEE SIMON — The glass transition behavior of materials under nanoconfinement is often different than their behavior in the bulk. A leading explanation is that enhanced mobility at free surfaces or neutral interfaces results in depressions in Tg, whereas attractive interfaces result in increases in Tg. In this work, we examine the Tg of a polycyanurate using differential scanning calorimetry for both material confined in cylindrical nanopores and for freely-standing nanocylinders. Preliminary results using an alumina nanofilter for the confining matrix indicate that the Tg depression for the supported and freely standing nanocylinders are similar. The implications of the results will be discussed.

C1.00266 Band Alignment of atomic layer deposited HfO2 on clean and N passivated Germanium surfaces , ABDUL RUMAIZ, Brookhaven National Laboratory, JOSEPH WOICIK, NIST, GABRIELLA CARINI, PETER SIDDONS, Brookhaven National Laboratory, ERIC COCKAYNE, NIST, PATRICK LYSAGHT, SEMATECH, DANIEL FISCHER, NIST — Hard x-ray photoelectron spectroscopy (HAXPES) has been used to study the band alignment between atomic layer deposited (ALD) HfO2 on clean Ge (100) and nitrogen treated Ge (100) surfaces. The position of the valence-band maximum was determined by convolving theoretically calculated density of states from first-principles calculations and comparing with experimental valence-band data. The valence-band offset was found to be 3.2 ± 0.1 and 3.3 ± 0.1 eV for the samples grown on clean and N passivated Ge, respectively. The oxide charge however shows a significant increase between the two samples. The small change in the band offset between the two systems strongly indicates negligible contribution of the interface to the conduction/valence-band barrier and the band alignment of the heterojunctions.

C1.00267 Spectroscopic Ellipsometry of Gadolinium Gallium Oxide Multilayers , KALEB GILBERT, KUNAL BHATNAGAR, STEVE JACKSON, Angelo State University, RAVI DROOPAD, WILHELMUS GEERTS, Texas State University — The dielectric parameters of Gadolinium Gallium Oxide (GGO) multilayer structures have been investigated with spectroscopic ellipsometry and modeled with a simplified modeling technique. The GGO thin films are of varying thickness and the simple four parameter model was effective in determining consistent values for the dielectric constants of this important high k dielectric material. Ellipsometric data was collected in two different acquisition configurations to insure the merit of the model. The model is further confirmed by the determination of film thickness values within an acceptable range when compared with those reported by the sample grower. The dielectric parameters are then used to determine the band gap of GGO.

C1.00268 The existence of an isopermitive point of water at low frequencies , HILDA MERCADO, ABRIL ANGULO, Cinvestav-Monterrey — Water has been studied extensively since the last past century and it continues to be a subject of great interest because it has special properties and a relevant role in biological functions. One of the most used techniques to study water is the dielectric spectroscopy. Normally, the studies with this method are carried out at frequencies higher than 1 MHz. We have studied the relative permittivity of water at low frequencies (100 Hz to 1 MHz), and we found that this varies strongly as a function of the frequency. In addition, we found a specific frequency where this parameter is independent of temperature and we called it the isopermitive point. Below this point the relative permittivity increase with temperature, above, it decreases. Our explanation of this behavior is that water can be considered as a system of two species: dipoles and ions. The first obey the Maxwell-Boltzmann statistics, while the second causes the Maxwell-Wagner-Sillars effect. At the isopermitive point the effect of both mechanisms in the relative permittivity compensate each other.

C1.00269 An *Ab Initio* Study of rare gases in uranium dioxide[1] , LI MA, ASOK RAY, University of Texas at Arlington — Hybrid density functional theory has been used to study the stability and behavior of rare gases (He, Ne, Ar, Kr and Xe) in uranium dioxide. The calculations have been performed using the all-electron full-potential linearized augmented plane wave plus local orbitals basis (FP-L/APW+lo) method. Three insertion sites are considered: the octahedral interstitial position and the oxygen and uranium substitution sites. The defect formation energy, the optimized lattice constants and the volume variation induced by gaseous atom incorporation, and the electronic structure are studied for each rare gas in anti-ferromagnetic UO_2 phase without and with spin-orbit coupling (scalar vs. "full" relativistic). The results indicate that the lattice constants and formation energies increase with the increase of the radius of the rare gases. The octahedral interstitial position is the most favorable occupation site. All incorporation energies are found to be positive implying an exothermic process.

[1]This work is partially supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525) and by the Department of Energy.

C1.00270 Ab initio study of adatom adsorption on topological insulator thin film , KYUNG-HWAN JIN, Department of Physics, Pohang University of Science and Technology, SEUNG-HOON JHI, Department of Physics and Division of Advanced Materials Science, Pohang University of Science and Technology — Recently topological insulator has attracted great attention due to its intriguing electronic and transport properties. Topological insulator has bulk energy gap but conducting surface states which are chiral with a linear energy-momentum relation. These surface states are robust against external perturbations as they are protected by the time reversal symmetry. We studied the electronic structure of topological insulator Bi_2Te_3 thin film and investigated how it is modified upon the adsorption of single atomic impurities using first-principles calculations. We chose nitrogen (N), oxygen (O), sodium (Na) and cobalt (Co) atoms to study their adsorption on top of Bi_2Te_3surface. We investigated the effect of non-magnetic and magnetic impurities on the surface states, and the band splitting due to the inversion symmetry-breaking by the Rashba field.

C1.00271 Phonons in Bi2Te3 and Bi2Se3 Thin Films[1] , SHANG-FEN REN, Illinois State University, WEI CHENG, Beijing Normal University — Bi2Te3 and Bi2Se3 are topological insulators attracted great research attention in recent years. In this research, some of calculated results on phonons in Bi2Te3 and Bi2Se3 bulk and single quintuple thin films are presented. The effects of spin-orbit couplings on phonon properties in these materials are discussed. Some features of Raman observations of these materials are explained.

[1]Acknowledgement: (1) Subcontract of Dr. Y. Cui's KAUST Investigator Award (No. KUS-l1-001-12). (2) Prof. D. S. Wang at Institute of Physics (CAS), his grant (NSFC-10634070), and Supercomputing Center of CAS in Beijing. (3) WC's visit to LBNL.

C1.00272 Performance of the spin- and angle- resolved photoemission spectrometer with highly efficient VLEED spin detector , K. MIYAMOTO, T. OKUDA, A. KIMURA, H. MIYAHARA, K. KURODA, H. NAMATAME, M. TANIGUCHI, Hiroshima univ. — Because of the growing scientific interests in the spin-related exotic materials such as topological insulators, spin- and angle- resolved photoemission with much improved efficiency is strongly desired. In this report, we present the current status of a new SARPES with significantly improved energy- (ΔE) and angular resolutions ($\Delta\theta$), which is under construction at beam line BL-9B in Hiroshima Synchrotron Radiation Center. The system consists of high performance hemispherical analyzer (VG-Scienta R-4000) and highly efficient spin detector based on very low energy electron diffraction of Fe(001)p(1x1)-O, which has 100 times higher efficiency than conventional Mott spin detector. Owing to the high efficiency of the detector, the highest ΔE and $\Delta\theta$ have been improved to be 7.5 meV and 0.37^o. Moreover, high-resolution ARPES measurement ($\Delta E \sim 2$meV, $\Delta\theta \sim 0.2^o$) and Fermi surface mapping in the sample temperature range from 8K to room temperature can be efficiently performed by hemispherical analyzer equipped with multi-channel detector and motorized 5 axis goniometer. These features of the SARPES enable us to observe detailed spin-dependent band structures of topological insulators very precisely and efficiently.

C1.00273 Statistics of Josephson vortices in topological superconductors , EYTAN GROSFELD, University of Illinois, ADY STERN, Weizmann Institute of Science — In recent years there has been an intensive search for Majorana fermions in condensed matter systems. Predicted to be localized on cores of vortices in certain non-conventional superconductors, their presence is known to render the exchange statistics of bulk vortices non-Abelian. In this talk I will present novel results regarding the persistence of Majorana zero modes into insulating barriers, providing a way to coherently and effectively manipulate them. A method to probe the Majorana modes will be presented.

C1.00274 Van der Waals epitaxial growth and transport properties of Bi2Se3 thin films[1] , JIAN-HAO CHEN[2], JACK HELLERSTEDT, WILLIAM CULLEN, MICHAEL FUHRER, Dept. of Physics, Materials Research Science and Engineering Center and Center for Nanophysics and Advanced Materials, Univ. of Maryland, College Park — Thin films of Bi_2Se_3 with high carrier mobility are grown with van der Waals epitaxy method in ultra-high vacuum environment on single crystal Sapphire (0001) and single crystal $SrTiO_3$ (111) surfaces. *Ex-situ* transport measurement revealed weak-antilocalization-like behavior at small out-of-plane magnetic field (B_o) and non-linear Hall conductance versus Bo. The carrier concentration of the Bi_2Se_3 can be substantially tuned with applied electric field through the $SrTiO_3$ substrate.

[1]This work was supported by the UMD NSF-MRSEC grant no. DMR 05-20741.

[2]Present address: Department of Physics, UC Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

C1.00275 Electronic properties at the interface in oxide $BiFeO_3$/Nb-doped $SrTiO_3$ semiconductor , YU-TING CHEN, YA-PING CHIU, MIN-CHUAN SHIH, Department of Physics, National Sun Yat-sen University, Kaohsiung, 804, Taiwan, ROC, JAN-CHI YANG, Department of Materials Science and Engineering, National Chiao Tung University, HsinChu, 300, Taiwan, ROC, YI-CHUN CHEN, Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan, ROC, YING-HAO CHU, Department of Materials Science and Engineering, National Chiao Tung University, HsinChu, 300, Taiwan, ROC — In oxide systems, the interface of the heterojunctions had attracted much attention due to the interesting properties of the low-dimensional electron confinement. In this work, by using cross-sectional scanning tunneling microscopy, the direct and local information of structural and electronic properties across the$p-n$ heterojunction in the multiferroic $BiFeO_3$ films grown on Nb-doped $SrTiO_3$ substrate was investigated. Spectroscopy analysis of the point-to-point electronic properties allows us to realize how the asymmetrically electronic band alignment is formed at the interface. Further analysis of the evolution of the potential field across the interface also reveals that surface charge states, spontaneous polarization, and the $p-n$ contact contribute to the formation of the build-in field pointing from $BiFeO_3$ films to Nb-$SrTiO_3$ semiconductors.

C1.00276 Size dependent anomalous dielectric behavior in nanoparticle Gd_2O_3 : SiO_2 glass composite system , SUDIP MUKHERJEE, YU-HSING LIN, TING-HUI KAO, C.C. CHOU, H.D. YANG, Department of Physics and Center for Nanoscience and Nanotechnology, National Sun Yat-Sen University, Kaohsiung, 804 Taiwan — Gd_2O_3 (0.5 mol%) nanoparticles have been synthesized in a silica glass matrix by the sol-gel method at calcination temperatures of 700 °C and above. Compared with the parent material SiO_2, this nano-glass composite system shows enhancement of dielectric constant and diffuse phase transition along with magnetodielectric effect around room temperature. Observed conduction mechanism is found to be closely related to the thermally activated oxygen vacancies. Magnetodielectric behavior is strongly associated with magnetoresistance changes, depending on the nanoparticle size and separation. Such a material might be treated as a potential candidate for device miniaturization.

C1.00277 Study of field-dependent coupling of mixed phases in highly-strained BFO by impedance spectrum , JHIH-WEI CHEN, Dept. of Physics, National Cheng Kung University, YI-CHUN CHEN, H.J. CHEN, W.I. LIANG, YING-HAO CHU — In this study, we investigated the dielectric mechanism of highly-strained BFO epitaxial films with Tetragonal (T)-like and rhombohedral (R)-like monoclinic phases. The ratio of R-like BFO to T-like BFO is controllable by varying the film thickness through the relaxation of substrate stress. The impedance spectrum of T-like and R-like samples showed conducting-system dispersive (CSD) peaks at 20 kHz and 6.7 MHz, respectively. By contrast, the T+R-BFO had an additional dielectric-system dispersive (DSD) mechanism at relatively low frequency of 4.2 kHz. Moreover, the distribution range of relaxation time for this mechanism depended on the switching history, implying that the mechanism is related to the ferroelastic interaction between the two monoclinic phases. This result suggested intermediate states through phase transformation will reduce energy barrier for polarization switching. The effect of interfacial capacitance between sample and electrode was also discussed.

C1.00278 Monoclinic phase transition in stress-induced BiFeO3 epitaxial films , YEN-CHIN HUANG, Department of Physics, National Cheng Kung University, Y.C. CHEN, C. CHENG, K.I. LIN, J.S. HWANG, W.I. LIANG, H.J. CHEN, Y.H. CHU — Material system near morphotropic phase boundary usually attracted a lot of attention due to their unique physical properties. The key issue of the mechanism is to reveal the coupling between the multiple phases or the intermediate states during phase transformation. Recently, highly-strained multiferroic BiFeO3 (BFO) films had been reported to possess a particular isosymmetric boundary between tetragonal(T) and rhombohedral(R) phases. In this study, we investigated the as-grown state of mixed-phase BFO and the evolution of phases under external stimulus. Through first principle study and Raman measurement, we found the mixed phase BFO films at room temperature included two monoclinic phases, MA(Cm) and MC (Pm). When the temperature was increased to about 420 K, MC phase transformed to a R-like phase. The MA and the R-like phase coexisted until 620 K; after that, the R-like phase disappeared while the MA lasted to higher temperatures. This result showed the possible path of transition near the morphotropic phase boundary.

C1.00279 Tunnel electroresistance in ferroelectric tunnel junctions , A. CHANTHBOUALA, A. CRASSOUS, V. GARCIA, K. BOUZEHOUANE, S. FUSIL, J. GROLLIER, C. DERANLOT, Unite Mixte de Physique CNRS/Thales, France, X. MOYA, N. MATHUR, University of Cambridge, UK, M. BIBES, A. BARTHELEMY, Unite Mixte de Physique CNRS/Thales, France — In tunnel junctions with a ferroelectric barrier, large resistance changes can arise upon switching the ferroelectric polarization direction. This tunnel electroresistance (TER) effect has recently been observed by scanning probe techniques on electrode/barrier bilayers (e.g. LSMO/$BaTiO_3$), yielding giant TER values in the 50000% range at room temperature. Beside their fundamental interest to elucidate the interplay between electrostatic effects, changes in the interfacial density of states, piezoelectricity and quantum-mechanical tunneling, ferroelectric tunnel junctions undoubtedly present a great potential for application as memory devices with simple, non-destructive readout and low-power write operations. We will present our progress towards the realization of solid-state ferroelectric tunnel junctions and discuss their potential as next-generation non-volatile memories.

C1.00280 Structural and Magnetic Study of $YCrO_3$ Doped with Calcium[1] , EDUARDO VERDIN, Departamento de Física, Universidad de Sonora, México, FRANCISCO MORALES, RAUL ESCAMILLA, ROBERTO ESCUDERO, Instituto de Investigaciones en Materiales, UNAM, México, ALEJANDRO DURAN, Centro de Nanociencias y Nanotecnologia, UNAM, Ensenada, B. C. México — In recent years there has been much interest in multiferroic materials. The coupling between ferromagnetic and ferroelectricity on the same material is important from both basic science and applications. Here we address the behavior observed in $YCrO_3$ doped with Ca. The pure material presents a ferroelectric transition at about 473 K, and ferromagnetism at about 140 K. The magnetic transition is due to canted spins, so ferromagnetism and antiferromagnetism coexist. In this presentation we will show the studies on Ca doped $YCrO_3$. We show that Ca does not affect the magnetic transition (T_N), but the dielectric behavior is strongly affected by the increase of the electrical conductivity (σ_{ac}) in the range of 35 to 200 °C.

[1]Thanks to DGAPA-UNAM through project no. IN112909.

C1.00281 Surface magnetization of a multiferroic with linear M-to-P coupling: The case of $FeTiO_3$, JAMES GLASBRENNER, KIRILL BELASHCHENKO, University of Nebraska-Lincoln — A multiferroic material with linear coupling between the magnetization **M** and electric polarization **P** could serve as an electric switch of magnetization. However, for applications it is necessary to couple its magnetization to a proximate ferromagnet through exchange bias at the interface. Symmetry considerations indicate that multiferroics with linear **M**-to-**P** coupling should also have a boundary magnetization, which is not directly coupled to **P** but is rather determined by the surface normal direction. This magnetization can present an obstacle for electric switching of exchange bias. Here we investigate the (001) surface magnetization of $LiNbO_3$-type $FeTiO_3$ using first-principles PAW calculations with spin-orbit coupling. The surface magnetization appears through spin canting of the surface moments. This canting is found for different surface terminations and compared with the bulk behavior.

C1.00282 Impact of Step Defect on Surface States of Topological Insulators , DEGANG ZHANG, C.S. TING, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, TX 77204 — Recent topological insulators have attracted much attention in the condensed matter community due to the existence of surface states. The Dirac-cone topological surface states, which preserve time-reversal symmetry, are produced by strong spin- orbit coupling. In recent STM experiments, the modulations of local density of states (LDOS) induced by a step defect were observed. In this work, we investigate electron tunneling in the presence of $\delta(x)$ or $\delta(y)$ potential on the surface of topological insulators in the framework of quantum mechanics and calculate the LDOS near the δ potential. The STM experiments could be interpreted by an additional spin torque term in the wave function. We also figure out the oscillatory features of the LDOS produced by the $\delta(x)$ and $\delta(y)$ potentials, respectively.

C1.00283 Current-Induced Spin Polarizations in Surfaces of Topological Insulators , TETSURO MISAWA, Tokyo Institute of Technology, SHUICHI MURAKAMI, Tokyo Institute of Technology, PRESTO, Japan Science and Technology Agency — Topological Insulators (TI) have gapless conducting states on their surfaces, which are largely spin-split. Former studies have showed that in spin-orbit coupled systems, current can induce a spin polarization. In this research, we calculate the response of the TI surface state to the dc electric field, that is, transverse conductivity and the induced in-plane spin polarization in the presence of delta-function impurities using Kubo formula. Additionally, in Bi_2Te_3, the shape of Fermi surface is warped to be 6-fold rotationally symmetric; thereby the transport properties are modified. In this warped Fermi surface, we predict that the current induces a component of spin polarization perpendicular to the surface as a nonlinear response. This out-of-plane polarization may be easier to detect than in-plane polarization. Using the 6-fold rotational symmetry, we discuss the nonlinear response of spin accumulation to the current and its implications on Bi_2Te_3. We also study another non-linear effect, the inverse Faraday effect, where the oscillating electric field induces the dc spin polarization.

C1.00284 GENERAL PHYSICS I —

C1.00285 Blowpipe Mineralogy for Physics/Environment: Highest-Possible-Tc SuperConductor (Beyond: (but via!!!) MgB2, Cuprates, Pnictides) Quest; BOTH PERMANENT FOREVER Carb-IDES SOLID-State Sequestration AND Drought(s)-Elimination , KURT SEGLER, WENDELL WILLIAMS, EDWARD SIEGEL, FLYING-WATER — Detailed are old blowpipe new applications: charcoal-block reduction of borates to yield ("N-NW" of MgB2) Overhauser-[PR 35,1,411(1987); Intl.J.Mod.Phys.1, 2 & 4, 927(1987)]-"land" predicted high-EST-POSSIBLE Tc SC ∼ "LiD2"; very-early: Siegel[Phys.Stat.Sol.(a)11,45(1972);Semiconductors.and Insulators 5: 39,47,62(1979)] carb-IDES SOLID-state phase-TRANSITIONED CHEMICALLY-REDOX"-REACTED STABLE PERMANENT LONG-term NOT "CO2" BUT C-sequestration: PROFITABLE "Grab and Sell" TRUMPS "cap and trade"!!!; Mott alloying/vertical metal-insulator transitions in "borax-(GLASS)-beads"; and very-earlySiegel [3rd Intl.Conf.Alt.Energy (1980)-vol.5/p.459!!!] "FLYING-WATER" Hindenberg-effect (H2-UP;H2O-DOWN) via Hydrogen-maximal-Archimedes-buoyancy "chemical-rain-in-pipelines", only via Siegel proprietary "magnetic-hydrogen-valve"(MHV): Renewables-Hydrogen-Water flexible versatile agile scaleable retrofitable integrated operating-system for PERMANENT drought(s)-elimination FOREVER!!!

C1.00286 Consciousness can reduce the voltage of the output signal of solar cell , DAYONG CAO, Beijing Natural Providence Science & Technology Development Co., Ltd — When the sun's light radiate on the solar cell, it can produce the output signal as the pho- tocurrent. We use the Data Acquisition Modules to record the voltage of the output signals. The v1 is voltage of the photocurrent of solar cell1; The v2 is the one of solar cell2. And these two solar cells stay side by side. When we record the voltages from the morning to the noon, the voltages will go up, and the v1 is bigger than the v2 during this time. But in other experi- menter, not only sun's light ratiade on two solar cells, but also consciousness act on two solar cells. Not only I can use consciousness to reduce the growth voltage of the output signals, but also can change the v1 to be littler than the v2. The experiment was conducted on Sep. 2010. When light of lamp radiate on two solar cells, I can reduce v1, at the same time, can augment v2. These experiments had been finished in Los Angeles, Oct. 26th. And the experiment show that the consciousness active function differ from the passive function of conditioned reflex (of Pavlov). There is the physical system of the mass, energy, space and time-MEST; There is the spirited system of the mind, consciousness, emotion and desire-MECD; the information system is the code system. We can use the consciousness change the electron-structure of solar cell by the interaction of the information.

C1.00287 FLYING-WATER Renewables-H2-H2O TERRAFORMING: PERMANENT Drought(s)-Elimination FOREVER!!! , G. ERTL, G. ALEFELD, W. YOUDELIS, H. RADD, G. OERTLE, EDWARD SIEGEL, FLYING-WATER — "H2O H2O everywhere; ne'er a drop to drink"[Coleridge(1798)]; now: "H2 H2 everywhere; STILL ne'er a drop to drink": ONLY H2 (or methane CH4) can be FLYING-WATER(F-W) chemical-rain-in-pipelines Hindenberg-effect (H2-UP;H2O-DOWN): {O/H2O}=[16]/[18] ∼90%; O already in air uphill; NO H2O pumping need! In global-warming driven H2O-starved glacial-melting world, rescue is possible ONLY by Siegel [3rd Intl. Conf. Alt.-Energy (1980)-vol.5/p.459!!!] Renewables-H2-H2O purposely flexible versatile agile customizable scaleable retrofitable integrated operating-system. Rosenfeld[Science 315,1396(3/9/2007)]-Biello [Sci.Am.(3/9/2007)] crucial geomorph-ology which ONLY maximal-buoyancy H2 can exploit, to again make "Mountains into Fountains", "upthrust rocks trapping the clouds to precipitate their rain/snow/H2O": "terraforming"(and ocean-rebasificaton!!!) Siegel proprietary magnetic-hydrogen-valve (MHV) permits H2 flow in already in-ground dense BCC/ferritic-steels pipelines-network (NO new infrastructure) counters Tromp[Science 300,1740(2003)] dire warning of global-pandemics (cancers/ blindness/famine) Hydrogen-economy CATASTROPHIC H2 ozone-layer destruction sobering cavat to dangerous H2-automotion-economy panacea hype!!!

C1.00288 FRAUD/SABOTAGE Killing Nuclear-Reactors Need Modeling!!!: "Super"alloys GENERIC ENDEMIC Wigner's-Disease/.../IN-stability: Ethics? SHMETHICS!!! , JOSEPH O'GRADY, fPa/PSEG/ASTM, ARLDEN BUMENT, fPa/BMI/NIST/NSF, EDWARD SIEGEL, failure-PREVENTION-asociates(fPa)/Westin"KL"ouse/PSEG/IAEA/ABB/ — Carbides solid-state chemistry domination of old/new nuclear-reactors/spent-fuel-casks/refineries/jet/missile/rocket-engines is austenitic/FCC Ni/Fe-based (so miscalled)"super"alloys(182/82;Hastelloy-X,600,304/304L-SSs,...690!!!) GENERIC ENDEMIC EXTANT detrimental(synonyms): Wigner's-disease(WD) [J.Appl.Phys.17,857 (46)]/Ostwald-ripening/spinodal-decomposition/overageing-embrittlement/thermal-leading-to-mechanical(TLTM)-INstability: Mayo[Google: < "If Leaks Could Kill" >;-Siegel[J.Mag.Mag.Mtls.7,312(78)=at flickr.com search on "Giant-Magnotoresistance" <<<"Fert" [PRL(1988)]-"Gruenberg"[PRL(1989)] 2007-Nobel]necessitating NRC inspections on 40+25=65 Westin"KL"ouse PWRs(12/2006)]-Lai [Met.Trans.AIME, 9A,827(78)]-Sabol-Stickler[Phys.Stat.Sol.(70)]-Ashpahani[Intl.Conf. Hydrogen in Metals, Paris(1977]-Russell [Prog.Mtls.Sci.(1983)]-Pollard [last UCS rept.(9/1995)]-Lofaro [BNL/DOE/NRC Repts.]-Pringle [Nuclear-Power:From Physics to Politics(1979)]-Hoffman [animatedsoftware.com], what DOE/NRC MISlabels as "butt-welds" "stress-corrosion cracking" endpoint's ROOT-CAUSE ULTIMATE-ORIGIN is WD overageing-embrittlement caused brittle-fracture cracking from early/ongoing AEC/DOE-n"u"tional-la"v"atories sabotage!!!

C1.00289 Horizons and Phase Space , RICHARD KRISKE, University of Minnesota — This author has previously suggested that the CMBR may not be entirely due to the generalized Red-Shift, but may be due to the curvature of the Universe in that the time dimensional axis would gradually tilt away from the observer at great distances in the same way that the height dimension tilts away from the observer on the surface of the Earth. There is a well known theory used by navigators that uses Euclidean Geometry to gauge this effect on the surface of the Earth, but when used in 4 space this method lacks the height needed to calculate the distance to the horizon in that the height is the time dimension. A similar height like variable can be found in QED however in the phase that is calculated from the Lagrangian. This author is suggesting that QED needs to be corrected in adding an additional phase that comes about from information conveyed in the wave-function at the time it is created giving it information about the direction of the time dimension which is rotated as the wave function moves and ultimately changes the frequency of the photon. This is field information that resembles current theories.

C1.00290 Interface Defect States and Charge Transport Properties in Low-Cost Photovoltaic Devices made from Scalable Deposition Methods[1]

, ANDREW MARIN, DAVID MUNOZ-ROJAS, DIANA IZA, TALIA GERSHON, JUDITH MACMANUS-DRISCOLL, University of Cambridge — Electrochemical deposition and Atmospheric Atomic Layer Deposition (AALD) are high-throughput, scalable methods that can be used to produce low-cost transition metal oxides for photovoltaic devices. Previous work by our group has used electrochemical deposition to fabricate ZnO/Cu_2O cells, however the performance of these cells is limited by poor Cu_2O transport properties and recombination at interface states. AALD has been shown to produce much smoother films of Cu_2O but little work has been done to characterize the electrical properties of these films. Similarly little work has been done to show the ability of AALD to reduce interface defect states. In this investigation, we use impedance spectroscopy and illuminated solar cell performance to examine the electrical properties of Cu_2O films and ZnO/Cu_2O photovoltaic devices. We also show how AALD can deposit seed layers for further improved electrochemical deposition.

[1]The authors would like to thank the Gates-Cambridge Trust and the International Copper Association.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D1 DCMP: New Developments in Quantum Criticality Ballroom A1

2:30PM D1.00001 Quantum critical points and novel phases in heavy fermion metals[1]

, QIMIAO SI, Rice University — Quantum criticality arises from competing interactions of correlated systems that favor rivaling ground states. It not only influences physical properties over a wide temperature and parameter ranges, but also gives rise to a plethora of new quantum phases. Magnetic heavy fermion metals represent a prototype system in this context, and have in particular provided the setting to study local quantum criticality that involves not only order-parameter fluctuations but also a Kondo breakdown [1]. Surprisingly, recent theoretical and experimental developments have revealed some unusual phases proximate to the heavy-fermion quantum critical points, thereby opening up an entirely new frontier on the relationship between quantum criticality and novel phases [1]. I will summarize the relevant recent experiments [2] and discuss them within the framework of a global phase diagram that was put forward several years ago [3] and has recently been discussed more extensively [4,5]. Our theoretical studies emphasize the interplay between two effects. One is the Kondo screening and its breakdown, and the other is the fluctuations in the quantum magnetism of local moments alone. The insights gained from these studies of the well-defined quantum criticality in heavy fermions may have broader relevance. Such implications will be discussed, in particular on the interplay between metallic antiferromagnetism, electronic localization and unconventional superconductivity.

[1] Q. Si and F. Steglich, Science 329, 1161 (2010).
[2] S. Friedemann et al., Nature Phys. 5, 465 (2009);[0pt] J. Custers et al., PRL 104, 186402 (2010).
[3] Q. Si, Physica B 378, 23 (2006); S. J. Yamamoto and Q. Si, PRL 99, 016401 (2007).
[4] Q. Si, Phys. Status Solidi B247, 631 (2010); S. J. Yamamoto and Q. Si, J. Low Temp. Phys. 161, 233 (2010).
[5] P. Coleman and A. H. Nevidomskyy, J. Low Temp. Phys. 161, 182 (2010).

[1]Supported by NSF and the Robert A. Welch Foundation.

3:06PM D1.00002 Two-dimensional Confinement of Heavy Fermions in Artificial Superlattices[1]

, HIROAKI SHISHIDO, Research Center for Low Temperature and Materials Sciences, Kyoto University, Kyoto, Japan — Low dimensionality and strong electron-electron Coulomb interactions are both key parameters for novel quantum states of condensed matter. A metallic system with the strongest electron correlations is reported in rare-earth and actinide compounds with f electrons, known as heavy-fermion compounds, where the effective mass of the conduction electrons are strikingly enhanced by the electron correlations up to some hundreds times the free electron mass. To date the electronic structure of all heavy-fermion compounds is essentially three-dimensional. We realized experimentally a two-dimensional heavy fermion system, adjusting the dimensionality in a controllable fashion. We grew artificial superlattices of $CeIn_3(m)/LaIn_3(n)$, in which m-layers of heavy-fermion antiferromagnet $CeIn_3$ and n-layers of a non-magnetic isostructual compound $LaIn_3$ are stacked alternately, by a molecular beam epitaxy [1]. By reducing the thickness of the $CeIn_3$ layers, the magnetic order was suppressed and the effective electron mass was further enhanced. The Néel temperature becomes zero at around $m = 2$, concomitant with striking deviations from the standard Fermi liquid low-temperature electronic properties. Standard Fermi liquid behaviors are, however, recovered under high magnetic field. These behaviors imply new "dimensional tuning" towards a quantum critical point. We also succeeded to fabricate artificial superlattices of a heavy fermion superconductor $CeCoIn_5$ and non-magnetic divalent Yb-compound $YbCoIn_5$. Superconductivity survives even in $CeCoIn_5(3)/YbCoIn_5(5)$ films, while the thickness of $CeCoIn_5$ layer, 2.3 nm, is comparable to the c-axis coherence length $\xi_c \sim$2 nm. This work has been done in collaboration with Y. Mizukami, S. Yasumoto, M. Shimozawa, H. Kontani, T. Shibauchi, T. Terashima and Y. Matsuda.superconductivity is realized in the artificial superlattices.

[1] H.Shishido *et al.*, Science **327** 980 (2010).

[1]This work has been done in collaboration with Y. Mizukami, S. Yasumoto, M. Shimozawa, H. Kontani, T. Shibauchi, T. Terashima and Y. Matsuda.

3:42PM D1.00003 Universal Signatures of Metamagnetic Quantum Criticality[1]

, FRANZISKA WEICKERT, Los Alamos National Laboratory, MPA-CMMS, Los Alamos, NM, 87545, USA — The continuous quest for quantum critical materials is inspired by the exotic phases and unusual phenomena that can be observed close to a zero-temperature instability. An appealing realization of such a critical point is found in metamagnetic materials where the magnetization shows a finite step at a certain magnetic field that becomes more pronounced at low temperatures. The most striking advantages of this kind of quantum criticality are that the critical point is i) symmetric in the associated thermodynamic phase diagram and not accompanied by a symmetry-breaking ordered phase and ii) the tuning parameter magnetic field H can be adjusted continuously and makes a very detailed and comprehensive study of this so called quantum critical end-point (QCEP) possible. In the presented talk the qualitative features of a field-driven QCEP are discussed, which result from very basic thermodynamic relations and the two general assumptions that i) the differential magnetic susceptibility diverges at the critical field H_c by definition and ii) the QCEP has Ising symmetry. We present real examples of metamagnetic systems, where the characteristics can be found experimentally. Particular emphasis will be placed on the well-known intermetallic material $CeRu_2Si_2$. We argue that a QCEP is approximately realized in this compound and confirm our claims by the combination of new high-resolution thermal expansion, magnetostricion and specific heat results. Very similar behavior was found recently on the prominent material $Sr_3Ru_2O_7$ whose metamagnetic quantum criticality is masked by the appearance of a phase proposed to be of nematic electronic nature. We believe that our work will facilitate and promote the experimental identification of further metamagnetic systems for quantum criticality in the future.

[1] *Weickert et al.*, Phys. Rev. B, **81**, 134438 (2010).

[1]This work was carried out at the MPI for Chemical Physics of Solids in Dresden, Germany.

4:18PM D1.00004 Quantum criticality and confinement effects in an Ising chain in transverse field

, RADU COLDEA, University of Oxford — The Ising chain in transverse field is one of the key paradigms for the theory of continuous zero-temperature quantum phase transitions. We have recently realized this system experimentally by applying strong magnetic fields to the quasi- 1D, low-exchange Ising ferromagnet CoNb2O6 to drive it to its quantum critical point where the spontaneous long-range magnetic order is suppressed by magnetic field [1]. Using high-resolution single-crystal neutron scattering we have probed how the spin dynamics evolves with the applied field and have observed a dramatic change in the character of spin excitations at the quantum critical point, from pairs of domain-wall (kink) quasiparticles in the magnetically-ordered phase, to sharp spin-flip quasiparticles in the paramagnetic phase. The weak, but finite couplings between the chains significantly enrich the physics by stabilizing a complex structure of two-kink bound states due to mean-field confinement effects. In zero field the rich spectrum of bound states can be quantitatitively understood following McCoy and Wu's analytic theory of weak confinement [2]. Just below the critical field the energies of the two lowest bound states approach the "golden ratio" as predicted by Zamolodchikov's E8 scaling limit solution of the off-critical Ising model in a weak longitudinal field [3].

[1] R. Coldea, D.A. Tennant, E.M. Wheeler, E. Wawrzynska, D. Prabhakaran, M. Telling, K. Habicht, P. Smeibidl, K. Kiefer, Science 327, 177 (2010).
[2] B. M. McCoy and T. T. Wu, Phys. Rev. D 18, 1259 (1978).
[3] A.B. Zamolodchikov, Int. J. Mod. Phys. A4, 4235 (1989).

4:54PM D1.00005 Strange metals and quantum phase transitions from gauge/gravity duality

, HONG LIU, MIT — Metallic materials whose thermodynamic and transport properties differ significantly from those predicted by Fermi liquid theory, so-called non-Fermi liquids, include the strange metal phase of cuprate superconductors, and heavy fermion systems near a quantum phase transition. We use gauge/gravity duality to identify a class of non-Fermi liquids. Their low-energy behavior is governed by a nontrivial infrared fixed point which exhibits non-analytic scaling behavior only in the temporal direction. Some representatives of this class have single-particle spectral functions and transport behavior similar to those of the strange metals, with conductivity inversely proportional to the temperature. Such holographic systems may also exhibit novel "magnetic instabilities", where the quantum critical behavior near the transition involves a nontrivial interplay between local and bulk physics, with the local physics again described by a similar infrared fixed point. The resulting quantum phase transitions do not obey the standard Landau-Ginsburg-Wilson paradigm and resemble those of the heavy fermion quantum critical points.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D2 DCMP: Topological Surface States Ballroom A2

2:30PM D2.00001 Visualizing surface states of topological insulators using spectroscopic mapping with the scanning tunneling microscope[1]

, PEDRAM ROUSHAN, Princeton University — In topological insulators, the spin texture of the surface states makes them distinct from conventional two-dimensional electron states, and leads to novel properties for these states. These surface states are expected to be immune to localization and to overcome barriers caused by material imperfections. We have used scanning tunneling microscopy and spectroscopy to study the topological surface states in $Bi_{0.9}Sb_{0.1}$, *Sb,* and Bi_2Te_3. By mapping the interference of the surface states scattering off random alloying disorder in $Bi_{0.9}Sb_{0.1}$, we have demonstrated that despite strong atomic scale disorder, backscattering between states of opposite momentum and opposite spin is absent, resulting from the spin texture [1]. Furthermore, we have measured the transmission and reflection of topological surface states of *Sb* through atomic terraces [2]. In contrast to Schottky surface states of noble metals, these surface states penetrate such barriers with high probability. To examine the possibility of disorder induced localization, we investigated the surface states of Bi_2Te_3 in the presence of local defects. In the presence of magnetic dopants, we have observed an interference pattern throughout a broad range of energies, even in the region of linear dispersion near the Dirac point [3]. We discuss the results of a statistical analysis of these patterns which can help to learn about the tendency toward localization for these surface states and how this trend is affected as the energy is tuned to the Dirac point. *Work was done in collaboration with J. Seo, H. Beidenkopf, L. Gorman, Y. S. Hor, C. Parker, D. Hsieh, and A. Richardella, M. Z. Hasan, R. Cava, and A. Yazdani.

[1] P. Roushan *et al.* Nature 460, 1106 (2009).
[2] J. Seo *et al.* Nature 466, 343 (2010).
[3] H. Beidenkopf *et al.* (2010).

[1]Supported by NSF-DMR, and MRSEC through PCCM. Infrastructure at Princeton Nanoscale Microscopy Laboratory are also supported by grants from DOE, and the W.M. Keck foundation.

3:06PM D2.00002 STM and STS studies of electronic states near macroscopic defects in topological insulators[1]

, ZHANYBEK ALPICHSHEV, Stanford University — Bi_2Te_3 and Bi_2Se_3 have been argued recently to be three-dimensional (3D) topological insulators (TI), exhibiting a bulk gap and a single, non-degenerate Dirac fermion surface band topologically protected by time-reversal symmetry. In this talk we will discuss the physics of topological insulators. We will show that Scanning tunneling spectroscopy (STS) studies on high-quality Bi_2Te_3 and Bi_2Se_3 crystals exhibit perfect correspondence to ARPES data, hence enabling identification of different regimes measured in the local density of states (LDOS). Unique to Bi_2Te_3, we will discuss observations of oscillations of LDOS near a step. Within the main part of the surface band we found that the oscillations are strongly damped, supporting the hypothesis of topological protection. At higher energies, as the surface band becomes concave, oscillations appear which disperse with a particular wave-vector that results from an unconventional hexagonal warping term in the surface-state-band Hamiltonian [1]. For both systems, a bound state was observed in the bulk gap region that runs parallel to the edge of the defect and is bound to it at some characteristic distance. An expression that fits the data, and provides further insight into the general topological properties of the electronic structure of the surface band near strong structural defects, can be obtained using the full three-dimensional Hamiltonian of the system.

[1] Zhanybek Alpichshev, J. G. Analytis, J.-H. Chu, I. R. Fisher, Y. L. Chen, Z. X. Shen, A. Fang, and A. Kapitulnik *Phys. Rev. Lett.* **104** 016401 (2010)

[1]In collaboration with J. G. Analytis, J.-H. Chu, I. R. Fisher, Y. L. Chen, Z. X. Shen, A. Fang, and A. Kapitulnik.

3:42PM D2.00003 Theory of Topological Insulators and Superconductors: Application to Cux-Bi2Se3

, LIANG FU, Harvard Univ — This abstract not available.

4:18PM D2.00004 Investigation and manipulation of the electronic properties of magnetically doped topological insulators[1] , KE HE, Institute of Physics, Chinese Academy of Sciences — Topological insulator (TI) is characterized by gapless surface/edge states which are protected by time reversal symmetry (TRS). Magnetic order in or adjacent to a TI can break its TRS, and thus result in various exotic phenomena, e.g. magnetic monopole, quantum anomalous Hall effect, and topological magneto-electric effect. Combining angle-resolved photoemission spectroscopy, scanning tunneling microscopy/spectroscopy, and transport measurement, we have investigated the electronic structures and properties of Bi2Se3 family three dimensional TIs doped with magnetic impurities. Gap opening at the Dirac surface states induced by magnetic impurities has been observed, suggesting the formation of long range magnetic order in the TIs. The Dependences of the gap size on impurity concentration, chemical potential and real space position and the (anomalous) Hall effect of the magnetically doped TIs have been systematically studied, the result of which reveals the nature and mechanism of the magnetic order. The present studies pave the road to the realization of the novel properties predicted in magnet/TI heterostructures.

[1]This work was supported by NSFC and MOST of China.

4:54PM D2.00005 Theory of surface phenomena in topological insulators , MARCEL FRANZ, University of British Columbia — Recently discovered topological insulators (TIs) are materials with bulk bandgap and robust gapless surface states protected by topological invariants that characterize their bulk band structure. After a brief introduction to the physics of TIs I will describe recent theoretical advances in understanding the behavior of surface electrons in the presence of both magnetic and non-magnetic impurities, surface steps, as well as magnetic and superconducting coating. The key property of the topological surface states – absence of backscattering from non-magnetic defects – leads to a number of features that stand in a stark contrast to the physics of ordinary non-topological states. Among these are vastly enhanced transmission through crystal steps, absence of quasiparticle interference patterns caused by non-magnetic impurities and formation of a gap in the presence of magnetic impurities.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D3 DMP GERA: Materials for Energy Ballroom A3

2:30PM D3.00001 Material tradeoffs in direct thermal to electric energy conversion systems , ALI SHAKOURI, Baskin School of Engineering, University of California, Santa Cruz — Thermoelectric devices allow direct conversion of heat into electricity without any moving parts. However the energy conversion efficiency has been limited due to parasitic Joule heating in the thermoelectric material as well as the heat leakage from the hot to the cold junction mainly through phonons. Using thermionic emission over heterostructures and electron energy filtering, high Seebeck coefficient and high electrical conductivity can be achieved simultaneously. Embedded nanoparticles can also be used to scatter mid and long wavelength phonons and reduce the lattice thermal conductivity with small impact on electrical transport. While the tradeoff in material properties can be reduced with nanoengineered structures, the overall efficiency/cost tradeoff has not been analyzed in detail. In a waste heat recovery system, in addition to the thermoelectric device, the heat sink and the electrical and thermal resistances have to be co-optimized. A recent analytic theory is reviewed which shows the potential of thermoelectric waste heat recovery in a wide range of applications. Co-optimization of the thermoelectric module with the heat sink will permit minimizing the amount of material used in the system and reduce the overall energy payback. Optimization of the thermoelectric system in maximum output power regime, which is important in many practical applications, lead to interesting conclusions about the asymmetric role of thermal resistances with hot and cold reservoirs.

3:06PM D3.00002 Photophysics of Strongly Confined Multiexcitons from the Perspective of Lasing and Solar Energy Conversion[1] , VICTOR KLIMOV, Los Alamos National Laboratory — Using semiconductor nanocrystals one can produce extremely strong spatial confinement of electronic wave functions not accessible with other types of nanostructures. One consequence of this effect is a significant enhancement in carrier-carrier interactions that lead to a number of novel physical phenomena including ultrafast mutiexciton decay due to Auger recombination and efficient generation of multiple electron-hole pairs by single photons via carrier multiplication. In this talk, I will discuss the implications of ultrafast Auger decay for lasing applications of the nanocrystals and describe several recent approaches developed in our group for resolving this problem by engineering carrier-carrier interactions in various types of heterostructured particles. I will also review the current status of carrier-multiplication research including experimental challenges in studies of this phenomenon, the role of extraneous effects, the competing energy relaxation channels, and applications of carrier multiplication in solar photovoltaics.

[1]This material is based upon work within the Center for Advanced Solar Photophysics, an Energy Frontier Research Center of the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

3:42PM D3.00003 Engineering Interfaces for Photovoltaic Energy Conversion , STACEY BENT, Stanford University — Dye-sensitized solar cells (DSSCs) and the related quantum dot-sensitized solar cells (QDSSCs) show promise as inexpensive, efficient next-generation photovoltaic technologies. A typical cell design consists of a sensitizer chemisorbed to a nanoporous TiO_2 substrate; the sensitizer absorbs a photon and an excited electron is injected into the TiO_2 where it diffuses to the anode. However, many devices suffer from a high rate of electron-hole recombination at the interface between TiO_2 and the hole conductive material, leading to reduced conversion efficiency. In this work we explore whether a passivating layer at the interface can improve efficiency by acting as a barrier against electron recombination. We have studied both organic and inorganic approaches to modifying the interfacial properties in DSSC and QDSSC devices. In studies of CdS-based QDSSCs, a series of organic self-assembled monolayers were formed at the interface, and their effect on CdS uptake and resulting optoelectronic and device properties was investigated. In DSSCs, nanoscale inorganic dielectric films of different thicknesses were applied to the interface using atomic layer deposition prior to dye absorption. The effect on device performance was measured experimentally and compared with predictions from kinetic models. The results of these investigations will be discussed in the context of the ability of interface engineering to improve photovoltaic energy conversion.

4:18PM D3.00004 Experimental and Theoretical Studies on Phonon Mean Free Path in Thermoelectric Materials[1] , GANG CHEN, MIT — Nanostructured thermoelectric materials have shown improved thermoelectric figure of merit due to reduced phonon thermal conductivity. To design nanostructures that effectively scatter phonons via interface and boundary scattering, it is important to know the phonon mean free path of thermoelectric materials in their bulk form. In this talk, we will present recent progress in experimental and theoretical investigation of phonon mean free path in thermoelectric materials. On the experimental side, we extend an optical pump-and-probe technique to measure contributions of phonons with different mean free paths to thermal conductivity via systematically changing the size of the heated regions. On the theoretical side, we apply first-principle calculations to extract anharmonic force constants, and compute the phonon relaxation time due to phonon-phonon scattering. We will present experimental and theoretical results obtained on silicon, half-heuslers, etc, and their implications to thermoelectric materials.

[1] This work is supported partially by S3TEC, a DOE BES funded EFRC, and by JSPS Excellent Young Researchers Overseas Visit Program.

4:54PM D3.00005 Progress in Materials for Solar Energy Conversion , EICKE WEBER, Fraunhofer-Institut fr Solare Energiesysteme ISE — This abstract not available.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D4 DCOMP DAMOP: Simulations Meet Experiments on Ultracold Quantum Gases

Ballroom A4

2:30PM D4.00001 Pairing states of a one-dimensional spin imbalanced Fermi gas accross a Feshbach resonance , ADRIAN FEIGUIN, University of Wyoming — A description of the BCS-BEC crossover in one dimension that properly accounts for the coexistence of fermions and bound pairs can be achieved in the framework of the Bose-Fermi resonance model, in which two fermions in an open channel couple resonantly to a diatomic molecule in the closed channel. In the case of a gas with spin imbalance, pairing correlations consistent with a phase of the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) type dominate a wide parameter range on the BCS side of the resonance. In the BEC regime, the FFLO correlations are suppressed, leading to a Bose-Fermi mixture consisting of a conventional bosonic superfluid in the molecular channel immersed into a gas of fermions that is either partially or fully polarized. I will present results of a comprehensive numerical study of this model using the density matrix renormalization group method, and determine the dependence of the critical polarization on filling and detuning. [F. Heidrich-Meisner, A.E. Feiguin, U. Schollwoeck, W.Z werger, Phys. Rev. A81, 023629 (2010)]

3:06PM D4.00002 Quantum Simulations with Ultracold Bosons in Optical Lattices and Superlattices , STEFAN TROTZKY, Ludwig-Maximilians-Universitat Munchen — Ultracold quantum gases in optical lattices have opened a new window for understanding strongly correlated many-body systems. They especially allow for ab-initio tests of fundamental condensed matter theories. In the presentation, I will discuss several examples, where static phases and non-equilibrium evolutions of ultracold quantum gases are compared to theoretical simulations. Among the examples that will be discussed are the measurement of the critical temperature for superfluidity in the vicinity of the quantum phase transition from a superfluid to a Mott insulator and the observation of a reentrant phase transition between superfluid and Mott insulating phases in a columnar superlattice. Finally, I will report on experimental and theoretical results that shed light on the question how isolated, strongly interacting quantum systems, can locally appear as if the system has equilibrated globally.

3:42PM D4.00003 Trapping, cooling and probing fermionic atoms into the Mott and Neel states[1] , JEAN-SEBASTIEN BERNIER[2], College de France and Ecole Polytechnique — A new form of quantum condensed matter physics has emerged from the study of ultra-cold fermionic atoms in optical lattices. Experiments have recently reached the incompressible Mott regime. Detailed comparison to theory and computational studies at intermediate temperatures have validated the concept of optical lattice emulation of many-body fermionic systems. Cooling these systems deeper into the quantum degenerate regime, and devising new spectroscopic probes to investigate physical issues of interest such as quasiparticle properties, are key challenges in this context. The presentation will be based in part on the following references: L. De Leo, C.Kollath, A.Georges, M.Ferrero and O.Parcollet Phys. Rev. Lett. 101, 210403(2008); J.-S. Bernier et al. Phys. Rev. A 79, 061601 (2009); R. Jördens et al. Phys. Rev. Lett. 104, 180401 (2010); J.-S. Bernier et al., Phys. Rev. A 81, 063618 (2010); L. De Leo et al., arXiv:1009.2761

[1]Collaboration with J.S. Bernier, L. De Leo and C.Kollath is especially acknowledged. Work supported in part by CNRS, the "Triangle de la Physique" and the DARPA-OLE program.

[2]In collaboration with Antoine Georges, College de France and Ecole Polytechnique.

4:18PM D4.00004 Generalized Thermalization in Integrable Systems[1] , MARCOS RIGOL, Georgetown University — Once only of theoretical interest, integrable models of one-dimensional quantum many-body systems can now be realized with ultracold gases. The possibility of controlling the effective dimensionality and the degree of isolation in the experiments have allowed access to the quasi-1D regime and to the long coherence times necessary to realize integrable models. In general, in integrable quantum systems that are far from equilibrium, observables cannot relax to the usual thermal expectation values. This is because of the constraints imposed by the non-trivial set of conserved quantities that make these systems integrable. Experimentally, relaxation of an observable to a non-thermal expectation value was recently observed in a cold-atom system close to integrability. At integrability, it is natural to describe the observables after relaxation by an updated statistical mechanical ensemble: the generalized Gibbs ensemble (GGE), which is constructed by maximizing the entropy subject to the integrability constraints. In recent studies, the GGE has been found to accurately describe various observables in the steady state of integrable systems, but a microscopic understanding of its origin and applicability remains elusive. In this talk, we review some of the early results on this topic and discuss the justification of the GGE based on a generalized view of the eigenstate thermalization hypothesis, which was originally introduced to explain thermalization in nonintegrable systems. **References:**

[1] M. Rigol, V. Dunjko, V. Yurovsky, and M. Olshanii, Phys. Rev. Lett. **98**, 050405 (2007).
[2] M. Rigol, A. Muramatsu, and M. Olshanii, Phys. Rev. A **74**, 053616 (2006).
[3] A. C. Cassidy, C. W. Clark, and M. Rigol, arXiv:1008.4794.

[1]This work was supported by the US Office of Naval Research.

4:54PM D4.00005 A quantitative analysis of small atomic systems , LODE POLLET, ETH Zurich — Ultracold atoms in an optical lattice provide a unique toolbox for emulating the prototypical models of condensed matter physics. Before the optical lattice system can be trusted as a quantum simulator however, it needs to be validated and benchmarked against known results, for which quantum Monte Carlo simulations are ideally suited. In this talk, an overview of recent numerical studies of ultracold bosonic and fermionic systems in an optical lattice will be given, starting with a full comparison based on experimental time-of-flight images of bosons in an optical lattice and ab-initio simulations. Next, the advantages of single-site resolution detection tools will be highlighted. Finally, the temperature and entropy in present experiments on fermions in an optical lattice will be estimated, and the full thermodynamics on approach to the Neel temperature will be presented. Nearest-neighbor spin-spin correlations are shown to be useful for thermometry.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D5 FIAP: Industrial Physics Forum: Frontiers in Physics

Ballroom C1

2:30PM D5.00001 Controlling how atoms respond to ultra-intense x-ray radiation[1] , LINDA YOUNG, Argonne National Laboratory — With the advent of the Linac Coherent Light Source, the world's first hard x-ray free electron laser, an era of exploration using ultrafast, ultra-intense x-ray pulses has arrived. One can deposit 100,000 x-ray photons into one square Angstrom within 100 fs, producing an electric field strength that exceeds that binding the electron in a hydrogen atom. How does matter respond under these conditions? Using neon atoms, we investigated the electronic response as the x-ray interaction is tuned from the outer to the inner shell. At photon energies above all inner-shell edges, fully stripped neon is produced via six-photon absorption. The route to bare neon proceeds through photoejection of 1s electrons that produces hollow atoms and an intensity-induced x-ray transparency. X-ray transparency can be induced in all atomic, molecular and condensed matter systems. Going beyond non-resonant x-ray atom interactions, we investigated the atomic response at inner-shell resonances and find evidence for x-ray induced Rabi cycling. These investigations provide a framework for understanding ultra-intense x-ray interactions with matter.

[1]Work supported by DOE, Office of Basic Energy Sciences.

3:06PM D5.00002 Scanning Tunneling Microscopy of Dirac Fermions at mK Temperatures , JOSEPH STROSCIO, NIST — Since the beginning of the last century new frontiers in physics have emerged when advances in instrumentation achieved lower experimental operating temperatures. Notable examples include the discovery of superconductivity and the integer and fractional quantum Hall effects. New experimental techniques are continually adapted in order to meet new experimental challenges. A case in point is scanning tunneling microscopy (STM) which has seen a wealth of new measurements emerge as cryogenic STM instruments have been developed in the last two decades. In this talk I describe the design, development and performance of a scanning probe microscopy facility operating at a base temperature of 10 mK in magnetic fields up to 15 T [1]. The microscope is cooled by a custom designed, fully ultra-high vacuum (UHV) compatible dilution refrigerator (DR) and is capable of in-situ tip and sample exchange. Sub-picometer stability at the tip-sample junction is achieved through three independent vibration isolation stages and careful design of the dilution refrigerator. The system can be connected to, or disconnected from, a network of interconnected auxiliary UHV chambers used for sample and probe tip preparation. Current measurements are focusing on Dirac fermions in graphene and in topological insulators. The history of the fractional quantum Hall states in semiconductor heterostructures suggests that studying graphene at lower temperatures and higher magnetic fields may reveal new quantum phases of matter. Scanning tunneling spectroscopy of graphene at mK temperatures reveals the detailed structure of the degenerate Landau levels in graphene, resolving the full quartet of states corresponding to the lifting of the spin and valley dengeneracies [2]. When the Fermi level lies inside the four-fold Landau manifold, significant electron correlation effects result in enhanced valley splitting and spin splitting. New many-body states are observed at fractional filling factors of 7/2, 9/2, and 11/2.

[1] *A 10 mK Scanning Probe Microscopy Facility*, Y. J. Song, A. F. Otte, V. Shvarts, Z. Zhao, Y. Kuk, S. R. Blankenship, A. Band, F. M. Hess, and J. A. Stroscio, Rev. Sci. Instrum. (in press).
[2] *High Resolution Tunneling Spectroscopy of a Graphene Quartet*, Y. Jae Song, A. F. Otte, Y. Kuk, Y. Hu, D. B. Torrance, P. N. First, W. A. de Heer, H. Min, S. Adam, M. D. Stiles, A. H. MacDonald, and J. A. Stroscio, Nature **467**, 185 (2010).

3:42PM D5.00003 Topological materials and their potential applications , SHOUCHENG ZHANG — In this talk I shall give a brief introduction on the physics of the recently discovered topological materials and discuss their potential applications.

4:18PM D5.00004 The Hottest Liquid on the Planet , BARBARA JACAK, Department of Physics and Astronomy, Stony Brook University — We generally expect high temperature matter to act like a gas. However, nature sometimes holds surprises. Collisions of heavy nuclei at very high energies produce a plasma of quarks and gluons which is a strongly coupled liquid. Its vanishingly small shear viscosity to entropy density ratio means it flows essentially without resistance, making it one of the most "perfect" liquids known. Astoundingly, a key tool for theoretical study of the dynamics of this novel liquid arises from the duality of string theory with black holes. I will describe how this liquid is studied, what we've learned about its properties at the Relativistic Heavy Ion Collider in the U.S. and at the Large Hadron Collider in Switzerland, as well as what we haven't figured out yet. I'll also discuss how the quark gluon plasma relates to other strongly coupled systems such as dusty plasmas, cold atomic gases, and strongly correlated condensed matter.

4:54PM D5.00005 Ultracold polar molecules , DEBORAH JIN, NIST, JILA, Univ. of Colorado — Ultracold quantum gases are model systems for studying many-body quantum physics. For example, superfluidity in ultracold Fermi gases of atoms realizes an electrically neutral analog of superconductivity. Recently, enormous progress has been made toward the goal of creating a new type of quantum gas where the constituent particles are polar molecules rather than atoms. In addition to new internal degrees of freedom of the particles, polar molecules introduce the possibility of long-range dipole-dipole interactions, which make the system fundamentally different from atom gases, which have short-range, or contact, interactions. I will discuss recent experimental work on a trapped gas of ultracold fermionic polar molecules.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D6 DBP DPOLY DCMP: Physics of Proteins I: Unifying Principles and Concepts

Ballroom C2

2:30PM D6.00001 Protein Dynamics , HANS FRAUENFELDER, Los Alamos National Laboratory — Proteins combine properties of solids, liquids, and glasses. Schrödinger anticipated the main features of biomolecules long ago by stating that they had to be solid-like, but able to assume many different conformations. Indeed proteins can assume a gigantic number of conformational substates with the same primary sequence but different conformations. The different substates are described as craters in a very-high-dimensional energy landscape. The energy landscape is organized in a hierarchy of tiers, craters within craters within craters. Protein motions are pictured as transition between substates - jumps from crater to crater. Initially we assumed that these jumps were controlled by internal barriers between substates, but experiments have shown that nature selected a different approach. Proteins are surrounded by one to two layers of water and are embedded in a bulk solvent. Structural motions of the protein are controlled by the alpha fluctuations in the solvent surrounding the protein. Some internal motions most likely involving side chains are controlled electrostatically by beta fluctuations in the hydration shell. The dynamics of proteins is consequently dominated by the environment (H. Frauenfelder et al. PNAS 106, 5129 (2009). One can speculate that this organization permits exchange of information among biomolecules. The energy landscape is not just organized into two tiers, alpha and beta, but cryogenic experiments have revealed more tiers and protein more properties similar to that of glasses. While proteins function at ambient temperatures, cryogenic studies are necessary to understand the physics relevant for biology.

3:06PM D6.00002 Engineering electron tunneling in natural and artificial proteins[1] , P.L. DUTTON, Johnson Research Foundation, Department of Biochemistry and Biophysics, University of Pennsylvania, Philadelphia, PA 19104 — Experimental investigation of oxidoreductases has revealed their naturally selected electron tunneling engineering that underlies oxidative and reductive catalysis. This engineering is relatively simple, which allows us to design artificial oxidoreductases from scratch, without the unnecessary complexity found in natural proteins. We have constructed a simple, four α-helix protein bundle protein framework that can be manipulated to support a range of cofactor and substrate binding, and redox and light driven actions. For example, by controlling water access and mobility, this framework can support hemoglobin-like oxygen transport without anything resembling a globin fold. The same framework provides a clear path to artificial proteins designed to catalyze single or multi electron tunneling coupled to chemistry.

[1]In collaboration with C.C. Moser, Johnson Research Foundation, Department of Biochemistry and Biophysics, University of Pennsylvania.

3:42PM D6.00003 The Physical Mechanism of Proton Transfer in Proteins , AIHUA XIE, Department of Physics, Oklahoma State University, Stillwater, OK 74078 — Proteins are able to perform an enormous variety of functions, while using only a limited number of underlying processes. One of these is proton transfer. The physical mechanism of proton transfer has been extensively studied, using a variety of experimental and computational methods. However, it remains unclear what determines the direction and rate of proton transfer reactions in proteins. We have developed and applied a new approach to this long-standing problem by integrating structural dissection, energy landscape, first principle calculation (quantum theory), and molecular dynamics simulation. Our proof of concept study reveals key structural elements that control the direction and rate of proton transfer in proteins. The results are of predictive power and can be generally applied to different proteins.

4:18PM D6.00004 Frustration and the Functional and Folding Landscape of Proteins , PETER WOLYNES, University of California, San Diego — The energy landscape for folding is funnel-like and largely correlates topology directly with energetics. Thus many of the "excited states" important for function are ensembles of structures in which entropy balances partial unfolding energy costs. I will discuss such spectra for cytochrome c. Another way of achieving low free energy excitations is via frustration which entails deviations from the simple funnel landscapes responsible for setting the overall protein shape. I will discuss interesting examples of the consequences of frustration for binding, allostery and for membrane protein systems.

4:54PM D6.00005 Dynamics and mechanism of water-protein interactions , DONGPING ZHONG, The Ohio State University — Water-protein interactions are essential to biology and such interactions are not static but dynamic in nature. With femtosecond spectroscopy and site-directed mutagenesis, we have systematically investigated protein surface hydration dynamics and the actual time scales of their fluctuations. These new results are significant to understanding the physics of protein dynamics at the most fundamental level.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D7 GSNP: From Molecular Control to Spatiotemporal Patterns in Bacteria and Beyond

Ballroom C3

2:30PM D7.00001 Bacterial strategies for chemotaxis response , MASSIMO VERGASSOLA, CNRS/Institut Pasteur — Bacteria respond to chemical cues by performing a biased random walk that enables them to migrate towards attractants and away from repellents. Bias is achieved by regulating the duration of the bacterial runs as a function of the environment, inferred from the history of chemoattractant detections experienced by the bacterium. This time-signal is processed using a time convolution function that can be assayed measuring the response of the bacterium to short pulses of chemoattractant. The convolution constitutes an elementary form of memory, which is encoded at the molecular level by the processes of (de-)methylation and (de-)phosphorylation of the underlying biochemical network. While the latter is being characterized in detail, the functional reasons shaping the bacterial chemotactic response are largely unknown. We show that the chemotactic response observed experimentally is the strategy that ensures the highest minimum (MaxiMin) uptake of chemoattractant, in any field thereof. The consequence is that adaptation of the chemotactic bacterial system appears to be evolutionary driven by the need to cope with space-time environmental fluctuations rather than the extension of the dynamic range of response.

3:06PM D7.00002 Arrested phase separation in reproducing bacteria: a generic route to pattern formation? , JULIEN TAILLEUR, University of Edinburgh — In this talk I will present a generic mechanism by which reproducing microorganisms can form stable patterns. This mechanism is based on the competition between two separate ingredients. First, a diffusivity that depends on the local population density can promote phase separation, generating alternating regions of high and low densities. Then, this is opposed by the logistic law for birth and death of microorganisms which allows only a single uniform density to be stable. The result of this contest is an arrested nonequilibrium phase separation in which dense droplets or rings become separated by less dense regions, with a characteristic steady-state length scale. I will illustrate this mechanism by considering a model of run-and-tumble bacteria, for which a density dependent diffusivity can stem from either a decrease of the swim speed or an increase of the tumbling rate at high density. No chemotaxis is assumed in this model, yet it predicts the formation of patterns strikingly similar to those believed to result from chemotactic behavior.

3:42PM D7.00003 A tunable sequential and periodic pattern formed by coupling cell motility with density , JIANDONG HUANG, The University of Hong Kong — The ability of living organisms to form patterns is an untapped resource for synthetic biology. We aim to generate unique patterns by rewiring the genetic circuitry controlling cell motility. Specifically, E. coli cells are programmed to regulate their movement by sensing local cell density. Interesting patterns are formed by newly engineered cells. An engineered low-density mover strain spreads outwards and autonomously forms a sequential and periodic pattern. Moreover, we build a theoretical model that satisfactorily fits our current experimental data, and also predicts some parameters which may significantly affect the pattern formation. The study of this self-organized spatial distribution of cells may help us to probe the principles underlying the formation of natural biological patterns, and to prepare for future engineering of biological structures.

4:18PM D7.00004 Self-organized biological patterns driven by growth and expansion , TERENCE HWA, Center for Theoretical Biological Physics, UC San Diego — The reaction-diffusion (RD) model, involving the diffusion of two types of morphogens ("activator" and "inhibitor") whose interaction stimulates their own synthesis, is an established paradigm to explain the autonomous generation of space-filling patterns in biology. Starting from random initial perturbations, the RD model typically generates patterns via the development of finite-wavelength dynamical instabilities in confined geometries. In this talk, I will describe examples where elements of the RD model, together with the open, expanding geometries offered by growing biological systems, give rise to novel strategies to generate well-defined patterns in space and time.

4:54PM D7.00005 Deadly competition between sibling bacterial colonies , AVRAHAM BE'ER, University of Texas at Austin, CNLD — As a result of stress due to nutrient limitation or antibiotics, competing individual bacteria within a single colony may lyse sibling cells to release nutrients (cannibalism) or DNA (fratricide). However, we have recently shown that competition is not limited to individuals, but can occur at the colony level [A. Be'er et al., PNAS 106, 428 (2009); A. Be'er et al., PNAS 107, 6258 (2010).] In response to the presence of an encroaching sibling colony, *Paenibacillus dendritiformis* bacteria secrete a lethal protein, lysing cells at the interface between the colonies. Analysis of the proteins secreted by these competing sibling colonies, combined with a mathematical model, shows how colonies maintain their growth by self-regulating the secretion of two proteins: subtilisin (a well-known growth promoter), and Slf (a previously unknown protein, which is lethal). The results also explain why a single colony is not inhibited by its own secretions.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D8 GMAG: Spin Currents Ballroom C4

2:30PM D8.00001 Spin Currents in Silicon[1] , IAN APPELBAUM, University of Maryland, College Park — I will discuss the results of our recent spin injection experiments using long-distance non-degenerate undoped (and n-type doped) Si devices. We have a unique capability to recover the details of electron transport on a sub-ns timescale through a "Larmor clock" transformation of spin precession data, despite using only quasistatic current measurements. I suggest that this is potentially a new tool for probing non-equilibrium phenomena in semiconductors, revealing both intrinsic and extrinsic materials properties through sensitivity to subtleties of the bandstructure and impurity spectrum.

[1]Supported by ONR and NSF.

3:06PM D8.00002 Spin Hall Effects in Ferromagnet-Semiconductor Heterostructures , MUN K. CHAN, University of Minnesota — The effect of spin-orbit coupling on charge transport has long been studied in the form of the anomalous Hall effect in ferromagnets. Charge current in a ferromagnetic channel is intrinsically spin polarized, and asymmetric transverse scattering of spin-up and spin-down electrons due to spin-orbit coupling leads to charge accumulation on the channel edges. Recent breakthroughs in the ability to inject and detect non-equilibrium spin populations in non-ferromagnetic materials have opened up new avenues to study related phenomena. Of particular interest is the spin Hall effect (SHE) in which an ordinary charge current induces a transverse spin current. The resultant spin accumulation at the channel edges was first detected optically [Y. K. Kato *et al.*, Science 306, 1910 (2004) ; J. Wunderlich *et al.*, Phys. Rev. Lett. 94, 047204 (2005)]. We report on an all-electrical measurement of the SHE in Fe/n-In$_x$Ga$_{1-x}$As heterostructures. The edge spin accumulation is detected with spin-sensitive Fe/Schottky tunnel barrier contacts. We investigate the bias and temperature dependence of the SHE and successfully determine the skew and side-jump contributions [E. S. Garlid *et al.*, Phys. Rev. Lett. 105, 156602 (2010)]. Additionally, we have studied the inverse spin Hall effect (iSHE), in Fe/n-GaAs devices. Spin current injected into n-GaAs by a biased Fe/Schottky contact results in a spin-dependent Hall voltage. The iSHE signal is an order of magnitude larger than that expected from SHE measurements in the same heterostructure. Temperature dependence, nuclear magnetic resonance, and field cycling measurements show conclusively that the iSHE is coupled to the dynamically polarized nuclear spins. We have therefore discovered a new contribution to spin Hall effects: the hyperfine coupling. Work done in collaboration with E.S. Garlid, Q.O. Hu, C.J. Palmstrøm, and P.A. Crowell. Funding provided by NSF DMR 0804244, ONR MURI, and NSF MRSEC and NNIN programs.

3:42PM D8.00003 Electrostatically Manipulated Ballistic Spin Currents[1] , MARK JOHNSON, Naval Research Laboratory — Two decades ago Datta and Das published a remarkable paper [1] concerning spin polarized ballistic electron currents in a semiconductor channel and the Rashba spin orbit interaction. They predicted that the source-drain conductance of a spin-injected Field Effect Transistor (spin FET) would oscillate periodically as a function of monotonically increasing gate voltage. We have observed Datta Das oscillations using spin-FETs with ferromagnetic metal electrodes as source and drain [2]. The channel is composed of a high mobility InAs single quantum well heterostructure with strong spin-orbit interaction. The source-drain length is less than the electron mean free path at T=1.8 K. Using the nonlocal geometry, diffusive carriers are removed at a remote ground and the channel conductance is dominated by a current of spin polarized ballistic electrons. A conductance that oscillates as a function of gate voltage is observed. The oscillation amplitude is calibrated from the lateral spin valve magnetoresistance. The spin-orbit interaction parameter is determined from beats in Shubnikov-de Haas data. Thus, the fit to theory has no adjustable parameters other than a small phase factor. Finally, we compare the temperature dependence of the oscillation amplitude with that of the carrier mean free path. The importance to Spintronics, which proposes the use of both spin and charge as state variables, is the demonstration that carrier spin orientation can be modulated by voltage, a parameter normally associated with charge.

[1] S. Datta and B. Das, Appl. Phys. Lett. v. 56, 665 (1990).
[2] H.C. Koo, J.H. Kwon, J. Eom, J. Chang, S.H. Han and M. Johnson, Science v. 35, 1515 (2009).

[1]In collaboration with H.C. Koo, J. Eom, S.H. Han and J. Chang. I acknowledge support from ONR.

4:18PM D8.00004 Logic Devices Based on Spin Current[1] , BEHTASH BEHIN-AEIN[2], Purdue University — The need to find low power alternatives to digital electronics circuits has led to increasing interest in alternative switching schemes like the magnetic quantum cellular automata that store information in nanomagnets which communicate through their magnetic fields. A recent proposal called all spin logic (ASL) proposes to communicate between nanomagnets using spin currents which are spatially localized and can be conveniently routed. In this talk we present a model for ASL devices that is based on established physics and is benchmarked against available experimental data. We investigate switching energy- delay of ASL devices and provide frameworks that allow simple comparisons with charge based devices like CMOS and can help to determine possible use of ASL in future logic implementation. Expected scaling of switching energy-delay of ASL devices as magnets are downscaled while retaining their stability against thermal fluctuations will be presented.

[1]This work was supported by Nanoelectronics Research Initiative (NRI) and Network for Computational Nanotechnology (NCN).
[2]First author would like to acknowledge his collaborators Angik Sarkar, Srikant Srinivasan and Supriyo Datta.

4:54PM D8.00005 Optical detection of spin currents[1] , HUI ZHAO, Department of Physics and Astronomy, University of Kansas — Extensive efforts are currently being devoted to developing spintronics. Several techniques have been developed to generate pure spin currents in many materials and structures. However, there is still no method available that can be used to directly detect pure spin currents, which carry no net charge current and no net magnetization. Currently, studies of pure spin currents rely on measuring the induced spin accumulation with optical techniques or spin-valve configurations. I will discuss observation of a second-order nonlinear optical effect of pure spin currents that can be used for the non-invasive, non- destructive, and real-time imaging of pure spin currents. This effect is caused by a subtle imbalance of the Faraday rotation of electrons with opposite spin orientations [1]. In our experiment, a transient pure spin current was injected in a GaAs crystal by a quantum interference and control technique using a pair of phase-locked ultrafast laser pulses. Second- harmonic generation of an ultrafast probe pulse with a central wavelength of 1760 nm was observed [2]. We systematically studied the second-harmonic power as a function of the probe delay, probe position, spin current density, and carrier density. All the observations are consistent with a second- order nonlinear optical effect induced by the pure spin current. Since this effect does not rely on optical resonances, it can be used to detect pure spin currents in a wide range of materials with different bandstructures. Furthermore, the control of nonlinear optical properties of materials with pure spin currents may have potential applications in photonics integrated with spintronics.

[1] J. Wang, B. F. Zhu, and R. B. Liu, Phys. Rev. Lett. 104, 256601 (2010).
[2] L. K. Werake and H. Zhao, Nat. Phys. 6, 875 (2010).

[1]Work supported by NSF under grant no. DMR-0954486.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D9 DFD: Patterns, Nonlinear Dynamics followed by General Fluid Dynamics D220

2:30PM D9.00001 Rayleigh Bénard Convection-A Case Study on Pattern Formation , HIRA SIDDIQUI, RUDOLF FRIEDRICH, WWU Muenster, Germany — Spiral turbulence in Rayleigh-Benard convection is studied numerically in the framework of generalized Swift Hohenberg equations. The model equation consist of an order parameter equation for the temperature field coupled to an equation for the mean flow field. In contrast to the earlier work, nonlinearities in the dynamics of the mean flow are retained leading to a two dimensional Navier-Stokes equation coupled to a Swift-Hohenberg equation. We present the numerical investigations of nonlinear effects due to the interaction of nonlinear two dimensional flows and the pattern forming process.

2:42PM D9.00002 A simple approach to localized convection , H. PLEINER, Max Planck Inst. for Polymer Research, Germany, M.G. CLERC, Univ. de Chile, Santiago de Chile, J. MARTINEZ-MARDONES, Pont. Univ. Catolica de Valparaiso, Chile, L.M. PEREZ, Dep. Ingeneria Metalurgica, Univ. de Santiago, Chile, D. LAROZE, Max Planck Institute for Polymer Research, Mainz and Inst. de Alta Investigacion, Univ. de Tarapaca, Arica, Chile — Localized structures can be found in many different (dissipative) driven systems [1], an example being stationary and traveling convection structures in the thermal instability of binary fluids. Here, the special localized structure is a convective state between two quiescent, conductive ones, and can been interpreted as a pinning phenomenon close to a stationary sub-critical bifurcation. Generally, localized structures are described by using higher dimensional, complex amplitude or phenomenological prototype (e.g. Swift-Hohenberg) equations or by direct numerical integration of the hydrodynamic equations. Here we show, using the binary mixture convection in porous media as an example, that the analytically derived one-dimensional amplitude equation amended by non-adiabatic (non-resonant) terms important close to convection fronts, well describes localized convection states, in particular the slanted homoclinic bifurcation diagrams.

[1] O. Descalzi, M. Clerc, S. Residori, and G. Assanto (Eds.), Localized States in Physics: Solitons and Patterns, Springer, 2011.

2:54PM D9.00003 The dynamics of cracks in torn thin sheets , YOSSI COHEN, ITAMAR PROCACCIA, Department of Chemical Physics, The Weizmann Institute of Science, Rehovot 76100, Israel — The stress field near the tip of a crack due to a mode III shear tearing of a thin plate of elastic material has a universal form but with a non-universal amplitude known as the Stress Intensity Factor. All the non-universal aspects of the stress distribution are collected in the Stress Intensity Factor which depends on everything, including the crack length, the boundary conditions and the history of the loads that drive the crack evolution. Although the equations of elasticity for thin plates are well known, there remains the question of selection of a path for a propagating crack. We invoke a generalization of the principle of local symmetry to provide a criterion for path selection and demonstrate the qualitative agreement of our results with the experimental findings. We also analyze the nature of the singularity at the crack tip with and without the nonlinear elastic contributions. Finally we present an exact analytic results for the stress intensity factor to the linear approximation for the crack developing in thin sheets.

3:06PM D9.00004 Chaotic Plume-Like Bursts in Rimming Flows , GABRIEL SEIDEN, VICTOR STEINBERG, Weizmann Institute of Science — We report a detailed experimental investigation of chaotic, plume-like bursts observed in rimming flows of polymer solutions within a partially filled horizontal cylinder. In particular, we investigate the attractive interaction between adjacent plumes and the effect of rotation rate and polymer concentration on the statistics of these unique bursts. A comparison is also made between the Newtonian and non-Newtonian cases.

3:18PM D9.00005 Cracks formation during blood drop evaporation , BENJAMIN SOBAC, DAVID BRUTIN, Université de Provence, UNIVERSITÉ DE PROVENCE TEAM — We firstly presented the pattern formation occurring when drops of whole blood desiccate in a recent publication [1]. The phenomena presented evidence to involve lots of physical field such as surface chemistry, haematolology, fluid mechanics, heat transfer, colloids science... All these mechanisms are acting together and produce an axisymetric and reproducible pattern. Dried cellular components are segregated and deposited by a capillary flow. During the evaporation, the system is slowly drying and cracks when stresses are too important leading to the final pattern observed. In this presentation, we will present the mechanisms involved in the formation of crack patterns. The phenomenon presented here with red blood cells as the main colloids involved is very similar to the drying of drop of nanoparticules [2]. We will explain the common point and the differences encountered.

[1] D. Brutin, B. Sobac, B. Loquet and J. Sampol, Pattern formation in drying drops of blood, Journal of Fluid Mechanics, underpress, 2010.
[2] L. Pauchard, B. Abou, K. Sekimoto, Infuence of Mechanical Properties of Nanoparticles on Macrocrack Formation, Langmuir, 25(12), 6672-6677, 2009.

3:30PM D9.00006 ABSTRACT WITHDRAWN –

3:42PM D9.00007 Pattern formation and coarsening in crystalline membranes , DANIEL A. VEGA, ALDO D. PEZZUTTI, Dep. de Física- IFISUR- Universidad Nacional del Sur - CONICET — We study through a Brazovskii-Helfrich Hamiltonian the process of defect formation, annealing and coarsening of two dimensional crystalline membranes. In good agreement with the cosmological model of Kibble and Zurek, proposed to determine the density of topological defects at the onset of a symmetry breaking phase transition, we found that the collision of orientationally uncorrelated domains produces a structure of grains with an average density of topological defects controlled by the temperature of the quench. The strain field of the dislocations and disclinations generated during the phase separation process can induce the buckling of the membrane, slowing down the Lifshitz-Safran mechanism of coarsening observed in flat systems.

3:54PM D9.00008 Pattern formation in ternary lipid membranes with composition-deformation coupling , MATTHEW DEMERS, Northwestern University Department of Applied Mathematics, FRANCISCO SOLIS, MONICA OLVERA DE LA CRUZ, Northwestern University Department of Materials Science — We study patterns formed in three-component lipid membranes, where composition is coupled to shape via differences in spontaneous curvature. The system is examined in the strong segregation regime. System morphology is determined by the competition of bending energy, surface tension, and line tension. We will present the phase behavior as determined by numerical minimization, as well as analytic solutions for select cases.

4:06PM D9.00009 Supercavitating flow past an elastic curvilinear hydrofoil[1] , YURI ANTIPOV, Louisiana State University — A nonlinear inverse fluid-structure interaction problem is considered. The obstacle is a curvilinear elastic hydrofoil, and the cavity formed behind is modeled according to the single-spiral-vortex model by Tulin. First, the model for a rigid polygonal supercavitating hydrofoil is solved by the method of conformal mappings. The mapping function is expressed through the solutions of two Riemann-Hilbert problems. To identify the vertices of the polygon where the jets break away from the foil, the Brillouin-Villat separation condition is applied. The unknown parameters of the conformal mapping are computed on solving a system of transcendental equations. Next, by increasing the number of vertices of a regular N-polygon, the cavitation problem for a circular arc is solved, pressure on the foil is defined, and a boundary- value problem for a thin shell subject to normal loading is stated. The elastic problem is solved exactly for an arc with clamped ends, and the new hydrofoil profile is determined. Finally, a new cavitation problem for the deformed foil is stated and solved. Numerical experiments reveals the presence of two thin partial cavities near the foil ends.

[1]This work was funded by NSF through grant DMS0707724.

4:18PM D9.00010 Drag calculations using the inviscid Euler equations alone , GALEN GISLER, PGP/University of Oslo — Recently Hoffman and Johnson[1] have proposed a new resolution of d'Alembert's Paradox, the problem that inviscid potential flow predicts zero drag on a body, in contrast to observations. They reject the commonly accepted resolution, that drag results from the very thin viscous boundary layer between the no-slip condition on the surface of the body and the free-flowing fluid. Instead they argue that drag results from turbulence in the body's wake, even if free-slip is assumed. They used a finite-volume code to verify their conclusions. While their calculations look promising, and offer prospects for calculation of rather more complex flows at modest resolution, it is desirable to perform independent verification. I will present independent tests of the Hoffman-Johnson resolution using a finite-volume Euler-equation code, studying the dependence of the inferred drag on meshing style and resolution.

[1] Johan Hoffman and Claes Johnson, J. Math. Fl. Dyn. 12, 321-334 (2010).

4:30PM D9.00011 Dynamics of induced dipole ER fluid: a continuous energetic approach , JIANWEI ZHANG, WENFENG LI, JIAXI LI, Dept. of Physics, Tongji University, Shanghai, China — We studied dynamics of Electrorheological (ER) fluid by continuum induced dipole fluid method [1]. We found that the velocity profile of ER fluid increases in high shear-rate region and solid particles are separated from colloid in high electric field. These findings demonstrated the breakdown of Bingham fluid model under high shear-rate and high electric field. Our continuum approach describes ER fluid's behaviors under most conditions. We also found that the shift of maximum shear stress under different electric field follows the same trend as that of the maximum static stress. This indicates that the static and dynamic stresses are both dominated by the same energetic process. A connection between micro-particles' structures and macro-dynamic properties under varying conditions is established by our continuum method. Our studies probe the physics of induced dipole ER fluid.

[1] Jianwei Zhang, Xiuqing Gong, Chun Liu, Weijia Wen, and Ping Sheng, Physical Review Letters 101, 194503, 2008.

4:42PM D9.00012 Velocity fluctuations in steadily sedimenting suspensions , K. VIJAY KUMAR[1], SRIRAM RAMASWAMY, CCMT, Department of Physics, Indian Institute of Science, Bangalore 560012 — The simplest model of a homogeneous suspension steadily sedimenting under gravity at low Reynolds number indicates that the velocity fluctuations should diverge with the system size. This is, however, not seen in experiments. We improve on a previously described coarse-grained model proposed for this problem by identifying certain crucial missing terms in the equations of motion. These terms are allowed by symmetry considerations and can be generated by a mechanism which is natural in the dynamics of low Reynolds number sedimentation. A dynamical renormalization group calculation of our model leads to the conclusion that these extra terms are always relevant. If these terms are stabilizing, this suggests a natural mechanism for suppressing fluctuations in sedimenting suspensions. We analyze the properties of the critical point where these extra terms vanish.

[1]Present Address: Departments of Mechanical Engineering & Materials Science and Physics, Yale University, New Haven, CT 06511

4:54PM D9.00013 Stabilization of toroidal droplets using viscoelastic media , EKAPOP PAIRAM, ALBERTO FERNANDEZ- NIEVES, School of Physics / Georgia Tech Team — We inject a viscous liquid through a needle into another rotating viscous liquid to generate toroidal droplets. These droplets are unstable and undergo a transformation into spherical droplets driven by surface tension: They either break ala Rayleigh-Plateau or grow fatter to become a single spherical droplet depending on the aspect ratio of the torus. By replacing the outer phase with a viscoelastic fluid with a non-zero yield stress we can stabilize these and other non-zero genus droplets. We will examine this stabilization mechanism and present criteria to effectively prevent the break-up of these droplets.

5:06PM D9.00014 Iron chemistry at aqueoues interfaces by near edge X-ray spectroscopy[1] , DAVID VAKNIN, WENJIE WANG, ALEX TRAVESSET, Ames Laboratory, and Department of Physics, Iowa State University, Ames, Iowa 50011, IVAN KUZMENKO, X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439 — Employing synchrotron X-ray absorption near-edge spectroscopy (XANES) combined with X-ray fluorescence (XF) and reflectivity (XR) techniques, we monitor the state of ferrous and ferric iron as it binds to charged carboxylic and phosphate groups. By subphase pH manipulation, arachidic acid and dihexadcyl phosphate monolayers can provide a range of surface charge density from nearly charge-neutral to a fully charged monolayer to which iron ions are attracted from solutions. Analysis of our results from fluorescence show that the driving forces attracting Fe^{3+} and Fe^{2+} to the interface originate from chemical interactions and electrostatic, respectively. XANES shows that the electronic and geometric structure of iron complexes at interface are different from those in the bulk. Moreover, the XANES results demonstrate that valence state and bonding of the interfacially bound Fe^{3+} and Fe^{2+} are practically indistinguishable. This, we argue, is due to the versatility of iron ions in behaving as electron acceptors (Fe^{3+}) or as donors (Fe^{2+}).

[1]Supported by the Office of BES, U.S. Department of Energy Cont. No. DE-AC02-07CH11358.

5:18PM D9.00015 Interfacial microrheology in viscoelastic membranes , GOPAL SUBEDI, KENNETH W. DESMOND, ERIC R. WEEKS, Emory University — Prior studies on interfaces using microrheology have typically been applied to interfaces with only a surface viscosity component and not an elastic one. We are extending the application of interfacial microrheology to viscoelastic lipid monolayers. We use a DPPC and cholesterol lipid monolayer in a Langmuir trough as a model system. The Langmuir trough gives us the flexibility to control the concentration and thus the phase of the monolayer. The microrheology technique allows us to measure the rheology at specific concentrations or in situations as the concentration is changed. The microrheology technique employs video microscopy to record the diffusive motion of micron size spheres placed at the interface. Since the diffusive motion of the microspheres is dominated by the interfacial rheology of the monolayer, the recorded motions of the microspheres are used to infer the rheological properties of the interface. We hope to extend our understanding of viscoelastic interfaces with the study.

Monday, March 21, 2011 2:30PM - 5:30PM –
Session D10 SPS: SPS Undergraduate Research II D221

2:30PM D10.00001 The ^{11}C Project:Measurement of Root Exudation at Elevated CO2 Levels in Low and High Nutrient Solutions , VERIDA LEANDRE, North Carolina AT SU, CALVIN HOWELL, Duke Univ. — Understanding the plant kingdom's mechanisms of resource management in variable environments is integral to predicting how plants will respond to an increase in atmospheric CO_2. The goal of this study is to determine the effects of changing nutrient conditions on the root exudation of barley plants at elevated CO_2 levels. The ^{11}C group at the Triangle Universities Nuclear Laboratory (TUNL) tags various species of plants with short-lived positron-emitting radioisotopes in order to analyze metabolite transport in response to changes in the environment. ^{11}C is produced at TUNL using a tandem Van de Graaff particle accelerator, then transported from TUNL to the Duke Univ. Phytotron (100m) where plants are labeled with ^{11}C in a growth chamber. The chamber allows researchers to control the light intensity, air temperature, humidity and concentration of CO_2 in the air. The plant absorbs $^{11}CO_2$ in a leaf that is placed inside a cuvette through which radioactive $^{11}CO_2$ gas flows. The sugars in the labeling leaf are tagged with ^{11}C and translocated throughout the plant similar to ^{12}C. Scintillation detectors are used to track the tagged sugars as they are translocated through the plant and exudated from the root into the nutrient solution or $^{11}CO_2$ gas is respired by the root. The labeling system, detector arrangement, electronics and data analysis will be described and preliminary results will be presented.

2:42PM D10.00002 A One Dimensional Stochastic Susceptible-Infectious-Recovered Model and its Variations: a Hamiltonian Approach , ALI HAMED, Washington and Lee University, DIA'A BISHARAT, MOHAMAD AMINE, IRINA MAZILU, Washington and Lee — The spread of an infectious disease is a random process, and a stochastic approach to the problem is justified. The susceptible-infectious-recovered model (SIR) describes the evolution of three types of individuals (in a small community) which undergo an infection and recovery mechanism. The model (and its variations) predicts the number of infected individuals over a certain period of time, gives an estimate of the maximum possible number of infected people, and predicts how long the disease will be threat to the examined community. Using a quantum mechanical approach, we investigate four variations of the original SIR model and compare our analytical findings with the computer simulation results. We also calculate correlations between infected and recovered individuals, and find a good agreement between theory and computer simulations.

2:54PM D10.00003 Exploring a Parasite-Host Model with Monte Carlo Simulations , NYLES BREECHER, JIAJIA DONG, Hamline University — We explore parasite-host interactions, a less investigated subset of the well-established predator-prey model. In particular, it is not well known how the numerous parameters of the system affect its characteristics. Parasite-host systems rely on their spatial interaction, as a parasite must make physical contact with the host to reproduce. Using C++ to program a Monte Carlo simulation, we study how the speed and type of movement of the host affect the spatial and temporal distribution of the parasites. By drawing on mean-field theoretics, we find the exact solution for the parasite distribution with a stationary host at the center and analyze the distributions for a moving host. The findings of the study provide rich behavior of a non-equilibrium system and bring insights to pest-control and, on a larger scale, epidemics spreading.

3:06PM D10.00004 Optical design of a robotic TV camera probe for minimally invasive abdominal surgery[1] , SUSANNA TODARO, Harvey Mudd College, WEIYI HE, DENNIS KILLINGER, University of South Florida — Minimally invasive techniques are a promising new field of surgery; however, they limit the surgeon's access points and maneuverability. In order to increase the number of access points in minimally invasive abdominal surgery, a proposed implantable medical probe braces to the abdominal wall and provides illumination and video signal. The probe is cylindrical, about 25 mm long and 10 mm in diameter. A ring of LEDs on the end of the probe illuminates the tissue, and the resulting image is focused onto an HD video detector. It was necessary to apply beam-shaping reflectors to collimate the light onto a small target area, to avoid illuminating areas not picked up by the video. These reflectors were designed and simulated using the optical ray tracing software TracePro. Two LED chip geometries and three types of reflector geometries were analyzed, and the parameters for each geometry were optimized. For the straight-edged reflectors, the intensity patterns and optimization were compared to experimental results. Although parabolic reflectors produced the best collimation, cone reflectors with a 20-degree half-angle produced significant collimation at a much cheaper price.

[1]This work was supported by NSF REU program (award No DMR-1004873).

3:18PM D10.00005 Developing a Procedure for the Characterization of Mechanical Properties of Collagen Gels[1] , CHRISTOPHER CHAMBERS, Northern Arizona University, HEATHER LOVELADY, GARRETT MATTHEWS, University of South Florida — The characterization of bulk mechanical properties of type I collagen gels is critical to understanding the role of collagen in the extracellular matrix (ECM), and developing biocompatible devices for use in the human body. Understanding the mechanical properties of the gel state of collagen can lead to the ability to adjust these properties for multiple uses. Here, we examined the Young's modulus of the synthesized gels. This project used a microrheological approach to discover these properties. Gels were first formed using a known process and magnetic microspheres were embedded in the gel prior to formation. An optical microscope was fitted with a magnetic chamber used to drive the embedded beads in two modes, an oscillatory motion and a pulse motion. Tracking software was modified and used to analyze the motion of the beads recorded with a CCD camera on the microscope. These techniques should be sufficient to obtain a reliable value for the Young's modulus of collagen gels, as well as other similar materials.

[1]This work was supported by NSF REU program (award No DMR-1004873).

3:30PM D10.00006 ABSTRACT WITHDRAWN –

3:42PM D10.00007 Does Thioflavin-T Detect Oligomers Formed During Amyloid Fibril Assembly[1] , CHRISTOPHER PERSICHILLI, Rensselaer Polytechnic Institute, SHANNON E. HILL, JASON MAST, MARTIN MUSCHOL, University of South Florida — Recent results have shown that oligomeric intermediates of amyloid fibril assembly represent the main toxic species in disorders such as Alzheimer's disease and type II diabetes. Thioflavin-T (ThT) is among the most commonly used indicator dyes for mature amyloid fibrils *in vitro*. We used ThT to monitor amyloid fibril formation of lysozyme (HEWL), and correlated ThT fluorescence to concurrent dynamic light scattering and atomic force microscopy measurements. Specifically, we tested the ability of ThT to discern among oligomer-free *vs.* oligomeric fibril assembly pathways. We found that ThT fluorescence did not detect oligomer growth; however, fluorescence increases did coincide with the formation of monomeric filaments in the oligomer-free assembly pathway. This implies that ThT fluorescence is not generally suitable for the detection of oligomeric intermediates. The results further suggest different internal structures for oligomeric *vs.* monomeric filaments.

[1]This research was supported, in part, by funding through the Byrd Alzheimer's Institute (ARG-2007-22) and the BITT-Florida Center of Excellence for M.M., an NSF-REU grant (DMR-1004873) for C. P. and an NSF-IGERT fellowship for S.H.

3:54PM D10.00008 The Design and Fabrication of Bismuth Hall Effect Biosensors , A.J. SIGILLITO, University of Dallas, M. RUDOLPH, V. SOGHOMONIAN, J.J. HEREMANS, Virginia Tech — Because of their high sensitivity, accuracy, and low cost, the use of Hall biosensors promises to be an effective diagnostic technique that may aid in the early diagnosis of diseases. In this research, Hall sensors were fabricated from thermally evaporated bismuth thin films. The bismuth films were deposited under high vacuum onto heated Si/SiO_2 substrates using a two layer deposition technique. The films varied in thickness from 60 nm to 75 nm and were etched into Hall bar geometries using photolithography and wet chemical etching. Magnetoresistance and Hall measurements were taken from 4 K to 300 K. The data indicate that the sensors may be characterized using a two carrier model with high mobility, low density holes and low mobility, high density electrons. Additionally, the sensors were exposed to magnetite nanoparticles and characterized using atomic force microscopy. The results will be reported. This research was funded by the National Science Foundation (NSF Grant DMR-0851662).

4:06PM D10.00009 EPR Study of Lithium Borovanadate and Lithium Silicate Glasses , BIKESH DAHAL, D. BLANE BAKER, William Jewell College, STEVE FELLER, Coe College — Lithium borovanadate and lithium silicate samples with varying molar ratios were prepared using both roller quenching and plate quenching methods. Electron paramagnetic resonance EPR spectra of those samples show that resolution of the hyperfine structure lines(hfs) depend on their molar ratio. When the molar ratio (K) is less than 0.5 in the borovanadate system, the hyperfine structure lines are well resolved and defined. However, when the molar ratio becomes greater than 0.5; the spectra starts to get less resolved; at molar ratio 0.7 there is no hyperfine resolution. Well resolved samples were modeled by using a modeling program in MATLAB to obtain Hamiltonian parameters. The Hamiltonian parameters that were obtained were $g_{parallel}$, $g_{perpendicular}$, $A_{parallel}$ and $A_{perpendicular}$. The Hamiltonian parameters were calculated to learn about the orientation of V^{4+} ions and electrons in the glass samples. According to our calculation $g_{parallel} < g_{perpendicular} < g_e$ which suggests that crystal field of the V^{4+} ions has a octahedral site with a tetragonal compression in the glass samples.

4:18PM D10.00010 EPR study of radical trapping of RAFT polymerization of Multifunctional Acrylates , AAYUSH REGMI, ASHUTOSH DAHAL, D. BLANE BAKER, William Jewell College, JOHN POJMAN, Louisiana State University, PATRICK BUNTON, William Jewell College — Electron Paramagnetic Resonance (EPR) was used to monitor radical trapping during Reversible Addition-Fragmentation chain Transfer (RAFT) polymerization of acrylate monomers with different degrees of functionality. Monomers used for the study were 1, 6-Hexanidiol Diacrylate (HDODA), Trimethylopropane Triacrylate (TMPTA), and Pentaerythritol Tetracrylate (PETA). X-band EPR spectra were obtained for approximately 0.2 g of samples in a 4 mm quartz tube heated at 50^0C inside the cavity. The trapped radicals' signals were first observed after the samples were heated for 400-500 minutes. Radical density continued to increase for an additional 180 -190 minutes. EPR spectra of RAFT samples of TMPTA and PETA were compared with subsequent spectra produced by traditional free radical polymerization.

4:30PM D10.00011 EPR study of Frontally Polymerized Multifunctional Acrylates[1] , ASHUTOSH DAHAL, AAYUSH REGMI, ANNA THOMA, ALECIA VALENCIA, William Jewell College, VERONIKA VINER, RAFAEL CUETO, Louisiana State University, D. BLANE BAKER, William Jewell College, JOHN POJMAN, Louisiana State University, PATRICK BUNTON, William Jewell College — Electron Paramagnetic Resonance(EPR) study of frontally polymerized Trimethylopropane Trimethacrylate(TMPTMA), Trimethylopropane Triacrylate(TMPTA), 1,6-Hexanidiol Diacrylate(HDODA) and Pentaerythritol Tetracrylate(PETA) was done to determine the absolute radical concentration. Higher radical concentrations were found in the frontally polymerized samples compared to the bulk polymerized samples for TMTPMA and PETA. The concentration of radicals was highest in TMPTMA frontal sample at 8.74 X 10^{-3} moles/kg. The lowest measureable concentration was in the HDODA bulk samples at 0.0266 X 10^{-3} moles/kg. For all frontally polymerized samples high radical concentrations were observed at the point of initiation after which the signal intensity decreased to steady state within a few centimeters down the front. An exponential growth in the radical signal was observed in the mixture of TMPTMA and TMPTA when the concentration of the TMPTMA was increased.

[1]Sponsored in part by Research Corporation

4:42PM D10.00012 First-principles investigation of graphene-metal interfaces[1] , ANDREW ROSS, Saint Anselm College, LYUDMYLA ADAMSKA, YOU LIN, IVAN OLEYNIK, University of South Florida — Epitaxial growth of graphene on Ni(111) substrates is one promising method of large-scale, high-quality graphene wafer production, due to the small lattice mismatch between these two materials. We present results of first-principles density functional theory (DFT) investigation of thestructural, electronic, and magnetic properties of graphene/Ni(111) interfaces relevant to experimental studies of graphene growth on nickel substrates. DFT calculations were performed to identify the favored interface geometries and binding sites for different interface configurations. Additional adlayers of Ni and Cu were either adsorbed on top of the graphene/metal interface, or placed between the graphene and substrate to model processes of metal intercalation. It was also found that the interaction between graphene/Ni(111) and the top Cu adlayer is much weaker compared to that for Ni adlayer. The atomic, electronic, and magnetic properties of these interfaces, including induced magnetic moments in graphene/Ni(111) and Cu,Ni/graphene/Ni(111) systems are also discussed.

[1]This work was supported by NSF REU supplement to the award CCF-0726842.

4:54PM D10.00013 Growth of Graphene on Metal Substrates[1] , TRAVIS MILLER, Grove City College, JAYEETA LAHIRI, RAFIK ADDOU, MATTHIAS BATZILL, University of South Florida — Graphene, a single layer of graphite, has large potential as an electronic material. For these applications large scale, high quality graphene wafers are required. A promising approach to achieve this is by growth on metal substrates. In this REU project I used Auger electron spectroscopy to study the growth of graphene on Ni(111) and its modification by Cu or Al additions. On pure nickel we found two graphene growth regimes. Below 480 °C graphene grows by converting a surface carbide phase while above 480 °C graphene grows on pure nickel. Addition of copper destabilizes the nickel carbide enabling the growth of graphene in the absence of a carbide at lower temperatures. Finally, aluminum intercalation through the Ni- supported graphene layer was investigated in an attempt to form an ordered Ni-Al alloy underneath the graphene. Surprisingly, we found that this intercalation process already occurs at only 100 °C. Furthermore, the intercalated Al is protected by the graphene against oxidation.

[1]This work was supported by NSF REU program (award No DMR-1004873)

5:06PM D10.00014 Single-Walled Carbon Nanotubes in Epoxy – Investigating Behavior under Strain and Alignment Using Fluorescence Spectroscopy[1] , TAMIKA THOMAS, KENA SENEGAL, SARENA SENEGAL, PAUL WITHEY, Northwestern State University, SERGEI BACHILO, R. BRUCE WEISMAN, Rice University — Single-walled carbon nanotubes (SWCNTs) have been successfully embedded into EPON 862/W epoxy both with and without a surfactant. Applying strain to the nanocomposite permitted the interfacial adhesion between the SWCNT and host to be studied at the single-particle level using near-infrared fluorescence spectroscopy. Load transfer from the host to an embedded CNT is clearly observed as a shift in the nanotube's spectral emission. Loss of adhesion, or slipping, is also detected. Attempts at enhancing CNT-alignment within the nanocomposite will also be discussed. Near-infrared fluorescence imaging and spectroscopy prove to be ideal methods for monitoring the behavior of SWCNTs within nanocomposites, especially at the single-particle level. Much of this work has been carried out by undergraduate physics and chemistry majors.

[1]Support from the Air Force Minority Leaders Program and generous use of facilities in the lab of Dr. R. Bruce Weisman at Rice University are gratefully acknowledged.

5:18PM D10.00015 An Ab-initio Study of Folded Armchair Graphene Nanoribbons , ADAM IAIZZI, Ithaca College, NAM LEE, LILIA WOODS, University of South Florida — We present a first principles approach to the characterization of armchair graphene nanoribbons folded along their long axis using density functional theory, along with ultrasoft psuedopotentials and the local density approximation for the exchange-correlation functional. Based on past studies, we anticipate that folding nanoribbons will produces changes in the band structure, possibly turning normally semiconducting nanoribbons into metallic nanowires. We determine the energy required to produce a number of different folded structures from nanoribbons as well as the energy and band structure as a function of width in single-fold structures. Ribbons as narrow as 13 carbon atoms formed stable folded structures.

Monday, March 21, 2011 2:30PM - 4:42PM –

Session D11 FIAP: Thermal Properties in Semiconductors and Nanostructures D222

2:30PM D11.00001 Thermoelectric Properties of Granular Materials[1] , ANDREAS GLATZ, Argonne National Laboratory, IGOR BELOBORODOV, California State University, Northridge — I will present our recent studies of thermoelectric properties of mono-phasic nanocrystalline semiconductors and metals in the weak coupling regime. The focus is in particular on the thermopower and figure of merit for temperatures less than the charging energy. I will show that the dimensionless figure of merit ZT, which is a measure for the performance of thermoelectric materials, has a maximum at certain temperatures and grain sizes which can be in the range of technological relevant values $ZT > 3$. The talk is based on: Phys. Rev. B **80**, 245440 (2009) and EuroPhys. Lett. **87**, 57009 (2009).

[1]Work supported by the U.S. DOE, Office of Science, under Contract No. DE-AC02-06CH11357.

2:42PM D11.00002 Thermal Conductivity Characteristics of Three-Layer Superlattices , JING ZHANG, HUA TONG, NELSON TANSU, Lehigh University — For thermoelectric applications, the thermal conductivity of the material needs to be reduced as low as possible in order to achieve higher thermoelectric efficiency of devices, as the device efficiency depends on the thermoelectric figure of merit ($Z*T$). Both theoretical and experimental data show that the cross-plane thermal conductivity of superlattices is much lower than that of the bulk materials The cross-plane thermal conductivity of three-layer superlattices is calculated by a numerical method, which is developed from the lattice dynamical theory. The phonon mean free path is included into the calculation, thus the minimum thermal conductivity occurs at the crossover of the particle-like model and wave-like model of the phonons. The studies focus on the effect of mass ratio, layer thickness, and mean free paths on the minimum thermal conductivity of the three-layer superlattice design. The minimum thermal conductivity of the three-layer superlattice structure is approximately half of that of the conventional two-layer superlattice structure. This finding indicates that the thermoelectric figure of merit for superlattice structure can further be enhanced by 2 times from the use of the three-layer superlattice design.

2:54PM D11.00003 Lattice thermal conductivity with first-principles anharmonic lattice model , TERUMASA TADANO, YOSHIHIRO GOHDA, SHINJI TSUNEYUKI, Department of Physics, The University of Tokyo — First-principles calculation of lattice thermal conductivity is important to design new devices such as high-efficiency thermoelectric materials. For lattice thermal conductivity calculations of complex materials and nanostructures, non-equilibrium molecular dynamics (NEMD) is more suitable than widely used Boltzmann transport theory. However, a combination of NEMD and FPMD is almost impossible because of its high computational cost, so that NEMD has been performed only with classical model potentials for specific materials. In order to overcome this limitation in materials, we have developed a new methodology for calculating lattice thermal conductivity without relying on any experimental values. In this method, the potential energy of a system is expressed as a many-body anharmonic model, that is, a Taylor expansion of the total energy with respect to displacements of atoms up to 4th order. Parameters of the anharmonic lattice model are determined with Hellmann-Feynman force of FPMD by least-square fitting. We performed thermal conductivity calculations with the anharmonic lattice model combined with NEMD and obtained reasonable agreements with experimental values.

3:06PM D11.00004 Surface roughness and phonon transport in thin Si nanowires: an atomistic study[1] , JESUS CARRETE, LUIS JAVIER GALLEGO, LUIS MIGUEL VARELA, Facultad de Fisica, Universidad de Santiago de Compostela, Spain, NATALIO MINGO, LITEN, CEA-Grenoble, France — Good thermal insulation is much harder to achieve than electrical insulation. Thus, the astonishingly low thermal conductivities recently reported on Si nanowires came as a surprise, since the displayed values were an order of magnitude lower than predicted by the diffuse boundary limit of Casimir's theory. Recent theoretical work has employed the Born approximation to predict a very much enhanced boundary scattering rate that would lead to a thermal conductivity well below the Casimir limit. We present a Green's function calculation that answers the question of whether the Casimir limit to the phonon mean free path can be overcome by roughness. Our results show that the mean free path (MFP) and the thermal conductivity of a nanowire are very close to the Casimir limit for shallow disorder, and can only be pushed below it using very deep surface roughness, well beyond previous estimates. We also explore the limits of the Born approximation in this context using vacancies and isotopic impurities as defects.

[1]This work was supported by the Spanish MICINN/FEDER (FIS2008-04894/FIS) and the Xunta de Galicia (INCITE09E2R206033ES). J.Carrete thanks the Spanish Ministry of Education for a FPU grant.

3:18PM D11.00005 Quantal Heating of 2D electrons in strong magnetic fields[1] , SERGEY VITKALOV, The City College of New York, New York, NY 10031, USA, ALEXEY BYKOV, Institute of Semiconductor Physics, 630090 Novosibirsk, Russia — Usually heating of conducting electrons by dc electric field increases electron temperature and effects weakly the electron transport. In this report we show that the dc heating of 2D electrons with a quantized spectrum is very peculiar and violates strongly the Ohm's Law [1]. The quantal heating establishes nontrivial electron distribution, which has the same broadening or an effective "temperature" as the unbiased system. The heating reduces significantly the dissipative electron transport, forcing the quantum conductors into a state with zero differential resistance (ZDR). Furthermore an apparent dc driven metal-insulator transition is found, which correlates with the transition into the ZDR state. This interesting correlation is unexpected and is not understood.

[1] J.-Q. Zhang, S.A. Vitkalov and A.A. Bykov, Phys. Rev. B 80, 045310 (2009); S. A. Vitkalov, International Journal of Modern Physics B, 23, 4727 (2009).

[1]Support: NSF DMR 0349049 and RFBR Projects No. 10-02-00285

3:30PM D11.00006 Light-induced thermodynamic metastability in amorphous silicon , DANIEL QUEEN, JULIE KAREL, FRANCES HELLMAN, University of California, Berkeley, QI WANG, RICHARD CRANDALL, EUGENE IWANICZKO, National Renewable Energy Lab — The efficiency of amorphous silicon photovoltaics is limited due to the generation of dangling bond defects upon light soaking which leads to a decrease in their efficiency known as the Staebler-Wronski Effect. These defects act as recombination centers for photoexcited electron-hole pairs and can be reversibly removed by annealing above 150°C. The electrical properties of these defects are well documented but the mechanism that gives rise to them is still an open question. It is known that hydrogen plays a crucial role in their formation and recovery but it is not clear if hydrogen participates in the defect formation. We present heat capacity data for a-Si:H films grown by the Hot-Wire CVD (HWCVD) technique and a-Si films grown by e-beam evaporationand measured using our MEMS based nanocalorimeter. Both materials have an excess heat capacity observed upon light soaking that is reversibly removed by annealing at 200°C. This excess is found to be independent of H content in the HWCVD films and is present but at a smaller magnitude in the e-beam evaporated a-Si. The lack of dependence on H content and the presence in the e-beam films indicates the light induced metastability is intrinsic to the amorphous silicon matrix.

3:42PM D11.00007 Thermodynamic properties of ZrSiO4 polymorphs from DFT based *ab initio* phonon calculations[1] , JINCHENG DU, MRUNAL CHAUDHARI — Zircon and Reidite are the polymorphs of $ZrSiO_4$minerals that are natural hosts of various radioactive elements in the crust of the earth. Its high permittivity also makes it a promising material for the gate dielectric material in metal-oxide semiconductors. Knowledge of the thermodynamic properties at high temperature and high is very important to consider its application as an effective natural storage for the radioactive wastes and high technology ceramics. These properties are thoroughly studied both computationally and experimentally for zircon, while significantly less attention was paid to reidite in the literature. We report studies of thermodynamic properties of Zircon and Reidite from phonon spectra calculations using *ab initio* based periodic density-functional theory (DFT) calculations. Various thermodynamic properties such as free energy, internal energy, entropy, enthalpy, heat capacity and thermal displacement as a function of temperature are calculated. Phoon dispersion curves and density of states are calculated and compared with the experimental data. Calculated bulk properties agree very well with the experimental data in the literature.

[1]This work is supported by UNT RIG.

3:54PM D11.00008 Vibrational and thermal properties of ternary semiconductors and their isotopic dependence: chalcopyrite CuGaS2[1] , ALDO ROMERO, CINVESTAV, Unidad Queretaro, M. CARDONA, R. KREMER, R. LAUCK, Max Planck Institute, Stuttgart, A. MUÑOZ, ULL, Spain — The availability of *ab initio* electronic calculations and the concomitant techniques for deriving the corresponding lattice dynamics have been profusely used in the past decade for calculating thermodynamic and vibrational properties of semiconductors, as well as their dependence on isotopic masses. The latter have been compared with experimental data for elemental and binary semiconductors with different isotopic compositions [1]. Here we present theoretical and experimental data for several vibronic and thermodynamic properties of a canonical ternary semiconductor of the chalcopyrite family: CuGaS2 [2]. Among these properties are the lattice parameters, the phonon dispersion relations and densities of states (projected on the Cu, Ga, and S constituents), the specific heat and the volume expansion coefficient. The calculations were performed with the ABINIT and VASP codes within the LDA approximation for exchange and correlation.

[1] Cardona *et al.*, PRB81, 075202 (2010)
[2] Gibin *et al.*, Solid State Commun Solid State Commun 133, 569 (2005); Sanati *et al.* S.S. Commun 131 229 (2004).

[1]Supported by CONACYT under projects J-59853-F and J-83247-F.

4:06PM D11.00009 Temperature dependence of band gap of highly confined CdSe and PbSe nanocrystals , JASON BYLSMA, PRASENJIT DEY, JASON REJMAN, University of South Florida, AARON ZAUBI, SARATH WITANACHCHI, PRITISH MUKHERJEE, DENIS KARAISKAJ, MATTHEW C. BEARD COLLABORATION[1] — We have recorded fluorescence spectra from PbSe and CdSe quantum dots in hexane/toluene respectively between 5K and 300K in order to investigate the temperature dependence of the electronic band gap of these highly confined nanostructures. The band gap for CdSe follows the known blue shift with decreasing temperature (dE/dt = -225 μeV/K). Olkhovets et. al. first reported a red shift of the band gap energy with decreasing temperature for small (d $<$ 4 nm) PbSe and PbS quantum dots [1]. Such behavior would contradict the expected blue shift of the band gap with decreasing temperature. We have measured the temperature dependence of the band gap of PbSe quantum dots for two different diameters below 4 nm and indeed observe a red shift of the band gap with decreasing temperature (dE/dT = 58 μeV/K), which is stronger for the smaller size quantum dots (dE/dt = 82 μeV/K). The origin of this peculiar behavior is not well understood and we are pursuing further theoretical and experimental studies in order to elucidate the mechanism behind it. [1] A. Olkhovets, et. al. Phys. Rev. Lett. 81, 3539 (1998).

[1]National Renewable Energy Laboratory

4:18PM D11.00010 Temperature and polarization dependent photoluminescence studies of WO_3 and WO_{3-x}single crystals , PRASENJIT DEY, University of South Florida, JUSTIN EASLEY, Massachusetts Institute of Technology, DENIS KARAISKAJ, University of South Florida, SATYEN DEB, National Renewable Energy Laboratory, TED CISZEK, Geolite/Siliconsultant, DANIEL DESSAU, University of Colorado, Boulder — WO_3 is an important material not only due to its interesting electronic properties but also for applications in electrochromics and energy storage. The mechanism behind the electrochromic effect has been debated for several decades.[1] We have studied two WO_3 single crystals, a transparent and a doped WO_{3-x}. A photoluminescence center around 865 nm is observed after sub-band gap excitation at 405 nm with relatively higher intensity in the crystal containing oxygen vacancies. The center appears as a broad transition of 35 nm FWHM and does not follow the band gap energy with temperature. However polarization dependent studies reveal at least two polarization dependent component of the center.

[1]Satyen K. Deb, Solar energy materials and solar cells **92**, 245 (2008), and the references therein.

4:30PM D11.00011 Mapping free-carrier diffusion in GaAs with radiative and heat-generating recombination[1] , TIM GFROERER, RYAN CRUM, Davidson College, MARK WANLASS, NREL — We use a tightly focused laser along with optical and thermal imaging to measure the diffusion-driven, free-carrier distribution in a GaAs/GaInP heterostructure. We find that temperature profiles are broader than their luminescence counterparts. This observation is consistent with how the underlying recombination mechanisms depend on carrier density: the rate of heat generation should be approximately proportional to the density of carriers, while the radiative rate should scale with the density squared. We show that the square root of the light signal follows the heat profile, giving consistent, independent measurements of the local carrier density.

[1]Acknowledgment is made to the donors of the American Chemical Society - Petroleum Research Fund for support of this research.

Monday, March 21, 2011 2:30PM - 5:18PM –

Session D12 DMP: Focus Session: Dopants and Defects in Semiconductors: Compound Semiconductors II D223/224

2:30PM D12.00001 Defect energy distribution in GaN/AlGaN heterostructures grown in Ga-rich and ammonia-rich conditions[1] , TANIA ROY, YEVGENIY PUZYREV, ENXIA ZHANG, DANIEL FLEETWOOD, RONALD SCHRIMPF, SOKRATES PANTELIDES — We use low-frequency noise measurements to estimate energy distributions of electrical-stress-induced defects in AlGaN/GaN high electron mobility transistors from 85 K to 450 K. The devices were grown under Ga-rich and ammonia-rich conditions using molecular beam epitaxy. The Ga-rich devices show a positive shift in pinch-off voltage and a decrease in gate leakage current with stress under a gate voltage of -3.6 V and a drain voltage of 20 V. These changes in response are associated with hydrogenated Ga vacancies in AlGaN. The ammonia-rich devices show a negative shift in pinch-off voltage and an increase in gate leakage current under the same stress conditions; these changes in device response are caused by N-antisite defects. The excess drain voltage power spectral density of the low frequency $1/f$ noise peaks at $\sim$ 100 K in both device types, which corresponds to a trap energy of 0.2 eV. We attribute this to N-vacancy-related defects, which are also observed in proton damage experiments.

[1]This work was supported in part by an ONR MURI grant.

2:42PM D12.00002 Thermal electron capture rate by Fe acceptor in GaN , J. DASHDORJ, M.E. ZVANUT, University of Alabama at Birmingham, T. PASKOVA, K. UDWARY, Kyma Technologies, Inc. — Doping GaN with Fe compensates the main residual impurities such as O and Si to produce semi-insulating substrates. Electron paramagnetic resonance measurements were made on GaN grown by hydride vapor phase epitaxy and doped with 1.5x10^{17} to 1.6x10^{18} cm^{-3} Fe. The Fe^{3+} spectra, angular dependence, and concentrations are consistent with literature and secondary ion mass spectroscopy data. During illumination with photon energies greater than 1.2 eV, the Fe^{3+} signal increased in the lowest doped sample, but decreased in the more highly doped samples. One possible interpretation of the results is that the $Fe^{2+/3+}$ and $Fe^{3+/4+}$ levels are about 1.2 eV below the conduction band. Due to our measurement resolution, the spectral separation between the levels cannot be determined. The time-dependence of the Fe^{3+} signal recovery after removal of 2.64 eV was recorded at temperatures between 3.5 and 297 K. Analysis show that capture rate of electrons by Fe^{3+} decreases from 6x10^{-16} to 5x10^{-17} cm^3/s with an inverse-square-root temperature dependence. The work is supported by the NSF.

2:54PM D12.00003 Direct atomic imaging of Mn in the GaN growth surface: High-density, Two-dimensional, Striped Superstructures[1] , KANGKANG WANG, Ohio University, NOBORU TAKEUCHI, ABHIJIT CHINCHORE, WENZHI LIN, ARTHUR SMITH — A class of novel well-ordered striped superstructures have been observed by depositing submonolayer Mn onto GaN(0001)-"1×1" surface. These superstructures consist of stripe domains along $[1\bar{1}00]_{GaN}$ with various widths, while scanning tunneling microcopy images resolved a common local $\sqrt{3}\times\sqrt{3}$-R30° structure for the stripes. Combined with first-principles calculations, a new two-dimensional structural model is proposed having a dense Mn_xGa_{1-x} surface layer. Mn atomic sites within the GaN surface are directly identified. A spin-induced asymmetry in the Mn electronic structure is revealed in real-space for the narrow stripes. These findings explain the behavior of Mn atoms in the GaN growth surface and herald the development of magnetic nanostructures on GaN surfaces.

[1]This work is funded by Department of Energy and National Science Fundation.

3:06PM D12.00004 Initial Phase of Sub-monolayer Iron Growth on GaN(0001) pseudo-1×1-1+1/12 Surface Studied Using Scanning Tunneling Microscopy and First Principles Theoretical Calculations[1] , WENZHI LIN, NOBORU TAKEUCHI, KANGKANG WANG, ABHIJIT CHINCHORE, MENG SHI, ARTHUR SMITH, Nanoscale and Quantum Phenomena Institute, Department of Physics and Astronomy, Ohio University, HAMAD ALBRITHEN, Physics and Astronomy Department, King Saud University — Iron/gallium nitride bi-layer structures have potential use for spintronic applications. Therefore, we have carried out an investigation of the initial phase of sub-monolayer iron growth on GaN(0001) pseudo-1×1-1+1/12 surface. To begin with, we verified an atomically smooth GaN growth surface with the assistance of *in situ* reflection high energy electron diffraction. STM shows smooth terraces separated by single and double height bilayer atomic steps. About 0.4 ML iron was deposited on the smooth GaN, and the subsequent STM images reveal Fe islands with a height of $\sim$ 2 Å growing in a two-dimensional step-flow mode outward from the GaN step edges of the pseudo-1x1-1+1/12 surface. A clear 6 × 6 structure is observed for the islands. First principles theoretical calculations are being carried out in order to interpret the experimental results.

[1]This work is supported by the U.S. Department of Energy (Grant No. DE-FG02-06ER46317).

3:18PM D12.00005 Atomic displacements in proton-irradiated AlGaN/GaN heterostructures , YEVGENIY PUZYREV, 1, TANIA ROY, ENXIA ZHANG, RONALD SCHRIMPF, DANIEL FLEETWOOD, 2, SOKRATES PANTELIDES, 1, DEPARTMENT OF PHYSICS AND ASTRONOMY DEPARTMENT, VANDERBILT UNIVERSITY TEAM, DEPARTMENT OF ELECTRICAL ENGINEERING AND COMPUTER SCIENCE, VANDERBILT UNIVERSITY TEAM — We report results of quantum molecular dynamics calculations of atomic recoils in AlGaN and GaN. The recoil energy required to create defects in a perfect AlGaN/GaN lattice is known to be over 40eV. However, drastic changes in atomic configuration occur when defect atom itself recoils with than 10eV. We show that both N antisite defects and N atoms near Ga vacancy require less than 10 eV to introduce N vacancies, divacancies and N interstitials. This phenomenon leads to additional donors that can account for a positive shift in threshold voltage, observed in our electrical measurements in AlGaN/GaN devices irradiated by 1.8 MeV protons.[1] In addition, divacancies and N vacancies have an electron transition level near the Fermi level in AlGaN which also provides explanation for the experimentally observed increase in 1/f noise after proton irradiation.[2]

[1]T. Roy, et. al., *IEEE Trans. Nucl, Sci.*, 2010. accepted
[2]T. Roy, et al, *Microelectron. Reliab.*, 2010, accepted.

3:30PM D12.00006 Nanoscale Potential Fluctuations in (GaMn)AsGaAs Heterostructures: From Individual Ions to Charge Clusters and Electrostatic Quantum Dots , PAUL KOENRAAD, INEKE WIJNHEIJMER, JENS GARLEFF, Eindhoven University of Technology, OLEG MAKAROVSKY, LAURENCE EAVES, RICHARD CAMPION, BRYAN GALLAGHER, University of Nottingham — During growth of the dilute p-type ferromagnetic semiconductor GaMnAs, interstitial manganese is formed when the Mn concentration exceeds 2%. This interstitial Mn acts as a double donor which compensates the free holes that mediate ferromagnetism. Annealing causes out-diffusion of these interstitials, thereby increasing the Curie temperature. Here, we use cross sectional scanning tunneling microscopy and spectroscopy to visualize the potential landscape which arises due to the clustering of interstitial Mn in annealed p-i-n (GaMn)As-GaAs double barrier heterostructures. We map the local minima in the potential landscape, link them to clusters of individual interstitial Mn ions, and show that the ions are doubly charged.

3:42PM D12.00007 Controlled layer-by-layer depth-profiling of GaAs(110) using scanning tunneling microscopy , DAVID GOHLKE, DONGHUN LEE, JAY GUPTA, Department of Physics, Ohio State University — The electronic properties of dopants in semiconductors such as GaAs vary depending on proximity to interfaces. We utilize a low temperature (5K) scanning tunneling microscope to realize a layer-by-layer peeling technique on p-GaAs(110). We apply positive voltage pulses near As vacancies to desorb surface-layer Ga and As atoms. Subsequent motion of the STM tip peels away the first layer from this starting point, fully exposing sections of the subsurface layer. The second and further layers can be readily peeled away by the same technique. This newly created pit allows depth-profiling of subsurface defects with STM. Funded by the Center for Emergent Materials at the Ohio State University, an NSF MRSEC (DMR-0820414). http://www.physics.ohio-state.edu/∼jgupta

3:54PM D12.00008 Time-Resolved Far-Infrared Magnetospectroscopy of Electron Relaxation in GaAs[1] , S.N. GILBERT[2], Vanderbilt Univ., G.L. CARR[3], Brookhaven National Lab — We report time-resolved magnetospectroscopy results for (S-I) GaAs at T∼10K and fields up to 10T. A pulsed Ti:sapphire laser produces photoelectrons with energy ∼10 meV above the conduction band minimum that are subsequently probed by far-infrared transmission spectroscopy. Both free electrons and exciton transitions are observed, including transitions involving Landau levels when the magnetic field is applied. We also observe a time-dependent change in these transitions and discuss a model for the relaxation of a warm (non-equilibrium) distribution of electrons on a ∼500 ps time scale.

[1]High-field magnet provided courtesy of J.J. Tu (CCNY)
[2]Supported by NSF-IGERT at Vanderbilt
[3]Supported by DOE contract DE-AC02-98CH10886 at Brookhaven

4:06PM D12.00009 Tunable control over the ionization state of single Mn acceptors in GaAs with defect-induced band bending[1] , DONGHUN LEE, JAY GUPTA, Dept. of Physics, Ohio State University — The continuous miniaturization of semiconductor devices will ultimately reach a point where control over the properties of single dopants is necessary. Recent STM studies have demonstrated the ability to control the ionization state of single dopants through tip-induced band bending. This change in ionization state appears in STM images as a ring-like feature centered on the dopant, whose diameter depends on voltage, tip-sample distance, and tip termination. Here we demonstrate an additional degree of freedom for controlling the charge state of single Mn acceptors in GaAs by utilizing nearby charged defects which can be positioned with atomic precision. Systematic changes in the ring diameter with the separation between Mn and defect allows us to separately extract contributions from defect-induced and tip-induced band bending. These methods provide non-volatile control over the ionization state of single dopants, even in the absence of probe electrodes or STM tip.

[1]Funding by the Arnold and Mabel Beckman Foundation and the Center for Emergent Materials (an NSF MRSEC DMR-0820414)

4:18PM D12.00010 Identification of the major cause of endemically poor mobilities in SiC/SiO_2 structures[1] , XIAO SHEN, SOKRATES T. PANTELIDES, Vanderbilt University — Mobility degradation at semiconductor-dielectric interfaces is generally attributed to defects at the interface or inside the dielectric, as is the case in Si/SiO_2 structures. In the case of SiC/SiO_2 structures, a decade of research focused on reducing or passivating interface and oxide defects, but low mobilities have persisted. It is known that during oxidation of Si, Si atoms are emitted into the substrate, but they do not form strongly-bonded complexes and their effects are usually benign. In contrast, during oxidation of SiC, C atoms are emitted into the substrate and they can form strongly-bonded carbon complexes. Here we identify one particular complex that explains a range of experimental defect signatures and electrical measurements. We propose that this complex is a major cause of the poor mobility in SiC/SiO_2 structures.

[1]This work is supported in part by NSF GOALI grant DMR-0907385.

4:30PM D12.00011 Electronic properties of Si-C interfaces[1] , XIANG-GUO LI, HAI-PING CHENG, Department of Physics, University of Florida, USA — In this work, we report our investigations of interfacial properties of Si-C systems. Electronic properties of Fe-doped carbon on silicon surfaces, Si-Fe-C layered structures and Si-graphene-Si junctions have been studied using first-principles calculations. Charge transfer at the interfaces, densities of states, and magnetization are fully analyzed. These problems are important because recent experiments show that Fe@C-Si materials have giant electro-resistance and magneto-resistance highly sensitive to the external magnetic field. The non-magnetic feature leads to very small magnetic noise. In addition, photovoltaic effects were also observed in some of these systems.

[1]Acknowledgement: funding support from DOE/BES/DE-FG02-02ER45995 and computing resource from NERSC and UF/HPC

4:42PM D12.00012 Polariton Formation Enhances Lifetimes of Dense Exciton Gasses in Cuprous Oxide by Suppressing Two-Exciton Decay[1] , N. LASZLO FRAZER, Northwestern University, R.D. SCHALLER, Argonne National Lab, Northwestern University, J.I. JANG, SUNY Binghamton, S.E. MANI, J.B. KETTERSON, Northwestern University — Collective excitonic states form at high densities, but in dense gases the long lifetime of excitons in cuprous oxide (Cu_2O) is compromised by two-exciton annihilation processes. Using the picosecond streak camera spectroscopy facility at the Center for Nanoscale Materials at Argonne National Laboratory we directly measured the decay of orthoexciton-polaritons generated by two photon absorption. The two-body decay lifetime is an order of magnitude longer than for excitons uncoupled to photons. The extended lifetime opens opportunities for experiments that manipulate polariton collective states. Unlike time-averaged measurements of two-body processes, streak camera detection shows decay suppression without effects from production efficiency or additional density dependent processes.

[1]Supported by the NSF IGERT program and the Northwestern Ryan Fellowship.

4:54PM D12.00013 Ultrafast carrier dynamics in Bi2Se3 thin films , KELIANG HE, LIGUO ZHU, CHEN XIA, BRIAN KUBERA, JIE SHAN[1], Department of Physics, Case Western Reserve University, 10900 Euclid Avenue, Cleveland, OH 44106, U.S.A. — Bismuth Selenide (Bi2Se3), a group V-VI narrow gap layered semiconductor, is a well-known efficient solid thermoelectric material at room temperature. It has recently also attracted much research attention due to its interesting topological properties. The carrier dynamics and charge transport, electron-phonon coupling, and its role in the transport properties in Bi2Se3 are fundamental issues in understanding its thermoelectric and topological properties. In this work, we employ the optical-pump terahertz-probe technique to study the transient photoconductivity in Bi2Se3 thin crystalline films as a function of the pump-probe delay time and the excitation fluence. The photoconductivity spectrum ranging from 0.3 to 1.9 THz reveals both a Drude and a Lorentz contribution. The former is attributed to a free electron response with a scattering time of 0.7 ps; and the latter, with both its amplitude and peak frequency dependent on the carrier density, arises from a coupled LO phonon-plasmon mode. The nature of this mode and its role in transport will be discussed.

[1]Corresponding author: jie.shan@case.edu

5:06PM D12.00014 Oxygen in B_2O_3 covered Czochralski-grown Ge , TOSHINORI TAISHI, Institute of Carbon Science and Technology, Shinshu University, HIDEAKI ISE, YU MURAO, TAKAYUKI OHSAWA, YUKI TOKUMOTO, YUTAKA OHNO, ICHIRO YONENAGA, Institute for Materials Research, Tohoku University — Ge has been regained keen interest in applications of Ge for ultra-fast CMOS and PV devices. High quality Ge crystals should be demanded for realization of such devices with higher performances in these circumstances. Oxygen impurity can be expected to enhance thermo-mechanical stability of Ge crystals due to dislocation locking similar to oxygen in Si. For the purpose, we grew oxygen-enriched Ge crystals by the Czochralski method from B_2O_3 covered melt added with GeO_2 powder in a silica crucible. To evaluate precious knowledge oxygen behavior in Ge, local vibrations of oxygen were evaluated by FT-IR spectroscopy. Concentrations of interstitially dissolved oxygen impurity in the crystals were in the range between 8.5×10^{15} and 5.5×10^{17} cm^{-3} determined from the FT-IR absorption at 855 cm^{-1} originating in local vibration of Ge-O_i-Ge quasi-molecules. Absorption peaks relating to GeO_x, SiO_x and Si-Oi-Si were not detected in the as-grown crystals. By prolonged annealing at 350_C, an absorption peak developed at 780 cm^{-1}, indicating formation of oxygen related thermal donors. Such donors disappeared by annealing at 550_C.

Monday, March 21, 2011 2:30PM - 5:30PM –
Session D13 GSNP: Statistical and Nonlinear Physics: General D225/226

2:30PM D13.00001 Stability and dynamical properties of Cooper-Shepard-Sodano compactons , ANDRES CARDENAS, New York University, BOGDAN MIHAILA, Los Alamos National Laboratory, FRED COOPER, Santa Fe Institute, AVADH SAXENA, Los Alamos National Laboratory — Extending a Pade approximant method used recently to study the properties of compactons in the Rosenau-Hyman (RH) equation [see B. Mihaila et al. Phys. Rev. E 81, 056708 (2010)], we study the numerical stability of single compactons of the Cooper-Shepard-Sodano (CSS) equation and their pairwise interactions. The CSS equation has a conserved Hamiltonian which has allowed several approaches for studying analytically the nonlinear stability of the solutions. We study three different compacton solutions and find they are numerically stable. Similar to the collisions between RH compactons, the CSS compactons reemerge with the same coherent shape when scattered. The time evolution of the small-amplitude ripple resulting after scattering depends on the values of the parameters characterizing the corresponding CSS equation. The simulation of the CSS compacton scattering requires a much smaller artificial viscosity to obtain numerical stability than in the case of RH compacton propagation.

2:42PM D13.00002 Pair Correlations for Charges in a Harmonic Trap , JEFFREY WRIGHTON, JAMES DUFTY, University of Florida, HANNO KÄHLERT, TORBEN OTT, PATRICK LUDWIG, MICHAEL BONITZ, Christian-Albrechts-Universität zu Kiel — A classical system of N identical charges in a harmonic trap exhibits both shell structure and orientational ordering due to Coulomb correlations. The shell structure can be reproduced accurately using approximate correlations from the bulk OCP [1]. Here we report additional relationships between correlations in the trap and those for the bulk OCP: 1) pair correlations calculated without reference to their location in the trap agree with those of the bulk OCP, 2) orientational pair correlations among particles within a shell are represented by those of the bulk OCP, when Euclidean distance is replaced by arc length (qualitative agreement using 3D OCP; quantitative agreement using 2D OCP). At stronger coupling, the correlations induce an ordering within the shells (spherical Wigner crystal). It is shown that the orientational correlations for this phase are described by those for the single sphere Thomson problem, i.e. the Thomson sites represent the "lattice" for the spherical crystal. Finite temperature effects for this phase are described as well. Research supported by DOE award DE-FG02-07ER54946, and by the Deutsche Forschungsgemeinschaft via SFB-TRR24.

[1] J. Wrighton, J. Dufty, H. Kaehlert, and M. Bonitz, Phys. Rev. E **80**, 038912 (2009); Contrib. Plasma Phys. **50**, 26-30 (2010).

2:54PM D13.00003 Quasi-bound state lifetimes and classical periodic orbits in HOCl , ALEX BARR, KYUNGSUN NA, LINDA REICHL, University of Texas at Austin — We use a discrete variable representation together with reaction matrix theory to calculate the quasi-bound states of a Chlorine atom scattering off a diatomic molecule of Hydrogen and Oxygen. The lifetimes of these quasi-bound states are found to vary over six orders of magnitude in a very small energy window. By examining Husimi distributions for various quasi-bound states we show that the longest-lived quasi- bound states are anchored by an island of stability surrounding a stable periodic orbit in the otherwise chaotic classical phase space. This stable periodic orbit, which corresponds to Chlorine rotating around the HO molecule, is responsible for the very long lifetimes of these quasi-bound states.

3:06PM D13.00004 An Infinite Order Phase Transition , PRADEEP KUMAR, University of Florida, AVINASH KHARE, Institute of Physics, Bhubaneshwar, AVADH SAXENA, Los Alamos National Laboratory — An infinite order phase transition, in the sense envisioned by Ehrenfest, must show no singularity in any finite (thermal or mechanical) derivative of the free energy. By considering the infinite p limit of a free energy that we have derived for a p-th order phase transition, we can derive a Landau type free energy. We will discuss the properties of the free energy and identify the features essential for a description of an infinite order phase transition. These include a logarithmic interaction between the fields and a novel dependence on spatial gradients. Contrary to popular belief, since some symmetry is broken at each finite p order, we submit that an infinite order phase transition does not exclude a symmetry being broken. Restricting to one dimension, we solve for domain wall solutions. Finally we show the relationship between an infinite order phase transition and Tachyon condensation. They are both analyzed as the infinite p limit of a class of p enumerated field theories. The mathematical difference being that the free energy for infinite order transition belongs to a potential that is negative (inverted) of the action for tachyon condensation.

3:18PM D13.00005 First Principles Derivation of Fading Models from Wave Chaos Theory , JEN-HAO YEH, University of Maryland — Wave chaos is the study of solutions to linear wave equations in situations where the ray dynamics recovered in the classical limit is chaotic. Fading is the observation of variations in signal strength measured at a receiver due to time-dependent variations in the propagation or multi-path scattering and interference. A quantitative statistical theory of wave chaos - random matrix theory (RMT) - can be applied to predict statistical properties of many quantities, such as the scattering matrix, of a wave chaotic system. Here we started from the statistical model of the scattering matrix [1] to establish a general fading model that includes Rayleigh fading and then combine the RMT fading model with our random coupling model that takes account system-specific features [2-4] to build a more general fading model that includes Rician fading. In the high loss limit, our model agrees with the Rayleigh/Rice models, however, it shows deviation in the limit of low loss. We have performed experiments [3,4] to verify the RMT fading model.
[1] http://publish.aps.org/search/field/author/Brouwer_P_W (P. W. Brouwer) and http://publish.aps.org/search/field/author/Beenakker_C_W_J (C. W. J. Beenakker), Phys. Rev. B 55, 4695 (1997). [2] James A. Hart, *et al.*, Phys. Rev. E 80, 041109 (2009). [3] Jen-Hao Yeh, *et al.*, Phys. Rev. E 81, 025201(R) (2010). [4] Jen-Hao Yeh, *et al.*, Phys. Rev. E 82, 041114 (2010).

3:30PM D13.00006 Quantum statistical mechanics on infinitely ramified fractals , JOE P. CHEN, Cornell University — I present the thermodynamics of identical particles confined in infinitely ramified, exactly self-similar fractals, such as the Sierpinski carpet (in 2D) and the Menger sponge (in 3D). Recent results from analysis on fractals have established that the heat kernel associated with the Laplacian on such fractals satisfy, in the short-time regime, a scaling relation with exponent $d_S/2$ (where d_S is the spectral dimension) modulated by log-periodic oscillations. I explain how such a scaling affects the partition function, and the resultant thermodynamics associated with blackbody radiation [1], Casimir effect, and electrons in the fractal box.

3:42PM D13.00007 Unified Approach to Quantum and Classical Dualities[1] , EMILIO COBANERA, GERARDO ORTIZ, Indiana University, Bloomington, IN, ZOHAR NUSSINOV, Washington University, St. Louis, MO — We discuss a new systematic and algebraic approach to searching for dualities in quantum systems. By associating "bond algebras" to quantum Hamiltonians we show how dualities can be characterized, recognized as unitary transformations, and mapped to dualities of classical partition functions. Hence our approach unifies classical and quantum dualities and provides a powerful method for determining exact properties of systems of interest. We show how duality transformations can be used always to eliminate gauge symmetries completely, and present a new duality between the Abelian Higgs model and a generalized Kitaev's extended toric code model in *three space dimensions* that illustrate this point. We also show new dualities for Z_p) gauge models.

[1]Phys. Rev. Lett. 104, 020402 (2010)

3:54PM D13.00008 Fluctuation-induced forces in strongly anisotropic critical systems , M. BURGSMÜLLER, H.W. DIEHL, Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany, M.A. SHPOT, Institute for Condensed Matter Physics, 79011 Lviv, Ukraine — Strongly anisotropic critical systems have two (or more) correlation lengths ξ_α and ξ_β that diverge as nontrivial powers $\xi_\alpha \sim \xi_\beta^\theta \to \infty$ upon approaching criticality. We investigate the effective (Casimir-like) forces that are induced between two confining parallel boundary planes at a distance L by fluctuations in such systems at bulk criticality. Two fundamentally distinct orientations of boundary planes must be distinguished: parallel, for which the planes are parallel to all of the available $1 \leq m < d$ α-directions, and perpendicular, for which they are perpendicular to an α-direction, but parallel to all other α- and β-directions. Using a RG approach, we show that universal Casimir amplitudes $\Delta_{\parallel,\perp}^{BC}$, depending on both the large-scale boundary condition (BC) at both plates and the type of surface plane orientation, can be introduced to characterize the asymptotic L-dependence of the critical fluctuation-induced force. This varies as $\mathcal{F} \sim -(\partial/\partial L)\,\Delta_{\parallel,\perp}^{BC}\,L^{-\zeta_{\parallel,\perp}}$, where the proportionality constant is nonuniversal. To corroborate these findings, $O(n)$ ϕ^4 models with m-axial Lifshitz points are investigated below their upper critical dimension $d = 4 + m/2$. Explicit one- and two-loop results for $\Delta_{\parallel,\perp}^{BC}$ are presented for both orientations and periodic or Dirichlet-like boundary conditions, along with large-n results.

4:06PM D13.00009 Multifractality of instantaneous normal modes at mobility edges , TEN-MING WU, Institute of Physics, Natl Chiao-Tung Univ, Hsinchu, Taiwan — In terms of the multifractal analysis, we investigate the characteristics of instantaneous normal modes (INMs) at mobility edges (MEs) of a simple fluid, where the locations of two MEs in the INM spectrum were identified in a previous work (Phys. Rev. E 79, 041105 (2009)). The mass exponents and the singularity spectrum of the INMs are obtained by both the box-size and system-size scalings under the typical average. The INM eigenvectors at a ME exhibit a multifractal nature and the multifractal INMs at each ME yield the same results in generalized fractal dimensions and singularity spectrum. Our results indicate that the singularity spectrum of the multifractal INMs agrees well with that of the Anderson model at the critical disorder. This good agreement provides a numerical evidence for the universal multifractality at the localization-delocalization transition. For the multifractal INMs, the probability density function and the spatial correlation function of squared vibrational amplitudes are also calculated. The relation between probability density function and singularity spectrum is examined numerically, so are the relations between the critical exponents of the spatial correlation function and the mass exponents of the multifractal INMs. All results will be appeared in Phys. Rev. E.

4:18PM D13.00010 Experimental study of memory erasure in a double-well potential , YONGGUN JUN, JOHN BECHHOEFER, Dept. of Physics, Simon Fraser University — We have experimentally demonstrated memory erasure in a time-dependent, double-well potential using a protocol suggested by Dillenschneider and Lutz [PRL 102, 210601 (2009)]. The protocol implements the erasure of information by removing the potential barrier, skewing the potential to one side, and then raising the barrier back. In this context, erasure means that no matter which well the particle started the cycle in, it ends up in a designated well. We implement the potential by placing an overdamped, charged Brownian particle in a feedback trap that uses electrophoresis to generate an arbitrary virtual two-dimensional potential. In a large system, Landauer's principle gives a lower bound for the heat dissipated in the erasure of a single bit (kT ln2). In a small system such as ours, thermal fluctuations allow for occasional violations. We quantify such violations as a function of barrier size and show that while averages are consistent with Landauer's principle, the tail of the distribution of dissipation per cycle—a fraction of trajectories—violates it.

4:30PM D13.00011 Cosmology in One Dimension: Fractal Geometry, Power Spectra and Correlation , BRUCE MILLER, Texas Christian University, JEAN-LOUIS ROUET, Universite d'Orleans — Concentrations of matter, such as galaxies and galactic clusters, originated as very small density fluctuations in the early universe. The existence of galaxy clusters and super-clusters suggests that a natural scale for the matter distribution may not exist. A point of controversy is whether the distribution is fractal and, if so,over what range of scales. One-dimensional models demonstrate that the important dynamics for cluster formation occur in the position-velocity plane. Here the development of scaling behavior and multifractal geometry is investigated for a family of one-dimensional models for three different, scale-free, initial conditions. A possible physical mechanism for understanding the self-similar evolution is introduced. It is shown that hierarchical cluster formation depends both on the model and the initial power spectrum. Under special circumstances a simple relation between the power spectrum, correlation function, and correlation dimension in the highly nonlinear regime is confirmed.

4:42PM D13.00012 ABSTRACT WITHDRAWN –

4:54PM D13.00013 Thermodynamics in a complete description of the Landau diamagnetism , S. CURILEF, F. OLIVARES, F. PENNINI, Universidad Catolica del Norte — We analyze some consequences that come from semiclassical measures as the Wehrl entropy and the Fisher information for the problem of a particle in a magnetic field starting from a complete description of the Husimi function. We discuss in the most complete form (three dimensions)[1] some results related to measures in contrast with the incomplete form (two dimensions)[2,3]. The formulation in two dimensions is sufficient unto itself to explain the problem whenever the length of the cylindrical geometry of the system is large enough. Our semiclassical description constitutes a useful framework to illustrate problems related to size effects, role of boundaries and other typical anomalies derived from the size of the system, which are refereed to two parameters as area and length and they explicitly appear in the form of the limiting temperature and magnetic field. In addition, we discuss that the zero temperature can be achieved only if the length of the system size is large enough, otherwise physical properties strongly depend on the size of the system. Moreover, from the quantization of the quantum Hall effect, we have obtained a family of quantized Wehrl entropies.

[1] F. Olivares, et al, PRE **81** 041134 (2010);
[2] D. Herrera, et al, Eur J Phys **29** 439 (2008);
[3] S, Curilef, et al, PRB **71** 024420 (2005).

5:06PM D13.00014 Newtonian trajectories as a tool for quantum dynamics in an electromagnetic field , FONS BROSENS, University of Antwerpen, WIM MAGNUS, imec-Leuven — In previous studies, we showed that the classical equations of motion provide a solution to quantum dynamics, if appropriately incorporated in the Wigner distribution function, exactly reformulated in a type of Boltzmann equation. However, this earlier work was limited to scalar potentials. In the presence of an electromagnetic field, we now show that this description in terms of classical paths remains valid, despite the fact that the definition of the Wigner distribution function is not gauge invariant. Some analytical results are also presented.

5:18PM D13.00015 The bond problem with an arbitrary percolation radius is solved! , VLADIMIR UDODOV, MARIYA BUREEVA, Katanov Khakas State University, KATANOV KHAKAS STATE UNIVERSITY TEAM — The results of investigations of main characteristics of a one-dimensional percolation theory (percolation threshold, critical exponents of correlation radius and specific heat) are presented for the problem of bonds and sites. It is shown that for a finite-size system the stability condition is fulfilled while the scaling hypothesis is inacceptable for one-dimensional bond problem. The correlation length exponent ν in a one-dimensional problem of bonds has been found to exceed the values of ν in the problem of sites for equal-length chains, and, in general, this exponent was found to be extraordinary large compared to the 2-D and 3-D cases for ordinary phase transitions in macrosystems. The scaling hypothesis is inapplicable to random (disordered) one-dimensional nanostructures containing hundreds of structural elements. The results obtained in this work can be used in modeling hopping conduction in semiconductors at low temperatures and polytype transformations in close-packed crystals. For the first time, using the method of computer simulation, we have solved the bond problem for the model of one-dimensional percolation in finite-size systems of tens of nanometers with an arbitrary percolation radius.

Monday, March 21, 2011 2:30PM - 5:30PM –
Session D14 GSNP: Systems Far From Equilibrium D227

2:30PM D14.00001 Fluctuation Relations for Currents[1] , NIKOLAI SINITSYN, Theoretical Division, Los Alamos National Laboratory, ALEXEI AKIMOV, Department of Chemistry, Rice University, VLADIMIR CHERNYAK, Deparment of Chemistry, Wayne State University, MICHAEL CHERTKOV, Theoretical Division, Los Alamos National Laboratory — We consider a non-equilibrium statistical system on a graph or a network. Identical particles are injected, interact with each other, traverse, and leave the graph in a stochastic manner described in terms of Poisson rates, possibly strongly dependent on time and instantaneous occupation numbers at the nodes of the graph. We show that the system demonstrates a profound statistical symmetry, leading to new Fluctuation Relations that originate from the supersymmetry and the principle of the geometric universality of currents rather than from the relations between probabilities of forward and reverse trajectories.

[1]NSF/ECCS-0925618, NSF/CHE-0808910 and DOE at LANL under Contract No. DE-AC52-06NA25396.

2:42PM D14.00002 Aging in coarsening ferromagnets with site and bond disorder[1] , HYUNHANG PARK, MICHEL PLEIMLING, Virginia Tech — Aging processes during phase ordering are studied in the random-site and random-bond Ising models in two dimensions through Monte-Carlo simulations. The dynamical correlation length $L(t)$ is numerically determined and the behavior of various two-time quantities is investigated. For both models deviations of $L(t)$ from an algebraic growth law $L(t) \sim t^{1/z}$ are observed. Using the correct form of $L(t)$ a simple scaling picture is recovered for the studied disordered ferromagnets in the coarsening regime. Thus various two-time quantities, as for example the autocorrelation function, the space-time correlation function and the time integrated linear response, show a scaling behavior that is fully consistent with simple aging [1]. The similarities and differences between the site-disordered and the bond-disordered models are discussed.

[1] H. Park and M. Pleimling, Phys. Rev. B **82**, 144406 (2010).

[1]This work was supported by the US Department of Energy through grant DE-FG02-09ER46613.

2:54PM D14.00003 Nonequilibrium phase transition in a driven Potts model with friction[1] , MICHEL PLEIMLING, Virginia Tech, FERENC IGLÓI, Research Institute for Solid State Physics and Optics, Budapest, Hungary, and Szeged University, Hungary, LOÏC TURBAN, University Nancy, France — We consider magnetic friction between two systems of q-state Potts spins which are moving along their boundaries with a relative constant velocity v. Due to interaction between the surface spins there is a permanent energy flow and the system is in a steady state which is far from equilibrium. The problem is treated analytically in the limit $v = \infty$ (in one dimension, as well as in two dimensions for large-q values) and for v and q finite by Monte Carlo simulations in two dimensions. Exotic nonequilibrium phase transitions take place, the properties of which depend on the type of phase transition in equilibrium. When this latter transition is of first order, a sequence of second- and first-order nonequilibrium transitions can be observed when the interaction is varied [1].

[1] F. Iglói, M. Pleimling, and L. Turban, arXiv:1010.0738.

[1]This work was supported in part by the US National Science Foundation through Grant DMR-0904999.

3:06PM D14.00004 Aging dynamics for the driven lattice gas[1] , GEORGE L. DAQUILA, UWE C. TÄUBER, Department of Physics, Virginia Tech — We numerically investigate the two-time behavior of the density-density auto-correlation function in driven lattice gases with particle exclusion and periodic boundary conditions in one, two, and three dimensions using precise Monte Carlo simulations. Starting from strongly correlated initial conditions we investigate the relaxation towards the nonequilibrium steady state. We obtain simple aging scaling behavior in one, two, and three dimensions. The simulation data confirm the density auto-correlation aging exponents determined from simple scaling arguments. For the one-dimensional case we connect with the KPZ surface growth model and establish a relation between the density-density and known height-height auto-correlation aging exponents.

[1]Research supported through the US Department of Energy (DOE-BES), grant no. DE-FG02-09ER46613.

3:18PM D14.00005 Effect of size distribution on metastability in magnetic nanoparticles , YOH YAMAMOTO, KYUNGWHA PARK, Virginia Tech, Blacksburg, VA — Magnetic nanoparticles that have been synthesized using various methods have size distributions. This results in distributions in the magnetic anisotropy of magnetic nanoparticles. Considering the particle size distributions, we investigate metastability in magnetic nanoparticles at low temperatures. To model this system, we use a spin $S = 1$ ferromagnetic Blume-Capel model on a square lattice with periodic boundary conditions. The particle size distribution is incorporated in the model such that the uniaxial magnetic anisotropy parameter has a Gaussian distribution. We perform kinetic Monte Carlo simulations of the Blume-Capel model with the Glauber dynamic to explore magnetization relaxation in the regime where a single droplet of flipped spins forms a critical droplet. We present the lifetime of the metastable state as a function of temperature and standard deviation of the magnetic anisotropy distribution as well as a finite-size effect on the lifetime.

3:30PM D14.00006 Phase Diagram for a 2-D Two-Temperature Diffusive XY Model[1] , MATTHEW REICHL, CHARO DEL GENIO[2], KEVIN E. BASSLER, University of Houston — Using Monte Carlo simulations, we determine the phase diagram of a diffusive two-temperature conserved order parameter XY model. When the two temperatures are equal the system becomes the equilibrium XY model with the continuous Kosterlitz-Thouless (KT) vortex-antivortex unbinding phase transition. When the two temperatures are unequal the system is driven by an energy flow from the higher temperature heat-bath to the lower temperature one and reaches a far-from-equilibrium steady state. We show that the nonequilibrium phase diagram contains three phases: A homogenous disordered phase and two phases with long range, spin texture order. Two critical lines, representing continuous phase transitions from a homogenous disordered phase to two phases of long range order, meet at the equilibrium KT point. The shape of the nonequilibrium critical lines as they approach the KT point is described by a crossover exponent $\varphi = 2.52 \pm 0.05$. Finally, we suggest that the transition between the two phases with long-range order is first-order, making the KT-point where all three phases meet a bicritical point.

[1]This work was supported by the NSF through grant No. DMR-0908286.
[2]Current affiliation: Max Planck Institut für Physik Complexer Systems

3:42PM D14.00007 Avalanches in gauge theories , STEFANOS PAPANIKOLAOU, Cornell University — I consider the non-equilibrium behavior of disordered systems which contain a residual gauge symmetry. Remarkably, in this limit each avalanche is a Wilson loop of the associated gauge theory. Such gauge invariant avalanches present interesting critical behavior that we characterize. Also, I show that, when the gauge symmetry is violated, the behavior drastically changes. Finally, the relation of these results to current experimental efforts on spin ice compounds is discussed.

3:54PM D14.00008 A framework for studying biased stochastic dynamics in continuous space[1] , S.M. ALI TABEI, YE TIAN, University of Chicago, MARTIN TCHERNOOKOV, Emory University, AARON DINNER, University of Chicago — Typically in the formalism of large deviation functions the biased dynamics are studied in a discrete space. However, in many realistic stochastic systems dynamics take form in a continuous rather than a discrete space. In recent work it was shown that the biased dynamics for continuous-space models can be calculated using transition path sampling: unbiased trajectories were generated by shooting with the original dynamics from an existing path and then accepted or rejected to obtain the biased path ensemble. Here, we instead develop a way to bias continuous-space dynamics directly in the form of a biased Langevin equation.

[1]Funded by the Human Frontier Science Program

4:06PM D14.00009 Measured first-passage-time distributions for a high-dimensional system: noise-induced current switching in semiconductor superlattices[1] , YURIY BOMZE, Duke University, HOLGER T. GRAHN, RUDOLF HEY, Paul-Drude-Institute, Berlin, Germany, STEPHEN W. TEITSWORTH, Duke University — We report the experimental measurement of first-passage-time distributions associated with current switching in weakly-coupled GaAs/AlAs superlattices, in a regime of nonlinear electronic transport where the static current-voltage ($I - V$) curves exhibit multiple branches and bistability. Precision, high bandwidth current switching data are collected in response to sequential steps in applied voltage to a final voltage V_f near to the voltage V_{th} corresponding to the end of a particular branch. For initial state preparation, a double step procedure is used to insure that the system is close to the true metastable state. For a range of V_f values, switching times reveal large stochastic fluctuations driven by internal shot noise. For smaller times ($< 3\mu$s), the switching time distributions show exponential tails, as expected for activated escape from an initial metastable state. However, at larger times (> 10 μs), the distributions exhibit power law tails (with exponent ranging from -2 to -1, and dependent on $|V_f - V_{th}|$). Possible sources for the power law decay include collective effects and the presence of multiple escape trajectories.

[1]Supported by NSF grant DMR-0804232

4:18PM D14.00010 Non-equilibrium Thermodynamics: Residual Entropy, Internal Variables, Maxwell Relations, and the Prigogine-Defay Ratio , PURU GUJRATI, The University of Akron — We extend a recently formulated [Phys. Rev. E 81, 051130 (2010)] non-equilibrium thermodynamic approach to an inhomogeneous system consisting of many smaller subsystems, each in internal equilibrium; their relative motions result in viscous effects. The correct Gibbs free energy of a subsystem contains the temperature and pressure of the medium, making our approach an extension of the classical non-equilibrium thermodynamics due to de Donder. The additivity of entropy requires quasi-independence of subsystems, so that the energy also becomes additive. We use Gibbs' entropy of the isolated system to derive the entropy for the system even when the latter is out of equilibrium. We use this entropy to discuss the residual entropy when the system is confined to one of the components in the phase space. The approach is extended to include internal variables that cannot be controlled by the observer during non-equilibrium evolution. We then identify the form of non-equilibrium Maxwell relations. We apply our formalism to evaluate the Prigogine-Defay ratio in glasses, which is found to be, in general, different from 1 at the apparent glass transition, as is normally seen in experiments.

4:30PM D14.00011 Generalized Gibbs distribution and energy localization in the semiclassical FPU problem , RAFAEL HIPOLITO, CUNY-College of Staten Island, IPPEI DANSHITA, Tokyo University of Science, VADIM OGANESYAN, CUNY-College of Staten Island, ANATOLI POLKOVNIKOV, Boston University — We investigate dynamics of the weakly interacting quantum mechanical Fermi-Pasta-Ulam (qFPU) model in the semiclassical limit below the stochasticity threshold. Within this limit we find that initial quantum fluctuations lead to the damping of FPU oscillations and relaxation of the system to a slowly evolving steady state with energy localized within few momentum modes. We find that in large systems this state can be described by the generalized Gibbs ensemble (GGE), with the Lagrange multipliers being very weak functions of time. This ensembles gives accurate description of the instantaneous correlation functions, both quadratic and quartic. Based on these results we conjecture that GGE generically appears as a prethermalized state in weakly non-integrable systems.

4:42PM D14.00012 Zero Droplet Stiffness Exponent: Probing Short Range Spin Glasses with Avalanches Induced by Long Range Interactions , GERGELY ZIMANYI, Physics Department, UC Davis, FERENC PAZMANDI — We probe the droplet excitations in short range spin glasses by adding a perturbative long range interaction that decays with distance as a power law: J/r^{σ}. It is shown that if the power law exponent σ is smaller than the spatial dimension d, the perturbation induces large scale avalanches which roll until they force the system to develop a pseudo gap in the excitation spectrum of the stabilities. This makes the perturbative long range interactions relevant for $\sigma < \sigma_c = d$. The droplet theory predicts that the critical exponent σ_c depends on the droplet stiffness exponent as $\sigma_c = d - \theta$. Combining these two results leads to a zero stiffness exponent $\theta = 0$ in the droplet theory of short range spin glasses.

4:54PM D14.00013 Introduction of a new thermodynamic property: "characteristic frequency" , MCKENDREE PEPPER, Chicago Bridge and Iron, and Lamar University, CRISTIAN BAHRIM, Department of Physics, RAFAEL TADMOR, Department of Chemical Engineering, Lamar University — Fluctuations of thermodynamic properties are observed in the critical region of fluids, multiphase regions, and in systems containing a small number of molecules. We describe the dynamics within the vapor-liquid *interfacial region* (IR) of a monatomic fluid in thermal equilibrium using fundamental principles of mechanics and thermodynamics. Our objective is to provide a new dynamic parameter which characterizes thermodynamic systems fluctuating near equilibrium, such as the IR. We call this new property *"characteristic frequency"*. Our model assumes that the IR is (1) a closed thermodynamic system, (2) has a linear response to a driving force generated by a thermodynamic fluctuation, and (3) has a unique characteristic (resonant) frequency. We find that mild oscillations from equilibrium of a thermodynamic system occur at the most probable speed, and that the amplitude of the oscillations depends solely on the partition functions of the vapor and liquid within the IR. Our conclusion is that fluctuating thermodynamic systems at thermal equilibrium can exhibit oscillations analogous to mechanical systems and manifest a similar resonant response as the classical oscillators near their characteristic frequency.

5:06PM D14.00014 An effective Fluctuation Theorem in Bidirectional Single-Electron Counting , YASUHIRO UTSUMI, Mie University, DIMITRY GOLUBEV, MICHAEL MARTHALER, Karlsruhe Institute of Technology, KEIJI SAITO, Graduate School of Science, University of Tokyo, TOSHIMASA FUJISAWA, NTT Basic Research Laboratories, GERD SCHOEN, Karlsruhe Institute of Technology — We investigate the direction-resolved full counting statistics of single-electron tunneling through a double quantum dot system and compare with predictions of the fluctuation theorem (FT) for Markovian stochastic processes. Experimental data obtained for GaAs/GaAlAs heterostructures appear to violate the FT. After analyzing various potential sources for the discrepancy we conclude that the nonequilibrium shot noise of the measurement device influence the tunneling statistics. Taking these modifications into account we show how the FT can be violated due to measurement effects and recovered for fast detection by introducing an "effective temperature."

5:18PM D14.00015 Landauer-Buettiker approach to current-induced forces in nanoelectromechanical systems , SILVIA VIOLA KUSMINSKIY, NIELS BODE, Dahlem Center for Complex Quantum Systems & Fachbereich Physik, Freie Universitaet Berlin, REINHOLD EGGER, Heinrich-Heine Universitaet, Duesseldorf, Germany, FELIX VON OPPEN, Dahlem Center for Complex Quantum Systems & Fachbereich Physik, Freie Universitaet Berlin — We study current-induced forces in nanoelectromechanical systems with coupling between electronic and mechanical degrees of freedom. We focus on the regime where the mechanical motion is slow and Coulomb blockade effects can be neglected. We derive the current-induced forces both in and out of equilibrium and give the conditions under which these forces can be expressed solely in terms of the S-matrix. We pay particular attention to situations with more than one mechanical degree of freedom which are characterized by several qualitatively new features. We apply our general results to some simple examples.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D15 DCOMP: Electronic Structure I D171

2:30PM D15.00001 ABSTRACT WITHDRAWN –

2:42PM D15.00002 ABSTRACT WITHDRAWN –

2:54PM D15.00003 ABSTRACT WITHDRAWN –

3:06PM D15.00004 Unfolding first-principles band structures[1] , WEI KU, T. BERLIJN, Brookhaven National Laboratory; Stony Brook University, C.-C. LEE, Brookhaven National Laboratory — A general method [1] is presented to unfold band structures of first-principles supercell calculations with proper spectral weight, allowing easier visualization of the electronic structure and the degree of broken translational symmetry. The resulting unfolded band structures contain additional rich information from the Kohn-Sham orbitals, and absorb the structure factor that makes them ideal for a direct comparison with angle resolved photoemission spectroscopy experiments. With negligible computational expense via the use of Wannier functions, this simple method has great practical value in the studies of a wide range of materials containing impurities, vacancies, lattice distortions, or spontaneous long-range orders.

[1] Wei Ku, T. Berlijn, and C.-C. Lee, Phys. Rev. Lett. **104**, 216401 (2010).

[1]supported by DOE BES No.DE-AC02-98CH10886

3:18PM D15.00005 ABSTRACT WITHDRAWN –

3:30PM D15.00006 ABSTRACT WITHDRAWN –

3:42PM D15.00007 Finite-basis correction applied to the optimized effective potential within the FLAPW method , CHRISTOPH FRIEDRICH, MARKUS BETZINGER, STEFAN BLÜGEL, Institut fuer Festkoerperforschung and Institute for Advanced Simulation, Forschungszentrum Juelich and JARA, 52425 Juelich, Germany — The optimized-effective-potential (OEP) method is a special technique to construct local exchange-correlation (xc) potentials from general orbital-dependent xc energy functionals for density-functional theory. Recently, we showed that particular care must be taken to construct local potentials within the all-electron full-potential augmented-plane-wave (FLAPW) approach. In fact, we found that the LAPW basis had to be converged to an accuracy that was far beyond that in calculations using conventional functionals, leading to a very high computational cost. This could be traced back to the convergence behavior of the density response function: only a highly converged basis lends the density enough flexibility to react adequately to changes of the potential. In this work we derive a numerical correction for the response function, which vanishes in the limit of an infinite, complete basis. It is constructed in the atomic spheres from the response of the basis functions themselves to changes of the potential. We show that such a *finite-basis correction* reduces the computational demand of OEP calculations considerably. We also discuss a similar correction scheme for GW calculations.

3:54PM D15.00008 ABSTRACT WITHDRAWN –

4:06PM D15.00009 ESTEST: A Framework for the Verification and Validation of Electronic Structure Codes[1] , GARY YUAN, FRANCOIS GYGI, University of California Davis, Davis, CA95616 — ESTEST is a verification and validation (V&V) framework for electronic structure codes that supports Qbox, Quantum Espresso, ABINIT, the Exciting Code and plans support for many more. We discuss various approaches to the electronic structure V&V problem implemented in ESTEST, that are related to parsing, formats, data management, search, comparison and analyses. Additionally, an early experiment in the distribution of V&V ESTEST servers among the electronic structure community will be presented. [1] G. Yuan and F. Gygi, Computational Science and Discovery (2010) (in press).

[1]Supported by NSF-OCI 0749217 and DOE FC02-06ER25777.

4:18PM D15.00010 The random phase approximation and beyond: an assessment for molecular binding energies and reaction barrier heights , XINGUO REN, PATRICK RINKE, MATTHIAS SCHEFFLER, Fritz Haber Institute (Berlin), JOACHIM PAIER, Humboldt University (Berlin), ANDREAS GRÜENEIS, GEORG KRESSE, University of Vienna (Vienna), GUSTAVO E. SCUSERIA, Rice University (Houston) — The random phase approximation (RPA) for the correlation energy has become a promising approach for describing electronic systems in various bonding situations. Recent efforts have focused mainly on correcting the general tendency of RPA to underestimate bond strengths e.g. by adding corrections from second-order screened exchange (SOSEX) [1,2] or single excitations (SE) [3]. In this work, we systematically assess the influence of SOSEX, SE and their combinations on the atomization energies of the G2-I molecular set, as well as the chemical reaction barrier heights of the HTBH38/04 and NHTBH38/04 benchmark sets [4]. We find that RPA+SOSEX+SE based on PBE gives the most balanced description. However, for reaction barrier heights standard RPA based on PBE turns out to be better and is surprisingly accurate. The underlying mechanism governing the performance of RPA and its variants in different circumstances will be analysed. [1] A. Grüneis *et al.*, J. Chem. Phys. **131**, 154115 (2009). [2] J. Paier *et al.* J. Chem. Phys. **132**, 094103 (2010). [3] X. Ren *et al.*, arXiv:cond-mat/1011.2724. [4] Y. Zhao *et al.* J. Phys. Chem. A **109**, 2012 (2005)

4:30PM D15.00011 Approximating Densities of States with Gaps[1] , ROGER HAYDOCK, C.M.M. NEX, Department of Physics and Materials Science Institute, University of Oregon — Reconstructing a density of states or similar distribution from moments or continued fractions is an important problem in calculating the electronic and vibrational structure of defective or non-crystalline solids. For single bands a quadratic boundary condition introduced previously [Phys. Rev. B 74, 205121 (2006)] produces results which compare favorably with maximum entropy and even give analytic continuations of Green functions to the unphysical sheet. In this paper, the previous boundary condition is generalized to an energy-independent condition for densities with multiple bands separated by gaps. As an example it is applied to a chain of atoms with s, p, and d bands of different widths with different gaps between them. The results are compared with maximum entropy for different levels of approximation. Generalized hypergeometric functions associated with multiple bands satisfy the new boundary condition exactly.

[1]Supported by the Richmond F. Snyder Fund.

4:42PM D15.00012 A New Boundary Condition for Embedding Atoms in Solids , G.A. BENESH, Department of Physics, Baylor University, Waco, TX 76798-7316, ROGER HAYDOCK, Department of Physics, University of Oregon, Eugene, OR 97403-1274 — Previously, Haydock and Nex [Phys. Rev. B 82, 205114 (2010)] formulated an approximation for embedding a finite discrete system into an infinite substrate by means of a new boundary condition. This boundary condition requires a maximum breaking of time-reversal symmetry (MBTS) in the sense that probability is carried away from the embedding surface at a maximal rate. The MBTS boundary condition has been useful in discrete systems for constructing accurate densities of states and other distributions from moments or continued fractions. In this work, we generalize the approach to the problem of embedding an atom or a cluster of atoms into an infinite solid. The new, continuous MBTS boundary condition has been applied to model systems and to the embedding of a hydrogen atom. Results are presented and compared with other methods.

4:54PM D15.00013 Reference Calculation of Temperature-dependent Behavior of Confined Many-electron Systems[1] , FRANK E. HARRIS, TRAVIS SJOSTROM, University of Florida — Confined many-electron systems at finite temperatures present a major challenge to density functional theory. Very little is known about the free energy behavior over the temperature range of interest, for example, in the study of warm dense matter, and as a result, it is difficult to assess the validity of proposed free energy density functionals. We present preliminary results on a comparatively simple but computationally feasible model, namely thermally occupied Hartree-Fock states for eight one-electron atoms in a box. We discuss the main technical task, evaluation of the required matrix elements, and summarize the results thus far obtained.

[1]We acknowledge support from US DoE Grant DE-SC0002139.

5:06PM D15.00014 Finite-temperature Exchange and Correlation Functionals in Self-Consistent Calculations[1] , T. SJOSTROM, V.V. KARASIEV, S.B. TRICKEY, University of Florida — Density functional theory is being used increasingly to investigate systems at substantial electron temperatures (e.g., warm dense matter, order of 1-10 eV or more). A common approach uses a ground-state (zero-temperature) exchange-correlation (XC) functional with thermal occupancy (Fermi distribution) of the Kohn-Sham states. Various finite-temperature extensions for XC free energy (Sommerfeld expansion, RPA, STLS, classical map) have been proposed, however. All have LDA form. We have implemented several in a pseudopotential code (SIESTA), and also extended them to have the PBE-GGA as the zero-temperature limit. We report equation of state calculations for Li from ambient density and temperature through the warm dense matter regime. Nontrivial variation is found.

[1]We acknowledge support from US DoE Grant DE-SC0002139.

5:18PM D15.00015 Finite Temperature Scaling of the Non-interacting Free Energy Density Functional[1] , J.W. DUFTY, V.V. KARASIEV, S.B. TRICKEY, Physics, Univ. Florida — The non-interacting free energy density functional is central to formulation of orbital-free DFT, yet its construction remains a challenge. Here, exact scaling relations and related bounds are obtained for guidance. First, that free energy is expressed as a functional of one-body reduced density operators that deliver the same average number density. For a one-component Fermion system, this functional has a minimum at the Fermi operator whose external potential assures the chosen number density. This is the formal definition of the non-interacting free energy density functional. The associated entropy and internal energy functionals are identified directly. A unitary transformation generating spatial scaling then determines how these functionals change under density scaling. As an application, these scaling laws are used to obtain inequalities and bounds for functionals at different values of the density and temperature. Relationships to similar recent work at finite temperatures, and the extensive prior zero-temperature results are noted.

[1]Work supported under US DOE Grant DE-SC0002139.

Monday, March 21, 2011 2:30PM - 5:30PM –
Session D16 GMAG: Magnetic Imaging and Characterization D173

2:30PM D16.00001 Single Shot Nanoscale Magnetic Imaging at the Linac Coherent Light Source[1] , BENNY WU, TIANHAN WANG, Stanford University, CATHERINE GRAVES, DILING ZHU, WILLIAM SCHLOTTER, JOSHUA TURNER, JOACHIM STOHR, Linac Coherent Light Source, ANDREAS SCHERZ, Stanford Institute for Materials and Energy Science — One of the major challenges of modern magnetism research is the manipulation and control of the magnetization on ultrafast timescales. Using the unprecedented brightness of the Linac Coherent Light Source (LCLS), we have been able to image the nanoscale magnetic worm domain structures in [Co/Pd] multilayer systems with a single x-ray pulse through x-ray Fourier transform holography on the Co L3 absorption edge. We established the threshold fluences for both non-destructive imaging and sample damage. In combination with the femtosecond pulses of LCLS, single shot coherent imaging will enable the observation of nanoscale magnetization dynamics on the sub-picosecond timescale for problems such as ultrafast demagnetization and all-optical magnetization reversal.

[1]This research was funded by the U.S. Department of Energy, Office of Basic Energy Sciences.

2:42PM D16.00002 Magnetic soft X-ray microscopy at 10nm spatial resolution[1] , PETER FISCHER, WEILUN CHAO, MI-YOUNG IM, ERIK ANDERSON, CXRO LBNL Berkeley CA — Magnetic soft X-ray microscopy, which combines high spatial and temporal resolution with elemental specificity by utilizing the specific features of X-ray magnetic circular dichroism effects is a unique and powerful analytical technique to image fast spin dynamics of nanoscale magnetism [1]. The spatial resolution is determined by Fresnel zone plate lenses used as diffractive optics. FZPs are fabricated by state-of-the-art lithography techniques and the challenge is to produce a dense, circular line pattern with a high aspect ratio to achieve high efficiency. Using an overlay technique [2-3], which requires high position accuracy of the e-beam writer, FZPs with 12nm outermost zone width could be fabricated. Implementing this optic at BL 6.1.2 at the ALS in Berkeley CA, we have demonstrated that a 10nm line and space test pattern can be clearly resolved. First magnetic images of a PtCo film with a pronounced perpendicular anisotropy will be presented. Further progress to below 10nm can be anticipated in the near future.

[1] P. Fischer, IEEE Transactions on Magnetics, 44(7) 1900 (2008)
[2] W. Chao, et al. Nature 435, 1210 (2005)
[3] W. Chao, et al., Optics Express 17(20) 17669 (2009)

[1]This work was supported by the U.S. Department of Energy under Contract No. DE-AC02-05-CH11231.

2:54PM D16.00003 New Developments in Magnetic Coherent Diffractive Imaging , ASHISH TRIPATHI, University of California, San Diego, SANGSOO KIM, Argonne National Laboratory, SEBASTIAN DIETZE, ERIK SHIPTON, ERIC FULLERTON, OLEG SHPYRKO, University of California, San Diego, IAN MCNULTY, Argonne National Laboratory — Magnetism at the nanoscale is central to understanding emergent complexity in transition metal oxides and engineered rare earth-transition metal multilayers, and in designing new magnetic data storage and spintronic technology. We study magnetism at the nanoscale here using coherent x-ray diffractive imaging (CXDI), which is a technique with potentially wavelength-limited spatial resolution that can probe deeply beyond surfaces, and potentially on ultrafast timescales using new x-ray laser sources. We look at the domain evolution vs. applied magnetic field over the whole hysteresis loop of a ferrimagnetic GdFe multilayer film using x-rays resonant at the Gd M5 edge for domain contrast. We explore complimentary and return point memory by imaging the multilayer over a large field of view. We lastly explore experimental and algorithmic improvements in CXDI using dichroism as contrast mechanism, as well as new opportunities for ultra-fast, single-shot imaging using a variation on the CXDI approach.

3:06PM D16.00004 Design of a Self-Aligned, 300mK-300K Temperature range Magnetic Force Microscope(MFM) with <10nm Resolution , OZGUR KARCI, NanoMagnetics Instruments Ltd. & Hacettepe University, IVAN KNEZ, Rice University, HILAL ATALAN, NanoMagnetics Instruments Ltd., RUI-RUI DU, Rice University, AHMET ORAL, Sabanci University, NANOMAGNETICS INSTRUMENTS LTD TEAM, HACETTEPE UNIVERSITY TEAM, RICE UNIVERSITY TEAM, SABANCI UNIVERSITY TEAM — We present the design of a self-aligned MFM, operating from 300mK to 300 K. Unique 'Self-Aligned' design uses cantilever alignment chips and eliminates the alignment procedure and sustains the alignment across the full temperature range. The MFM is very compact, 23.6mm OD, and is adopted to fit into Oxford Instruments Heliox TL system. A fiber interferometer with $\sim$12fm/$\sqrt{}$Hz noise level is designed and used to detect cantilever deflection. Stick slip coarse approach mechanism is used to bring the sample in to close proximity of the sample. We can also move the sample in XY directions within 3 mm range, while we measure the position with capacitive encoder with 3μm accuracy. We can also operate the LT-MFM in high magnetic fields. The microscope has been successfully operated between 300mK-300K and we can achieve <10nm resolution. MFM images of 394 Gbpsi Harddisk at 1.5-300K and CoPt Multilayers at 350mK will be presented.

3:18PM D16.00005 Monolithic diamond probes for nanoscale magnetic imaging using single spins in diamond , PATRICK MALETINSKY, SUNGKUN HONG, MICHAEL GRINOLDS, BIRGIT HAUSMANN, RON WALSWORTH, MIKHAIL LUKIN, MARKO LONCAR, AMIR YACOBY, Harvard University — Sensitive detection of magnetic fields at the nanoscale is a challenging problem in biological and physical sciences with great relevance to technological applications. Recent experimental demonstrations have shown the outstanding performance of diamond nitrogen-vacancy (NV) centers in magnetic field sensing [1, 2]. Here, we present a robust experimental realization of a scanning NV-magnetometer that exploits the full coherence properties of the NV-center for magnetic imaging. Our apparatus consists of a combined atomic force (AFM) and optical microscope, where the AFM tip is formed by a high purity diamond nanopillar containing a single NV center at its end. This geometry ensures high spatial resolution, long NV coherence times and waveguiding of NV fluorescence through the pillar, which combine to give maximal magnetic field sensitivity. We demonstrate the performance of our nanoscale magnetometer by imaging various magnetic field sources, including few tens of nm wide domains of a magnetic memory.

[1] Nature 455, 648 (2008)
[2] Nature 455, 644 (2008)

3:30PM D16.00006 A stroboscopic approach to combining diamond magnetometry with Atomic Force Microscopy , SUNGKUN HONG, MICHAEL GRINOLDS, PATRICK MALETINSKY, MIKHAIL LUKIN, RONALD WALSWORTH, AMIR YACOBY, Harvard University — Nitrogen-Vacancy (NV) defect centers in diamond have been recently considered as a promising candidate for sensitive magnetic field detection[1, 2] with nanometric spatial resolution. Most applications requiring high spatial resolution necessitate stabilizing the NV center in close proximity to the sample of interest, which can be accomplished using standard Atomic Force Microscopy (AFM) techniques[2]. However, the fluctuations associated with AFM tip oscillation set limits to both spatial resolution and magnetic field sensitivity[2]. Here we demonstrate a stroboscopic approach that locks the magnetic signal acquisition to a particular position of the tip. Our approach allows us to reach the sensitivity and spatial resolution given by the intrinsic properties of NV centers.

3:42PM D16.00007 High sensitivity SQUID susceptibility measurements , B. KALISKY, J.R. KIRTLEY, L.C. QIAN, B.L. DWYER, K.A. MOLER, Stanford, J. NGAI, Y. SEGAL, J. REINER, F. WALKER, C. AHN, Yale, A.M. HAMILTON, B. RUTT, A.C. MATIN, Stanford, O.M. AUSLAENDER, Technion, D.A. BONN, R. LIANG, W.N. HARDY, UBC, J.G. ANALYTIS, J.-H. CHU, I.R. FISHER, Stanford — Scanning superconducting quantum interference device (SQUID) sensors have high sensitivity to magnetic flux ($10^{-6}\Phi_0/\sqrt{Hz}$) and magnetic moment ($\sim$ 100 electron spins) under reasonable scanning conditions. In addition, a single turn field coil co-centered with the SQUID sensing loop provides excitation for simultaneous measurement of low field susceptibility, with sensitivity of $\chi \sim 10^{-6}$ at a spatial resolution of a few microns. I will present our recent measurements on several systems which exhibit weak susceptometry signals: thin film paramagnetic LaNiO3 that are (hopefully) the precursors to engineered superconducting films; individual magnetotactic bacteria, which are used as MRI contrast agents; and twinned high critical temperature cuprate and pnictide superconducting samples that may experience variations in the superfluid density at the twin boundary.

3:54PM D16.00008 Magnetic Characterization of Individual Magnetotactic Bacteria , LISA QIAN, Stanford University, BEENA KALISKY, Stanford Unversity, AMANDA HAMILTON, BO DWYER, A.C. MATIN, KATHRYN MOLER, Stanford University — Magnetic nanoparticles 5-50nm in size are of wide interest in the biological and medical fields. In particular, magnetotatic bacteria containing chains of nanoscale magnetite particles show potential for MRI contrast agents and targeting tumors. Magnetic characterization is typically done in large ensembles, where variations in shape and structure cannot be determined and interparticle coupling may cause bulk properties from those of isolated particles. We report the detection and magnetic characterization of individual magnetotatic bacteria using a variable temperature scanning SQUID microscope (SSM). SSM is ideal for this challenge due to its high spin sensitivity, ∼100 mu_B/sqrt(Hz). AC and DC modes of operation allow for direct probing of susceptibility and magnetic moment. We will also discuss calculation techniques used to obtain values for the magnetic moment, anisotropy energy and magnetosome chain length of individual bacteria.

4:06PM D16.00009 Magneto-resistance based First Order Reversal Curve (MR-FORC) analysis of MgO based MTJs , JOSHUA POMEROY, JOHN READ[1], National Institute of Standards and Technology (NIST) — MR-FORC utilizes partial magneto-resistance hysteresis loops to reveal the coercive and interaction field distributions in the free layer of MgO based magnetic tunnel junctions. The interpretation of the FORC diagrams will be discussed with emphasis on the identification of coercive values, the interlayer exchange properties, the magnetic after-effect and a reversible magnetic instability under study.

[1]Now at Hitachi Global Storage

4:18PM D16.00010 Stress and Depth Dependence of Stochastic Processes in the Barkhausen Effect , DAVID JILES, Iowa State University, Ames, Iowa 50011, LUKASZ MIERCZAK, EUGENE MELIKHOV, Wolfson Centre for Magnetics, Cardiff University, United Kingdom, IOWA STATE UNIVERSITY TEAM, WOLFSON CENTRE FOR MAGNETICS TEAM — Magnetic Barkhausen Noise (MBN) consists of discontinuous stochastic changes in flux density caused by sudden irreversible changes in magnetization as the magnetic field H changes continuously. These changes can be detected at the surface by a magnetometer, which in its simplest form can be in the form of voltage pulses caused in a pickup coil. The amplitude of such pulses has been shown to depend on the microstructure and stress in the material. Propagation of Magnetic Barkhausen emissions in magnetic materials is frequency dependent and therefore information from different depths inside the material is contained in the frequency spectrum of the detected Barkhausen signal at the surface. However the depth dependent information, although present, is difficult to extract from the measurements. Despite this extracting the depth dependent information about material conditions, such as variations in microstructure and/or the presence of residual stress is of a great interest. This work presents a new method for extracting this information from measured MBN signals.

4:30PM D16.00011 Cluster-deposited high-anisotropy magnetic nanoparticles[1] , BALAMURUGAN BALASUBRAMANIAN, RALPH SKOMSKI, XINGZHONG LI, DAVID SELLMYER, Nebraska Center for Materials and Nanoscience and Department of Physics and Astronomy, University of Nebraska, Lincoln, NE-68588 — Magnetic nanoparticles of size less than 10 nm with high magnetocrystalline anisotropy are highly desirable to understand the nanoscale effects on their magnetic properties and create building blocks for modern applications such as ultra-high-density recording media and high-performance permanent magnets. In the present study, monodisperse Co-based nanoparticles with an average particle size of 3 -10 nm, such as YCo_5 and $Co_{1-x}Pt_x$ ($x < 0.2$), were produced using an inert-gas-condensation cluster-deposition system and characterized using XRD, TEM, EDX and SQUID magnetometer. These nanoparticles were directly ordered into high-anisotropy crystal structures during the cluster-aggregation process and exhibit high anisotropic constant of order 10^7 ergs/cm^3. Size-effects on the structural and magnetic properties of YCo_5 and Co_xPt_{1-x} nanoparticles will be discussed.

[1]This work is supported by DOE, ARPA-E, BREM, NSF-MRSEC, and NCMN.

4:42PM D16.00012 Improved evaluation of magnetic nanoparticle susceptibility in hyperthermia, spectroscopy, and imaging[1] , YONG WU, ZHEN YAO, TIMOTHY ATHERTON, LISA BAUER, MARK GRISWOLD, ROBERT BROWN, Case Western Reserve University — Magnetic nanoparticles are becoming increasingly important for both diagnosis (through applications such as MRI and magnetic particle imaging (MPI), which comes from the nonlinear magnetization of nanoparticles and provides images with both high spatial and temporal resolutions) as well as for therapy (through focal heating). Thus understanding and modeling of the magnetic susceptibility of the nanoparticles is critical. In hyperthermia calculations, a constant chord susceptibility approximation is used to get a lower bound estimate of the power dissipated. In later work, this approximation has been adapted to examine the decay effects due to nanoparticle relaxation under oscillating magnetic fields in the MPI modality. We provide in the present paper both analytical and numerical work to understand where it is, or is not, appropriate to make this approximation. In addition, we provide a more general approach that does not rely on the above approximations, and may provide new insight to manufacture optimal nanoparticles for applications.

[1]Supported by the Ohio Third Frontier Funding

4:54PM D16.00013 The Spin-Lattice Relaxation of Hyperpolarized ^{89}Y Complexes , ASHISH JINDAL, LLOYD LUMATA, UT Southwestern Med. Cntr., YIXUN XING, UT Dallas, MATTHEW MERRITT, UT Southwestern Med. Cntr., PIYU ZHAO, UT Dallas, CRAIG MALLOY, DEAN SHERRY, ZOLTAN KOVACS, UT Southwestern Med. Cntr. — The low sensitivity of NMR can be overcome by dynamic nuclear polarization (DNP). However, a limitation to the use of hyperpolarized materials is the signal decay due to T_1 relaxation. Among NMR-active nuclei, ^{89}Y is potentially valuable in medical imaging because in chelated form, pH-sensitive agents can be developed. ^{89}Y also offers many attractive features – 100 % abundance, a 1/2 spin, and a long T_1, up to 10 min. Yet, developing new ^{89}Y complexes with even longer T_1 values is desirable. Designing such complexes relies upon understanding the mechanism(s) responsible for T_1 relaxation. We report an approach to hyperpolarized T_1 measurements that enabled an analysis of relaxation mechanisms by selective deuteration of the ligand backbone, the solvent or both. Hyperpolarized ^{89}Y – DTPA, DOTA, EDTA, and deuterated EDTA complexes were studied. Results suggest that substitution of low-gamma nuclei on the ligand backbone as opposed to that of the solvent most effectively increase the ^{89}Y T_1. These results are encouraging for in vivo applications as the presence of bound water may not dramatically affect the T_1.

5:06PM D16.00014 Magnetic Thermal Hysteresis in Dy nanolayers , AJANI ROSS, ALI KOYMEN, University of Texas Arlington — Magnetic thermal hysteresis is observed when the temperature dependent magnetic properties of a material are reliant on the starting point of the measurement. Trilayer samples of pure Dysprosium (Dy) and Gadolinium (Gd) were grown on substrates of glass ($Gd_n/Dy_m/Gd_n$), n and m constitutes the number of layers. We observed magnetic thermal hysteresis in these thin films at low values of constant external magnetic field strengths. The temperature is swept from 20K to 300K at constant field, then back (300K to 20K) under the same field. In these temperature sweeps differences in magnetic moment were observed near the low end of the temperature range. Experiments are being done, currently, to confirm the existence of alternate helicity (AH-state) and helical (H-state) states in these trilayer films, which are believed to be the cause of the observed thermal hysteresis according to theoretical calculations. In addition, the temperature dependence of entropy change for these samples is calculated.

5:18PM D16.00015 Chain formation in a magnetic fluid under the influence magnetic fields. , MATT BARRETT, ANDREAS DESCHNER, McMaster University, JAN EMBS, ETH Zurich & Paul Scherrer Institut, AN-CHANG SHI, MAIKEL RHEINSTADTER, McMaster University — We studied the aggregation of magnetic particles into simple chainlike structures in a Cobalt-based magnetic fluid, exposed to external magnetic fields [1]. The length of chain segments in very strong magnetic fields of up to 2 T was measured using small angle neutron scattering in-situ. Although it was predicted that the chain length can be described by a Langevin function, leading to chains several hundred particles in length, we observe a maximum correlation length of $\sim$ 650 Å, or 4-5 particles. To gain insight into the molecular mechanisms involved, our experiments were complemented by Monte Carlo simulations. We observed that the chains which formed increased in length as the magnetic field increased until reaching equilibrium at 4 particles, in excellent agreement with our experimental findings. We speculate that the interplay between the entropy and energy of the system combined with the particular properties of the magnetic dipole-dipole interaction ultimately decide the length of the particle chains. We observed attractive or repulsive interaction between chain segments depending on their relative position. [1] *"Chain formation in a magnetic fluid under the influence of magnetic fields"*, M. Barrett, A. Deschner, J.P. Embs, A.-C. Shi, M.C. Rheinstädter, submitted to Physical Review Letters.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D17 DMP GMAG: Focus Session: Bulk Properties of Complex Oxides - Cobaltites D174

2:30PM D17.00001 Possible link of a structurally driven spin flip transition and the insulator-metal transition in the perovskite $La_{1-x}Ba_xCoO_3$, DESPINA LOUCA, University of Virginia — The intricate nature of the magnetic ground state near the insulator-metal transition (IMT) in $La_{1-x}Ba_xCoO3$ was investigated via neutron scattering. For x less than the critical concentration, x_c $\sim$0.22, a commensurate antiferromagnetic (AFM) phase initially appears. As x approaches x_c, the AFM component continuously weakens while ferromagnetic (FM) order sets in the rhombohedral lattice. The two magnetic phases appear to be growing in different domains and have different ordering temperatures, with the FM order parameter setting in first at higher temperatures while the AFM order parameter occurs at lower temperatures. At x_c, a spin flip to a new FM state occurs while the crystal transforms to an orthorhombic (Pnma) symmetry. The magnetic Pnma phase coincides with the minimum saturation reached in the resistivity. It is proposed that the orbital overlap in the Pnma phase is the most conducive to charge hopping.

3:06PM D17.00002 Phase Control of Magnetic Order in (Y,Lu)$BaCo_4O_7$, JOHN MITCHELL, HONG ZHENG, SEVDA AVCI, Argonne National Laboratory, LAURENT CHAPON, DMITRY KHALYAVIN, ISIS Facility, OMAR CHMAISSEM, Northern Illinois University, ASHFIA HUQ, Oak Ridge National Laboratory — The $RBaCo_4O_7$ (R=Ca, Y, Tb-Lu) provides a novel topology for studying geometric frustration, in which face-sharing tetrahedra of magnetic ions link to form trigonal bipyramids on a Kagomé lattice. Here we describe the structural and magnetic behavior of the Lu member and the solid solution joining Lu to Y as a chemical means to tune between magnetically ordered and disordered ground states. Mean-field models of the generic magnetic phase diagram of $RBaCo_4O_7$ determined recently by our group (D. D. Khalyavin et al. Physical Review B 82, 094401 (2010)) show a variety of magnetic states as a function of two exchange parameters: J_{ab} and J_c, where J_{ab} links Co ions in the Kagomé planes and J_c links Co ions from the Kagome plane to the interleaving triangular layer. Experimentally, we find that $YBaCo_4O_7$ has a long-range ordered antiferromagnetic ground state, while $LuBaCo_4O_7$ appears to be disordered above 2 K. We use the solid solution to interpolate between these endpoints and discuss these results with respect to the mean-field phase diagram.

3:18PM D17.00003 Determination of magnetic moments and orbital occupancy in the spin chain compound $Ca_3Co_2O_6$[1] , JONATHAN DUFFY, MATTHEW BUTCHERS, University of Warwick, JONATHAN TAYLOR, ISIS, STEPHEN DUGDALE, TOM HAYNES, University of Bristol, STEFANO AGRESTINI, MARTIN LEES, University of Warwick — The one-dimensional cobaltate $Ca_3Co_2O_6$ exhibits a number of intriguing phenomena, including several metamagnetic steps as a function of applied magnetic field. Although it has attracted a considerable amount of research, the origin of the magnetism has not yet been fully determined. We report a measurement of the spin density in $Ca_3Co_2O_6$ using magnetic Compton scattering. The bulk spin moment was determined to be 3.78 $\pm$ 0.05μ_B at 7 T, confirming the existence of a large unquenched Co orbital moment of 1.4 $\pm$ 0.1 μ_B. In combination with molecular orbital calculations, the results reveal that double occupation of the $d_{x^2-y^2,xy}$ orbital is responsible for the observed large unquenched orbital moment. Fitting the model to the experimental data shows that there is an induced oxygen moment of 0.8 $\pm$ 0.1 μ_B. Unexpectedly, further comparison with KKR-SPA electronic structure calculations strongly indicates the existence of a Fermi surface.

[1]We acknowledge the support of the UK EPSRC via grant EP/F021518.

3:30PM D17.00004 Theory of the carrier concentration-dependent behavior in layered cobaltates , HONGTAO LI, University of Arizona, R. TORSTEN CLAY, Mississippi State University, SUMIT MAZUMDAR, University of Arizona — Layered cobaltates – anhydrous Na_xCoO_2, Li_xCoO_2 and the "misfit" cobaltates $[Bi_2A_2O_4] \cdot [CoO_2]_m$, where A = Ba, Sr or Ca – have attracted wide attention for their 2D layered structure and metallicity (both reminescent of 2D cuprates), and the tunability of the carrier concentration over a wide range. The Co ions form a 2D triangular lattice, and their formal charge in Na_xCoO_2 and Li_xCoO_2 can be tuned from Co^{3+} at $x = 1$ to Co^{4+} at $x = 0$. Charge carriers in all cases are holes, with the carrier concentration given by the fraction of Co-ions that are in the S = 1/2 Co^{4+} state. Experiments have indicated remarkable carrier concentration dependent magnetic susceptibility and thermoelectric power that remains unexplained to date. Specifically, all three systems show weakly correlated behavior at small nonzero x (large carrier concentration), and strongly correlated behavior at large x (small carrier concentration). In this talk we give clear theoretical explanation of the observed carrier concentration dependence within an a_{1g}-only one-band extended Hubbard Hamiltonian. The key to understanding the x-dependence is to have realistic finite on-site correlation U and significant intersite Coulomb interaction V. We present exact numerical results for triangular lattices upto 20 sites, and make detailed comparisons to experiments.

3:42PM D17.00005 Probing the Na atomic order in Na_xCoO_2, x=0.67 and 0.71 by NMR spectroscopy[1] , BEN-LI YOUNG, P.-Y. CHU, J.Y. JUANG, Department of Electrophysics, National Chiao Tung University, Taiwan, G.J. SHU, F.-T. HUANG, M.W. CHU, F.C. CHOU, Center for Condensed Matter Sciences, National Taiwan University, Taiwan — The sodium cobaltate Na_xCoO_2 has a layered structure, consisting of alternating triangular CoO_2 and Na planes. Evidences of Na atomic ordering have been reported at certain Na contents by different diffraction experiments. The Co magnetism, strongly influenced by the Na ordering, gives a unique phase diagram in Na_xCoO_2. In order to investigate the Na ordering and the Co magnetism, we conducted ^{23}Na and ^{59}Co NMR experiments in single crystals Na_xCoO_2 for x=0.67 and 0.71. We found that $Na_{0.67}CoO_2$ does not have well-defined Na structural order. However, the oxygen slightly-deficient sample $Na_{0.67}CoO_{1.98}$ shows a superstructure, as evidenced by the narrow and well-resolved NMR spectrum. As for $Na_{0.71}CoO_2$, Na ordering is also observed. We have tried to solve the Na ordering pattern from our NMR spectra. The results will be discussed and be compared with the existing structural models.

[1]This work was supported by NSC 98-2112-M-009-016-MY3 and the MOE ATU Program.

3:54PM D17.00006 Synthesis and anisotropic magnetic and transport properties of cubic $SrCoO_3$ single crystal , YOUWEN LONG, YOSHIO KANEKO, ERATO-MF, JST, Wako 351-0198, Japan, SHINTARO ISHIWATA, Dep. Appl. Phys., Univ. Tokyo, Tokyo 113-8656, Japan, YASUJIRO TAGUCHI, CMRG and CERG, RIKEN-ASI, Wako 351-0198, Japan, YOSHINORI TOKURA, ERATO-MF, JST, CMRG and CERG, RIKEN-ASI, Wako 351-0198, Japan; Dep. Appl. Phys., Univ. Tokyo, Tokyo 113-8656, Japan — Solid state oxides containing transition metals with unusually high valence states exhibit interesting physical properties. However, due to the unstableness of these high valence states, high pressure is often needed to stabilize such high valence states. We were successful in growing a large-size $SrCoO_3$ single crystal by using high-pressure technique. This material shows good metallic behavior with high ferromagnetic Curie temperature about 305 K, and the easy magnetization axis is <111> direction. The spin moment of Co^{4+} ion measured at 2 K and 7 T is about 2.50 μ_B, suggesting an intermediate spin configuration as predicted by theoretical calculations. Although $SrCoO_3$ has a highly symmetric cubic crystal structure (Pm-3m), it exhibits significant anisotropic magnetoresistance at low temperatures.

4:06PM D17.00007 The origin of the temperature dependence of the magnetic susceptibility and the large thermoelectric power in metallic layered cobaltites , IVÁN GONZÁLEZ, Centro de Supercomputación de Galicia, Avda. de Vigo s/n, E-15705 Santiago de Compostela, CAMILO X. QUINTELA, Applied Physics Department, University of Santiago de Compostela, 15782 Santiago de Compostela, Spain, MANUEL BAÑOBRE-LÓPEZ, FRANCISCO RIVADULLA, Physical-Chemistry Department, University of Santiago de Compostela, 15782 Santiago de Compostela, Spain — We perform detailed measurements of the thermoelectric power and the static magnetic susceptibility on metallic Na_xCoO_2 and $Ca_3Co_4O_9$, as representatives of layered Co oxides with a triangular Co-lattice. We propose that the observed large thermoelectric power and the Curie-Weiss temperature dependence of the susceptibility have a common origin related to metallic character of these compounds. Thermoelectric power measurements are compared to Boltzmann transport theory calculations. The Curie-Weiss behaviour of the susceptibility is explained within the framework of the self-consistent renormalization theory for spin fluctuations proposed by Moriya for itinerant magnets. Our results clarify the apparent duality in the localised/itinerant behaviour of the electron spin in these systems and provide a unifying view on the physics of metallic layered cobaltites.

4:18PM D17.00008 TEM imaging and in-situ EELS study of multiple ferroic transitions in LaCoO3[1] , TIANTIAN YUAN, ROBERT KLIE, University of Illinois at Chicago, Department of Physics, NINA ORLOVSKAYA, University of Central Florida — The perovskite oxide LaCoO3 has attracted increasing attention due to its reported room-temperature ferroelastic behavior, and a ferromagnetic transition observed at around 90K in epitaxially strained thin films. To advance our understanding of these nanoscale properties of LaCoO3, a combination of analytical TEM techniques, including the atomic-resolution Z-contrast imaging and electron energy-loss spectroscopy in combination with in-situ cooling experiments have been used to study the relationship of the multiple ferroic transitions in bulk LaCoO3. In particular, we find that the bulk LaCoO3 samples compressed above the coercive stress exhibit ferromagnetic transitions, similar to the ferromagnetic behavior of the epitaxially strained LaCoO3 thin film. While the bulk LaCoO3 samples compressed below the coercive stress do not exhibit any ferromagnetic transitions down to 5K. We will further correlate this ferromagnetic property to the ferroelastic property of LaCoO3, and show how the strain of the LaCoO3 affects the ferromagnetic property of the sample.

[1]Funded by: NSF CAREER Award DMR-0846748

4:30PM D17.00009 Magnetocaloric effect across the coupled structural/magnetocrystalline anisotropy transition in $Pr_{1-x}Sr_xCoO_3$ (x=0.3-0.5) , N.S. BINGHAM, M.H. PHAN, H. SRIKANTH, University of South Florida, M.A. TORIJA, C. LEIGHTON, University of Minnesota — Large magnetocaloric effects (MCE) are often observed in materials exhibiting a first order magnetic transition coupled with a crystal structure change. Since the magnetic and structural changes are coupled, it is difficult to decouple the structural entropy contribution from the magnetic entropy contribution to the total MCE. Therefore a clear understanding of the structural entropy change and its field dependence in such materials is lacking. A recent study revealed that $Pr_{1-x}Sr_xCoO_3$ (x>0.35) undergo a coupled structural/magnetocrystalline anisotropy transition at T_A, in addition to the paramagnetic-ferromagnetic transition at T_C. Since the structural change at T_A in PSCO is not associated with any magnetic transition, it is an excellent system for studying the structural entropy change and its contribution to the MCE. We report systematic studies of the MCE in $Pr_{1-x}Sr_xCoO_3$ (x=0.3, 0.35, 0.4, 0.5) compounds. The results show significant entropy change at T_A, whose magnitude can be tuned by controlling the magnetocrystalline anisotropy.

4:42PM D17.00010 Magneto-electronic Phase Separation in $Pr_{1-x}Ca_xCoO_{3-\delta}$: Intrinsic Exchange Spring Magnetism[1] , S. EL-KHATIB, American University of Sharjah, S. BOSE, C. HE, J. KUPLIC, University of Minnesota, M. LAVER, J.A. BORCHERS , Q. HUANG, J.W. LYNN, NIST Center for Neutron Research, J.F. MITCHELL, Argonne National Laboratory, C. LEIGHTON, University of Minnesota — We present a neutron diffraction, small-angle scattering, and magnetometry study of the narrow bandwidth perovskite cobaltite $Pr_{1-x}Ca_xCoO_3$, demonstrating an unusual form of magneto-electronic phase separation where long-range ordered ferromagnetism coexists spatially with short-range ferromagnetism. The two phases have very different coercivities and, remarkably, are strongly exchange coupled. The electronic phase separation thus leads to spontaneous formation of a hard-soft nanocomposite, exhibiting prototypical exchange-spring behavior in the absence of chemical interfaces.

[1]Work at UMN supported by DoE (neutron scattering) and NSF.

4:54PM D17.00011 The nature of magneto-elastic coupling with the isovalent substitution at the B-site in $LaCo_{1-y}B_yO_3$, JUAN YU, DESPINA LOUCA, Physics Department, University of Virginia — The influence of magnetic ion doping on the interplay of the lattice with magnetism in $LaCo_{1-y}B_yO_3$ (B = Ni or Fe, y= 0.1, 0.4) has been investigated via neutron scattering techniques. The substitution of either Ni^{3+} ($3d^7$) or Fe^{3+} ($3d^5$) does not alter the crystal symmetry which remains rhombohedral (R-3c) at all temperatures. With doping, the degree of cooperative octahedral rotations about the (111) axis increases, but it is only with Ni that such a rotation is accompanied by a compression along the trigonal axis. The observed crystal distortion is invoked to break the degeneracy of the magnetic Co^{3+} ions, while maintaining the Co-O bonds at a constant length. The absence of two distinct types of Co-O bond lengths in the local structure with the substitution of Fe^{3+} or Ni^{3+} for Co^{3+} ($3d^6$) is indicative that, unlike in the hole doped cobaltites with Ba^{2+} or Sr^{2+} previously studied, the intermediate spin state of Co is either absent or suppressed. This leaves us to question the origin of the magnetic interactions, which most likely arises from a high-spin state of the Co ion.

5:06PM D17.00012 First Principles Study of Misfit-Layered Calcium Cobaltite Using Fibonacci Approximants[1] , ALEJANDRO REBOLA, ROBERT KLIE, SERDAR OGUT, University of Illinois at Chicago — Cobalt oxides have been the focus of many recent studies due to the wide variety of electrical, magnetic, structural and thermoelectrical properties they exhibit. In this talk we present a first-principles study on the misfit-layered $Ca_3Co_4O_9$. This material can be more accurately described as $[Ca_2CoO_3][CoO_2]_{1.61}$ and consists of two substructures that are incommensurate to each other. Taking into account that the composition ratio is very close to the golden mean (1.6180...), and that this number can be obtained as the limit of the sequence of the ratios of consecutive Fibonacci numbers: 3/2, 5/3, 13/8, . . . , F(n+1)/F(n)..., we model the structure by using supercells of composition $[Ca_2CoO_3]_{F(n)}[CoO_2]_{F(n+1)}$. In this way, structural, electronic, transport and lattice properties can be calculated as a function of cell size. We compute the atomic and electronic structures, defect energetics of a series of rational approximants to $Ca_3Co_4O_9$within the framework of DFT+U, and examine the convergence of such properties with respect to size, thus allowing us to identify the most realistic and smallest structural model for this misfit-layered compound.

[1]This work is in part supported by the US Army Research Office (W911NF-10-1-0147).

5:18PM D17.00013 Complex ferrimagnetic state induced by zigzag oxygen-vacancy stripes in $Sr_3YCo_4O_{10.72}$, D.D. KHALYAVIN, L.C. CHAPON, ISIS facility, Rutherford Appleton Laboratory, E. SUARD, Institut Laue-Langevin, J.E. PARKER, S.P. THOMPSON, Diamond Light Source, A.A. YAREMCHENKO, V.V. KHARTON, University of Aveiro — The nature of high temperature ferromagnetic behaviour in $Sr_3YCo_4O_{10+\delta}$ perovskite has been studied by neutron powder diffraction supplemented with synchrotron X-ray diffraction measurements. The present analysis of the magnetic structure takes into account the complex superstructure formed by oxygen vacancy ordering. These vacancies create zigzag strips in the oxygen-deficient $CoO_{4+\delta}$ layers providing three distinct coordinations for Co ions. The values of the ordered moments were found to be essentially different for the distinct coordinated units and clearly correlate with the coordination number. The symmetry of the superstructure in conjunction with strong antiferromagnetic interactions between neighbour spins results in a net moment whose origin has been the subject of considerable debates.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D18 GMAG DMP: Focus Session: Low D/Frustrated Magnetism - Kagome Lattices

D172

2:30PM D18.00001 Highly frustrated magnets: a class of emergent gauge systems , MICHAEL LAWLER, Binghamton University — Condensed matter exhibit a wide variety of exotic emergent phenomena, such as the topological order in the fractional quantum Hall effect, and the "cooperative paramagnetic" response of geometrically frustrated magnets. The classical and quantum dynamics of spins exploring the large configuration space associated with the latter are not well understood analytically. I consider the constrained classical Hamiltonian dynamics of spins exploring such a configuration space as a starting point from which a complete classical and semi-classical description may be reached. The method I employ, introduced by Dirac [1] and now forms the basis of gauge theory, applies to any frustrated system constrained to a continuous set of configurations. Remarkably, in the kagome lattice model I consider as an example, these dynamics are similar to the "topological" (Chern-Simons) dynamics of electrons in the fractional quantum Hall effect and have non-locally entangled edge modes as the only degrees of freedom. In principle, these edge states may be found in any kagome-like Heisenberg antiferromagnets such as Herbertsmithite, the Jarosites, $SrCr_{8-x}G_{4+x}O_{19}$ and $Na_4Ir_3O_8$.

[1] Dirac, P. A. M. *Generalized hamiltonian dynamics.* Can. J. of Math. **2**, 129-148 (1950)

2:42PM D18.00002 Predictions for the ARPES spectral function of kagome antiferromagnetic insulators[1] , SUMIRAN PUJARI, Cornell University, MICHAEL J. LAWLER, Binghamton University, Cornell University — There are now a number of spin liquid candidate materials possibly with exotic spin-1/2 "spinon" excitations. Motivation by these discoveries, we consider the scaling properties of the hole spectral function for the frustrated Kagome Heisenberg antiferromagnet assuming Dirac Spin Liquid(DSL) ground state proposed for Herbertsmithite [2]. We predict a sublinear in energy power law dependence of the ARPES spectral function at certain wave vectors. Using Renormalization group techniques, we show how (gauge) fluctuations of the DSL mean field give an anomalous exponent to spinons[2] and no anomalous exponent to holons thereby leading to the sublinear power law. If this behavior is observed in experiments, they would provide strong evidence for the existence of spinons in highly frustrated magnets.[2]

[1]S.P. gratefully acknowledges support from NSF grant DMR-1005466

[2]Y. Ran et al, Phys. Rev. Lett. 98, 117205 (2007)

2:54PM D18.00003 Exact Chiral Spin Liquid with Stable Spin Fermi Surface on the Kagome Lattice[1] , VICTOR CHUA, Department of Physics, University of Texas at Austin, HONG YAO, Department of Physics, University of California, Berkeley, California, GREGORY FIETE, Department of Physics, University of Texas at Austin — We study an exactly solvable quantum spin model of Kitaev type on the kagome lattice. We find a rich phase diagram which includes a topological (gapped) chiral spin liquid with gapless chiral edge states, and a gapless chiral spin liquid phase with a spin Fermi surface. The ground state of the current model contains an odd number of electrons per unit cell which qualitatively distinguishes it from previously studied exactly solvable models with a spin Fermi surface. Moreover, we show that the spin Fermi surface is stable against weak perturbations.

[1]This work is supported in part by NSF grant DMR-0955778 (VC and GAF) at Austin and DOE grant DE-AC02- 05CH11231 (HY) at Berkeley.

3:06PM D18.00004 Quantum criticality in the kagome staircase system $Co_3V_2O_8$ in transverse magnetic field , K. FRITSCH, McMaster Univ., K.C. RULE, Helmholtz-Zentrum Berlin, K.A. ROSS, McMaster Univ., Y. QIU, J.R.D. COPLEY, NCNR NIST, K. KIEFER, K. HABICHT, Helmholtz-Zentrum Berlin, H.A. DABKOWSKA, B.D. GAULIN, BIMR and McMaster Univ. — $Co_3V_2O_8$ (CVO) belongs to the kagome staircase family of orthorhombic materials in which Ising-like Co^{2+}, S=3/2 magnetic moments decorate a stacked and buckled version of the two-dimensional kagome lattice. In zero applied magnetic field, this material displays a complex series of five different magnetically ordered phases below ∼11 K which culminate in a simple ferromagnetic state below Tc∼6 K. Previous inelastic neutron scattering work[1] on this quasi-two-dimensional system showed that the exchange interactions within the kagome planes are rather weak (J∼1.25 meV), making this system an ideal candidate for the study of transverse field-induced quantum critical phenomena as have been observed in $LiHoF_4$ or recently in $CoNb_2O_6$. We have investigated the phase diagram of CVO with the transverse field applied along the stacking direction using magnetization as well as single crystal neutron scattering techniques. We will discuss how the ground state magnetic structure and spin dynamics of CVO evolve upon tuning the transverse magnetic field through the quantum critical point near Hc∼6 T. [1] M. Ramazanoglu et al., PRB 79, 024417 (2009).

3:18PM D18.00005 Herbertsmithite: a slightly less than ideal kagomé antiferromagnet[1] , YUAN WAN, ZHIHAO HAO, OLEG TCHERNYSHYOV, Johns Hopkins University — Herbertsmithite, one of the best realizations of the Heisenberg antiferromagnet on kagomé, shows no signs of magnetic order down to the lowest accessible temperatures and likely possesses a quantum-disordered ground state. A recent site-specific X-ray diffraction experiment [1] shows deviations from the ideal model, most notably in the form of excess copper spins residing outside of kagomé planes. We study the influence of these impurities on the magnetic properties of herbertsmithite, focusing on locally induced Jahn-Teller distortions in kagomé planes and on exchange interactions between the excess spins.

[1] Danna E. Freedman *et al*, J. Am. Chem. Soc. **132**, 16185 (2010).

[1]The work is supported by DOE grant No. DEFG02-08ER46544.

3:30PM D18.00006 Magnetic studies of S=1/2 kagomé lattice single crystals , TIANHENG HAN, MIT, JOEL HELTON, ANDREA PRODI, CLAUDIO MAZZOLI, PETER MULLER, DEEPAK SINGH, JOSE RODRIGUEZ, COLLIN BROHOLM, DANIEL NOCERA, SHAOYAN CHU, YOUNG LEE — The Zn-paratacamite mineral family, $Zn_xCu_{4-x}(OH)_6Cl_2$, presents a promising system for studies of frustrated magnetism on a S=1/2 kagomé lattice. Here we report a new synthesis method, by which high quality single crystals of Zn-paratacamite can be produced. The x = 1 mineral herbertsmithite is a spin-liquid candidate. This compound displays a magnetic susceptibility that is anisotropic at high temperatures. A small anisotropy is observed in specific heat measurements with magnetic field applied in-plane and normal-to-plane. Inelastic neutron scattering has been performed and we will discuss the observed structure factor in the context of various theoretical expectations.

3:42PM D18.00007 Terahertz conductivity of a metal-organic hybrid Kagomé lattice: A candidate spin liquid , DANIEL PILON, ALEX FRENZEL, DANNA FREEDMAN, DANIEL NOCERA, NUH GEDIK, MIT — Recent theoretical studies predict that the optical conductivity of a spin liquid should exhibit power law behavior in frequency at low temperatures. Materials with the Kagomé structure are the most promising candidates for observing spin liquid behavior due to their high degree of magnetic frustration. We have measured the optical conductivity of Cu(1, 3-bdc), a spin-1/2 Kagomé lattice material, in the range 0.5 - 2 THz. We compare these results to the theoretical predictions and comment on the implications for the existence of a spin liquid state in this material.

3:54PM D18.00008 Valence-bond crystal in the extended Kagomé spin-$1/2$ quantum Heisenberg antiferromagnet: A variational Monte Carlo approach , FEDERICO BECCA, CNR, Istituto Officina dei Materiali and SISSA, Trieste, YASIR IQBAL, DIDIER POILBLANC, Laboratoire de Physique Theorique, Universite' de Toulouse — The highly-frustrated spin-$1/2$ quantum Heisenberg model with both nearest (J_1) and next-nearest (J_2) neighbor exchange interactions is revisited by using an extended variational space of projected wave functions that are optimized with state-of-the-art methods. Competition between modulated valence-bond crystals (VBC) proposed in the literature and the Dirac spin liquid (DSL) is investigated. We find that the addition of a $small$ ferromagnetic next-nearest-neighbor exchange coupling $|J_2| > 0.09J_1$ leads to stabilization of a 36-site unit cell VBC, although the DSL remains a local minimum of the variational parameter landscape. This implies that the VBC is not trivially connected to the DSL: instead it possesses a non-trivial flux pattern and large dimerization.

4:06PM D18.00009 Magnetization ramp of the Kagome lattice antiferromagnet , TORU SAKAI, JAEA, SPring-8, HIROKI NAKANO, Graduate School of Material Science, University of Hyogo — Magnetization process of the S=1/2 isotropic Heisenberg antiferromagnet on the Kagome lattice is studied. Data from numerical-diagonalization method up to 39-spin systems, are reexamined from the viewpoint of the derivative of the magnetization with respect to the magnetic field. We find that the behavior of the derivative around the 1/3 height of the magnetization saturation is quite different from the cases of typical magnetization plateaux. The magnetization process of the Kagome-lattice antiferromagnet reveals a new phenomena, which we call the "magnetization ramp." We also compare it with the 1/3 magnetization plateau of the triangular antiferromagnet.

[1] H. Nakano and T. Sakai: J. Phys. Soc. Jpn. 79 (2010) 053707, arXiv:1004.2528.

4:18PM D18.00010 Spin dynamics in the hyperkagome compound $Gd_3Ga_5O_{12}$, OLEG PETRENKO, University of Warwick, UK — We present the first neutron inelastic scattering results on the magnetic state of the frustrated hyperkagome compound $Gd_3Ga_5O_{12}$ (GGG) at low temperatures and in applied magnetic field. Our neutron scattering studies reveal a remarkable range of timescales. Short-range spatial correlations appear static within the instrumental resolution (50 μeV). Three distinct inelastic modes are found at 0.04(1), 0.12(2) an 0.58(3) meV at 0.06 K. The application of a magnetic field up to 2.5 tesla reveals disparate behavior of the magnetic excitations. In zero applied field, the lowest and highest energy excitations show spatial dependencies indicative of dimerized short-range antiferromagnetic correlations that survive to high temperatures, comparable to the nearest neighbor exchange interactions. Our results suggest that the ground state of a three dimensional hyperkagome compound differs distinctly from its frustrated counterparts on a pyrochlore lattice and reveal a juxtaposition of cooperative paramagnetism and strong dimerized coupling. These results are surprising since GGG is often classified as a strongly frustrated system with a manifold of connected states for which one would expect a continuum of gapless excitations.

In collaboration with: Pascale Deen, Institut Laue Langevin; G. Balakrishnan, Department of Physics, University of Warwick; B.D. Rainford, Department of Physics and Astronomy, Southampton University; C. Ritter, Institut Laue-Langevin; L. Capogna, Istituto Officina dei Materiali, IOM-CNR; H. Mutka and T. Fennell, Institut Laue-Langevin.

4:54PM D18.00011 Effects of doping on the geometrically frustrated Heisenberg antiferromagnet Gadolinium Gallium Garnet , D.M. SILEVITCH, M.A. SCHMIDT, James Franck Institute/University of Chicago, S. GHOSH, University of California, Merced, G. AEPPLI, University College, London, T.F. ROSENBAUM, James Franck Institute/University of Chicago — Geometric frustration in the Heisenberg antiferromagnet Gadolinium Gallium Garnet (GGG) gives rise to a set of quantum protectorates where clusters of spins decouple from the overall spin liquid state. At 110 mK, there is a partial transition to an ordered AF state. Here, we examine the effect of lightly doping GGG with Nd ions, which partially alleviates the underlying frustration. We examine the size and binding energy of the spin clusters as a function of doping and temperature, and also characterize the suppression of the Neel temperature as the dopant concentration is increased.

5:06PM D18.00012 Electron magnetic resonance studies of the $Pr_3Ga_5SiO_{14}$ and $Nd_3Ga_5SiO_{14}$ kagóme systems , SANHITA GHOSH, Florida State University, SAITI DATTA, HAIDONG ZHOU, National High Magnetic Field Laboratory, MICHAEL HOCH, STEPHEN HILL, Florida State University — In recent years, there has been considerable interest in materials exhibiting magnetic frustration due to their novel ground state properties. $Pr_3Ga_5SiO_{14}$ (PGS) and $Nd_3Ga_5SiO_{14}$ (NGS) have trigonal crystal structures in which the rare earth ions are arranged in corner sharing triangles to form a distorted kagomé lattice. We report high frequency electron magnetic resonance (EMR) measurements on single crystals of NGS and PGS in order to ascertain the nature of their ground states. Both compounds exhibit extremely rich EMR spectra at low temperatures, with a large number of sharp peaks. For each frequency investigated, the peak positions display a strong, systematic dependence on the temperature. However, the usual paramagnetic resonance frequency/field variation is not observed, with the pattern of peaks varying dramatically from one frequency to the next. We thus conclude that the observed spectra correspond to collective excitations associated with finite size ordered clusters that persist on EMR time scales.

5:18PM D18.00013 Valence Bond Crystal on the Hyperkagome Antiferromagnet , EMIL BERGHOLTZ, ANDREAS LAUCHLI, RODERICH MOESSNER, Max Planck Institute for the Physics of Complex Systems — We describe our recent work that indicates that the ground state of the antiferromagnetic spin-1/2 Heisenberg model on the highly frustrated, three-dimensional, hyper-kagome lattice is a valence bond crystal (VBC). Performing a series expansion around an arbitrary dimer covering on the hyper-kagome we find that a ground state with a huge (72 site) unit cell is selected by the quantum fluctuations. The regularity and favorable energetics of our series expansion establishes the VBC as a serious contender to the earlier spin liquid proposals. We find that the ground state supports many, very low lying, excitations in the singlet sector and that the low energy spinful excitations (spinons and triplons) are effectively confined to various emergent lower-dimensional structures. If applicable to the recently studied sodium iridate compound, $Na_4Ir_3O_8$, this scenario has interesting observable implications, such as spatially anisotropic neutron scattering spectra and possibly multiple finite temperature signatures in the magnetic specific heat due to a multi-step breaking of discrete symmetries. Most saliently, here—as for several proposed states for analogous kagome and pyrochlore magnets—one might expect a clearly resolved Ising transition at relatively high temperature.

Ref: E.J. Bergholtz, A.M. Läuchli and R. Moessner, Phys. Rev. Lett., in press (2010) [arXiv:1010.1345]

Monday, March 21, 2011 2:30PM - 5:30PM –
Session D19 GMAG: Low Dimensional Magnetism and Spin Tunneling D170

2:30PM D19.00001 GMAG Student Dissertation Award Talk: Effects of Nanoscale Structure on the Magnetism and Transport Properties of Chromium and Chromium-Aluminum Alloys[1] , ZOE BOEKELHEIDE, University of California, Berkeley — Bulk Cr has an incommensurate spin density wave (ISDW) due to nesting of the Fermi surface which is easily disrupted by perturbation. Thus, the properties of Cr are sensitive to small amounts of dopant atoms, application of pressure, etc. which has been well studied in bulk. We have taken advantage of thin film growth techniques to study the effects of nanoscale structure on the properties of Cr and Cr1-xAlx alloys. The first part of my talk will discuss our research on polycrystalline Cr thin films, where variables such as strain and disorder crucially affect the SDW. We find that Cr thin films can be ISDW like in bulk Cr, or transition to commensurate SDW (CSDW) or mixed depending on deposition conditions and the resulting thin film microstructure. The transport properties are also strongly affected, as quasilocal defect states inside the SDW gap cause resonant scattering. This results in anomalous features such as residual resistivity ranging between 3 and 400 μO -cm and significant resistivity minima at low temperature. Further evidence of quasilocal states inside the SDW gap is seen in the enhanced electronic density of states (DOS) from specific heat measurements of Cr thin films. The second part of my talk will discuss Cr1-xAlx alloys. The addition of Al to Cr causes the ISDW to transition to CSDW for x = 0.03. Cr1-xAlx also exhibits previously unexplained semiconducting behavior for x = 0.15-0.30. I will discuss our ongoing theoretical and experimental research which suggests that a chemically ordered, rhombohedrally distorted Cr3Al structure occurs in nanosized domains and causes a hybridization gap on part of the Fermi surface. The CSDW causes a gap on another part of the Fermi surface, so that the semiconducting behavior can be explained by a combination of structural and magnetic affects.

[1]Supported by the DOE under Contract No. DE-AC02-05CH11231.

3:06PM D19.00002 Suppression of Macrospin Tunneling by Nanomechanical Interference , LORIEN HAYDEN, Department of Physics and Astronomy, University of Missouri, Columbia, ALEXEY KOVALEV, Department of Physics and Astronomy, University of California, Los Angeles, GERRIT BAUER, Kavli Institute of NanoScience, Delft University of Technology, YAROSLAV TSERKOVNYAK, Department of Physics and Astronomy, University of California, Los Angeles — This research considers the quantum dynamics of a nanomechanical resonator coupled to a macrospin of a magnetic nanoparticle. Suppression of macrospin tunneling by nanomechanical interference is demonstrated. By approximating the macrospin molecule as a two level system, the results are extended to the magnetopolariton splitting between resonantly coupled Fock states in which are observed similar interference patterns. The mentioned interference effects should be observable in a single molecule magnet bridged between two leads.

3:18PM D19.00003 Spin Tunneling in a Rotating Nanomagnet , MICHAEL O'KEEFFE, EUGENE CHUDNOVSKY, CUNY Lehman College and Graduate Center, LEHMAN COLLEGE THEORETICAL CONDENSED MATTER PHYSICS TEAM — We study spin tunneling in a magnetic nanoparticle with biaxial anisotropy that is free to rotate about its anisotropy axis. Exact instanton of the coupled equations of motion is found that connects degenerate classical energy minima. We show that mechanical freedom of the particle renormalizes magnetic anisotropy and increases the tunnel splitting.

M. F. O'Keeffe and E. M. Chudnovsky, cond-mat, arXiv:1011.3134.

3:30PM D19.00004 Theory of Raman Scattering in One-Dimensional Quantum Magnets , MASAHIRO SATO, Aoyama Gakuin University, HOSHO KATSURA, Gakushuin University, NAOTO NAGAOSA, University of Tokyo — Raman scattering is one of the powerful tools to study the quantum dynamics of the spin systems, and has been studied for a long term. Conventionally, Raman scattering spectra have been interpreted in terms of the two-magnon processes, from which the exchange coupling can be estimated. However, it is known that the magnon is not a good elementary excitation in low- dimensional quantum spin systems, especially in 1D, and the theoretical studies on the Raman processes in 1D have not been developed compared with those for other electromagnetic processes such as NMR and ESR. Here we have developed a theory for Raman scattering of 1D quantum magnets. We show that Raman spectrum can detect some interesting excitations such as spinon pairs, solitons, etc, depending on the additional interactions to the conventional Heisenberg one and polarization direction of external electromagnetic wave.

3:42PM D19.00005 Surface ferri-magnetism in some antiferromagnetic materials , YONGBIN LEE, Ames Laboratory; Dept. of Physics and Astronomy, Iowa State University, Ames, BRUCE HARMON, Ames Laboratory; Dept. of Physics and Astronomy, Iowa State University, Ames — In an antiferromagnetic material with inversion symmetry the electronic energy bands are spin degenerate because of time reversal symmetry. However, at the surface the inversion symmetry is broken, which opens the possibility of breaking the spin degeneracy and inducing a significant net moment on the surface. As an example of this spin degeneracy breaking, we discuss the electronic structure of antiferromagnetically ordered $BaMn_2As_2$. Unlike the bulk bands, its surface bands can individually possess a net spin polarization. Also the bulk bands in this material have a gap, however the calculated spin polarized surface states cross the Fermi level. Our calculations show that an applied field perpendicular to the surface and along the spin axis induces a significant net surface magnetization, which does not extend significantly into the bulk. - Work at the Ames Laboratory was supported by the US DOE, Basic Energy Science, under contract No. DE-AC02-07CH11358.

3:54PM D19.00006 Spin-orbit interactionsand magnetic field in antiferromagnetic triangular molecular magnets , J.F. NOSSA, M.F. ISLAM, C.M. CANALI, Linnaeus University, M.R. PEDERSON, Naval Research Laboratory — Frustrated triangular molecular magnets such as Cu_3 are characterized by a doubly generate S=1/2 ground-state (GS) with opposite chirality. Recently it has been proposed theoretically [1] and verified by ab-initio calculations [2] that an external electric field can efficiently couple these two chiral spin states, even in the absence of spin-orbit interaction (SOI). SOIs are nevertheless important, since they introduce a splitting in the GS manifold. In this talk we will discuss different schemes on how to evaluate within spin density functional theory the effect of the SOIs on the chiral states. The connection between SOI and the Dzyalozhinsky-Moriya interaction will be discussed. We will also present calculations of the energy dependence on an external magnetic field, whose presence is important to achieve full control of the spin-electric coupling within the manifold of the GS chiral doublets.

[1] M. Trif et. al. Phys. Rev. B 82, 045429 (2010) and M. Trif et. al. Phys. Rev. Lett. 101, 217201 (2008)
[2] F. Islam et. al. Phys. Rev. B 82, 155446 (2010)

4:06PM D19.00007 Real-space imaging of Kondo screening in a two-dimensional Kondo lattice[1] , YING JIANG, YANNING ZHANG, JUEXIAN CAO, RUQIAN WU, WILSON HO, Department of Physics and Astronomy, University of California, Irvine, CA 92697-4575 — Kondo lattice systems exhibit nonuniversal many-body behaviors, mainly resulting from the competition and interplay between onsite Kondo screening and intersite coupling. In reduced spatial dimensions, the many-body correlation effects are expected be to more relevant. We report the realization of a two-dimensional (2D) Kondo lattice formed by self-assembled triplet oxygen molecules on the Au (110)-1×2 reconstructed surface. By mapping the Kondo resonance in the 2D O_2 lattice with a scanning tunneling microscope, the interplay between the intermolecule coupling and the onsite Kondo effect was manifested as the unexpected coexistence of both local and nonlocal Kondo screening at the atomic level. While the latter provides evidence of the collective deconfinement of magnetization in Au, the former shows local hybridization between the Kondo clouds of nearest-neighbor O_2 molecules, as revealed by density functional calculations. These findings may assist in our understanding of the unusual electronic properties in various strongly correlated electron systems, such as heavy fermion compounds and Kondo insulators.

[1]Corresponding author: wilsonho@uci.edu

4:18PM D19.00008 Single oxygen and CO molecules on Au(110): what can we learn?[1] , YANNING ZHANG, YING JIANG, WILSON HO, RUQIAN WU, University of California, Irvine — Studies of O_2 and CO molecules on the reconstructed Au (110) surface are crucial for the understanding of unusually high activity of Au nanostructures that are useful in heterogeneous catalysis. Moreover, the O_2/Au system is ideal to probe the Kondo effect using surface science techniques, due to the persisting magnetization of triplet O_2 in physisorption systems. In this work, scanning tunneling microscope (STM) measurements and density functional calculations were performed to investigate the adsorption geometries and physical properties of single O_2 and CO molecules on Au(110). The calculated atomic structures and vibration frequencies are comparable favorably with our STM experimental results at low temperature, allowing efficient establishment of structural models. Interestingly, the O_2 molecule takes a defect site over the Au row, with a tilted geometry. The magnetic moment of O_2 is still as large as 1.9 μ_B, which furthermore induces a pronounced Kondo resonance in a large spatial region. The cloud of Kondo enhancement was found to closely follow the distribution of the calculated spin density at the fermi level, a correlation which is important for the understanding of Kondo effect in molecular systems.

[1]Work was supported by DOE, Basic Energy Science, and NERSC

4:30PM D19.00009 Universal chiral magnetism in low-density 2D Kondo lattice model , DMITRY SOLENOV, DMITRY MOZYRSKY, IVAR MARTIN, Los Alamos National Laboratory — We demonstrate that (quasi-)two-dimensional systems comprised of localized moments and itinerant electrons form non-coplanar magnetic crystal states when the Kondo coupling energy is smaller than the chemical potential. These states arise for fully isotropic local exchange coupling between electrons and magnetic ions and do not require a spin-orbit (Dzyaloshinskii-Moriya) interaction or magnetic field. We give an analytical argument on instability of simple co-planar states and show that the states with non-zero chirality (degree of non-coplanarity) are energetically favorable. Numerical modeling is performed to estimate the ground state configurations.

4:42PM D19.00010 Low temperature magnetic dynamics in one-dimensional Co(II) molecular chains , A. AMJAD, Department of Physics, University of Central Florida, USA, G.M. ESPALLARGAS, J.M. CLEMENTE-JUAN, Instituto de Ciencia Molecular, Universidad de Valencia, Spain, R. KLEMM, E. DEL BARCO, Department of Physics, University of Central Florida, USA, E. CORONADO, Instituto de Ciencia Molecular, Universidad de Valencia, Spain, M. EVANGELISTI, ICMA, CSIC - Universidad de Zaragoza, Spain — We present a low-temperature study of one-dimensional Co-based molecular chains, trans-[$CoCl_2$(3,5-Br_2py)$_2$]. Ac and dc susceptibility experiments show that the cobalt ions tend to form anisotropic ferromagnetic chains, whose properties are dictated by the thermal excitations of 1D domain walls. The observation of anomalies in the hysteresis loops of the sample on increasing the magnetic field sweep rate reveals interesting dynamical effects at the individual chain level. On decreasing the temperature, no evidence for 3D ordering was observed in specific heat measurements, although the magnetization was strongly irreversible below ∼450 mK. Possible sources for this absence of a magnetic phase transition could be the weakness of the interchain interactions, the presence of single-ion anisotropy at skew angles, disordered domains, and lattice defects, etc. These possibilities will be studied both experimentally and theoretically.

4:54PM D19.00011 ABSTRACT WITHDRAWN –

5:06PM D19.00012 Spatial confinement effect on $TbMn_2O_5$ nanorods , CHUN CHUEN YANG, JING HUEI WANG, WEI LUEN HUANG, CHANG YU WENG, Department of Physics, Chung Yuan Christian University, CIH LIAN HONG, YANG YUAN CHEN, Institute of Physics, Academia Sinica, DEPARTMENT OF PHYSICS, CHUNG YUAN CHRISTIAN UNIVERSITY COLLABORATION, INSTITUTE OF PHYSICS, ACADEMIA SINICA COLLABORATION — Series of $TbMn_2O_5$ nanorods were fabricated by hydrothermal method with different annealing temperatures. Three samples which width by length equal to 10(4) nm $\times$ 38(14) nm, 25(6) nm $\times$ 64(18) nm, and 101(25) nm $\times$ 216(54) nm are identified by TEM images, x-ray diffraction, and SAED schemes. Furthermore discovery show that the preferred growth direction is along c axis (length). Ac magnetic susceptibility and specific heat measurements revealed incommensurate ($\sim$41 K) and commensurate ($\sim$38 K) Mn antiferromagnetic ordering peaks are only appeared in 101(25) nm $\times$ 216(54) nm sample. In this case, the small size effect resulted entropy difference of Mn magnetic ordering is 27 % less than bulk one. At 5 K, a small hysteresis loop was also observed in the identical sample and indicated the FM domains occurred. No such magnetic and thermal behaviors were found in another two samples. We believe this is attributing to spatial limitation and distortion caused by low surface-volume ratio. The estimated magnetic correlation length of Mn is in between 25 and 64 nm.

5:18PM D19.00013 Tetrairon(III) Single Molecule Magnet Studied by Scanning Tunneling Microscopy and Spectroscopy , YOUNGTEK OH, HOGYUN JEONG, MINJUN LEE, JEONGHOON KWON, JAEJUN YU, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea, SHARIFUL ISLAM MAMUN, GAJENDRA GUPTA, JINKWON KIM, Department of Chemistry, Kongju National University, Chungnam 314-701, Korea, YOUNG KUK, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea — Tetrairon(III) single-molecule magnet (SMM) on a clean Au(111) has studied using scanning tunneling microscopy (STM) and spectroscopy (STS) to understand quantum mechanical tunneling of magnetization and hysteresis of pure molecular origin. Before the STM studies, elemental analysis, proton nuclear magnetic resonance (NMR) measurement and Energy Dispersive X- ray Spectroscopy (EDS) were carried out to check the robustness of the sample. The STM image of this molecule shows a hexagonal shape, with a phenyl ring at the center and surrounding six dipivaloylmethane ligands. Two peaks are observed at 0.5 eV, 1.5 eV in the STS results, agreeing well with the first principles calculations. Spin-polarized scanning tunneling microscopy (SPSTM) measurements have been performed with a magnetic tip to get the magnetization image of the SMM. We could observe the antiferromagnetic coupling and a centered- triangular topology with six alkoxo bridges inside the molecule while applying external magnetic fields.

Monday, March 21, 2011 2:30PM - 5:30PM –
Session D20 FIAP: Bionanotechnology D168

2:30PM D20.00001 Multifunctional nanoparticles ($Au@SiO_2@Y_2O_3{:}Er^{3+}$) for biological and photonic application[1] , MADHAB POKHREL, JIANHUI YANG, University of Texas at San Antonio, PARESH C. RAY, Jackson State University, DHIRAJ K. SARDAR, University of Texas at San Antonio — Due to plasmon at the surface, the absorption and scattering of electromagnetic radiation by metal nanoparticles are strongly enough. These properties provide the potential of designing multifunctional nanoparticles which are optically active for simultaneous molecular imaging and photothermal cancer therapy. Gold nanorods with suitable aspect ratios can absorb and scatter strongly in the NIR region. In the present work, we have demonstrated the application of multifunctional nanoparticles ($Au@SiO_2@Y_2O_3{:}Er^{3+}$) as contrast agents for both molecular imaging and photo thermal therapy. These multifunctional naoparticles has shown the enhancement in Er^{3+}fluorescence through plasmon interaction and enhancement in Raman spectrum, which made these nanoparticles potential for biosensor for detecting the biological and chemical molecule.

[1]This research is supported by NSF PREM Grant no DMR-0934218.

2:42PM D20.00002 Fundamental Interactions between Deoxyribonucleic Acid (DNA) Oligomers and Au Nanoparticles: Experimental and Theoretical Studies , MOLLESHREE KARNA, Science and Math Academy, Aberdeen High School, Aberdeen, MD 2100, Army Research Lab, Aberdeen Proving Ground, MD 21005, RADHAKRISHNAN BALU, MARK GRIEP, GOVIND MALLICK, Army Research Lab, Aberdeen Proving Ground, MD 21005 — **E**xperimental and theoretical investigations were performed to understand the nature of fundamental interactions between gold nanoparticles (GNPs) and single stranded DNA (ss-DNA). Atomic force microscopic imaging and UV-Visible spectroscopic measurements revealed binding of NPs with ss-DNA under mildly acidic conditions.. *Ab initio* quantum chemical calculations within the framework of density functional theory provided a possible charge transfer pathway from the DNA base guanine to Au atoms and thus characterizing the interaction as electrostatic. The calculations outline the possible effect of the presence of other bases to guanine mediated charge transfer. Specifically, the presence of an adenine base alters the charge localization at the guanine base and thus prevents charge transfer to NPs.

2:54PM D20.00003 Modeling the effect of dynamic surfaces on membrane penetration , REID VAN LEHN, ALFREDO ALEXANDER-KATZ, MIT — The development of nanoscale materials for targeted drug delivery is an important current pursuit in materials science. One task of drug carriers is to release therapeutic agents within cells by bypassing the cell membrane to maximize the effectiveness of their payload and minimize bodily exposure. In this work, we use coarse-grained simulations to study nanoparticles (NPs) grafted with hydrophobic and hydrophilic ligands that rearrange in response to the amphiphilic lipid bilayer. We demonstrate that this dynamic surface permits the NP to spontaneously penetrate to the bilayer midplane when the surface ligands are near an order-disorder transition. We believe that this work will lead to the design of new drug carriers capable of non-specifically accessing cell interiors based solely on their dynamic surface properties. Our work is motivated by existing nanoscale systems such as micelles, or NPs grafted with highly mobile ligands or polymer brushes.

3:06PM D20.00004 Microsphere whispering gallery optical resonators for biomedical microfluidic devices , O. SVITELSKIY, A. DARAFSHEH, D. SUN, V.N. ASTRATOV, University of NC at Charlotte, M. SUMETSKY, OFS Laboratories, NJ 08873 USA, A. LUPU, M. TCHERNYCHEVA, Institut d'Electronique Fondamentale, Université Paris-Sud XI, 91405 Orsay, France — These resonators are potential candidates for broad application range as sensors of various physical quantities, and as key elements for photonic and optomechanical systems. Most of the biomedical applications involve deployment of resonators in fluidic environment. However, closeness of refractive indices of sphere n_s and fluid n_f obstructs excitation of the resonant modes. Moreover, an attempt to increase n_s can deteriorate coupling of light between fiber and sphere. To address these challenges we explore a series of high-Q resonators using a specially developed tapered optical microfiber microfluidic platform. The coupling strength between the cavity and the microfiber taper is shown to depend on the contact position of the microsphere along the taper and on the refractive index contrast between the microsphere and the fluid. We demonstrate that barium titanate glass beads with $n_s \sim 2$ can be suitable for practical tasks.

3:18PM D20.00005 Utilizing nonlinear optical properties in nanoparticles for imaging[1] , BRIAN YUST, NEEMA RAZAVI, DHIRAJ SARDAR, The University of Texas at San Antonio — Optical phase conjugation is a nonlinear effect in which light incident upon a nonlinear medium may be conjugated so that the output signal is in the opposite direction of the input, as seen in four-wave mixing. Recently, we have seen that these nonlinear effects may still be seen in various nanocrystals and nanoparticles. Barium titanate (BaTiO3) is a good candidate for phase conjugation on the nano-scale, because of its large third order susceptibility. BaTiO3 particles of varying size are synthesized through precipitation and hydrothermal methods and analyzed optically and morphologically. The nonlinear absorption, four wave mixing signal in the forward and counter-propagating geometries, and third order susceptibilities are characterized in both the visible and infrared. Possible uses for the unique optical properties of these nanoparticles in imaging, microscopy, and photonics will also be discussed.

[1]This work is supported in part by National Science Foundation PREM Grant No. DMR - 0934218 and UTSA Collaborative Research Seed Grant Program (CRSGP).

3:30PM D20.00006 Gold Nanostars for Photo-Thermal Ablation of Single Neurons[1] , ZURAB KERESELIDZE, Dept. Physics and Astronomy, UTSA, VICTOR ROMERO, CIO, Mexico, WASKAR EGIDO, CHRISTOPHER VALDES, EMMANUEL MICHAELIDES, Dept. Biology, UTSA, XOMALIN PERALTA, MIGUEL JOSE-YACAMAN, Dept. Physics and Astronomy, UTSA, FIDEL SANTAMARIA, Dept. Biology, UTSA — Nanoparticle mediated photo-thermal ablation therapy is a technique for removing cells within a tissue with minimal collateral damage. It works by exciting the surface plasmon resonance of metallic nanoparticles so there is an amplification of the absorption of the incident electromagnetic field which is then transformed into heat and results in photo-thermal ablation. Little is known about its effects at the single-cell level. We fabricated various sized and shaped gold nanoparticles, including nanostars, with a surface plasmon mode in the near infrared. Neurons of mouse cerebellar slices internalize bare nanostars during incubation periods of $<$3 hrs. We imaged the slices and excited surface plasmon mode of the nanostars. Our results show that we are capable of destroying individual nanostar containing cells without affecting the neighbors. Other shapes attach to the cell membrane but are not internalized. Therefore nanoparticles can provide a technique for a neuron single-cell photo-thermal without any functionalization.

[1]NSF PREM (#0934218), UTSA

3:42PM D20.00007 Biochemically Selective Nanoarrays: From Protein-DNA Interactions to Bio-Inorganic Nanoscale Assembly , JUSTIN ABRAMSON, MATTEO PALMA, ALON GORODETSKY, COLIN NUCKOLLS, MICHAEL SHEETZ, SHALOM WIND, JAMES HONE — The ability to control the arrangement of both biomolecules and bio-inorganic structures on surfaces with nanometer resolution is of great interest in the field of nanoscience and nanotechnology. Nanopatterned arrays of biomolecules can offer unmatched sensitivity in molecular diagnostics. Furthermore, templated assembly of bio-inorganic structures at the nanoscale makes possible interesting quantum optical structures, including switchable photonic cavities. Here we describe different strategies to control the immobilization of single- and double-stranded DNA, as well as quantum dots, on nanopatterned surfaces, with features down to the sub-30nm regime. The bio-functional chemistry allows for the formation of non-sterically hindered DNA nanodomains where the dsDNA attached to the nanodots is accessible and maintains its native conformation, as confirmed by restriction enzymes studies at the single molecule level. We will further highlight the broader utility of such nanopatterned surfaces for the self-organization of quantum dots, demonstrating the ability to both biochemically and covalenty assemble single quantum dots on our nanopatterns.

3:54PM D20.00008 Nanoscale open-ended coaxial line proximity sensor array for spatio-temporal impedance imaging[1] , JEFFREY R. NAUGHTON, BINOD RIZAL, MICHAEL J. BURNS, GREGORY MCMAHON, STEPHEN SHEPARD, MICHAEL J. NAUGHTON, Boston College — We describe the development of a dielectric impedance measurement array comprised of open-ended nanoscale coaxial proximity sensors. The device offers the capability of on-chip dielectric impedance tomography for imaging *e.g.* biological cells with $\sim$micron pixel density. Computer simulations of the response of individual pixels and of discrete arrays to changes in dielectric properties of proximate media are presented. Experiments with biological cells on 1st-generation arrays will be discussed.

[1]naughton@bc.edu

4:06PM D20.00009 Nonlinear Optical Properties of ZnO for BioimagingCell and Cell Destruction , BEN URBAN, SAMUDYATHA CHAKKI, University of North Texas, OS SENTHILKUMAR, KASILINGAM SENTHILKUMAR, YASUHISA FUJITA, Shimane University, ARUP NEOGI, University of North Texas — As of recent years nanotechnology has been at the forefront of scientific research. It promises to have a broad range of applications from turning unhealthy foods into health foods, making computers faster and curing cancer. We present results on using nonlinear optical processes of ZnO nano-crystals to detect, track and destroy cells. By incorporating ZnO into a hydrophobic nano-hydrogel matrix with trace amounts of H_2O_2, we can attach antibodies or microRNA for specific cell targeting and, using the heat generating properties of the third order nonlinear process, release H_2O_2 in the cell causing instant cell death. Theoretically, with the appropriate sequence for microRNA or the appropriate antibodies, we could target cancer cells in the body and destroy them. This presentation gives our results until now.

4:18PM D20.00010 Polymeric Nanoelectrodes for Investigating Cellular Adhesion[1] , PREM THAPA, GOVIND PANERU, BRET FLANDERS, Kansas State University — Polyethylene dioxythiophene nano-filaments were grown on lithographic electrode arrays by the recently developed directed electrochemical nanowire assembly technique. These filaments are firmly attached to the electrode but are not attached to the glass substrate. Hence, they behave like cantilevered rods (with one free end). Individual cells of the slime mold *Dictystolium discoideum* initiate contact by extending pseudopods to the nanoelectrodes when cultured on the electrode arrays. Scanning electron micrographs of the interfaces show the contact area to be of the order of 0.1 μm^2. Confocal images reveal the focal adhesions in the cell-electrode contact region. Deflection of the nanoelectrode by an individual cell can be used to measure the force exerted by the cell. Recent results on this innovative force sensing approach will be discussed.

[1]NSF

4:30PM D20.00011 Detecting Lyme disease using antibody-functionalized carbon nanotubes , JENNIFER DAILEY, University of Pennsylvania, Department of Physcs and Astronomy, MITCHELL LERNER, BRETT GOLDSMITH, University of Pennsylvania, Department of Physics and Astronomy, DUSTIN BRISSON, University of Pennsylvania, Department of Biology, A.T. CHARLIE JOHNSON, University of Pennsylvania, Department of Physics and Astronomy — We combine antibodies for Lyme flagellar protein with carbon nanotube transistors to create an electronic sensor capable of definitive detection of Lyme disease. Over 35,000 cases of Lyme disease are reported in the United States each year, of which more than 23 percent are originally misdiagnosed. Rational design of the coupling of the biological system to the electronic system gives us a flexible sensor platform which we can apply to several biological systems. By coupling these antibodies to carbon nanotubes in particular, we allow for fast, sensitive, highly selective, electronic detection. Unlike antibody or biomarker detection, bacterial protein detection leads to positive identification of both early and late stage bacterial infections, and is easily expandable to environmental monitoring.

4:42PM D20.00012 Fluorescence-Based DNA-Nanotube Platform with Single Molecule Resolution , PRAKRIT JENA, ANKUR JAIN, University of Illinois at Urbana-Champaign, DANIEL HELLER, Massachusetts Institute of Technology, MARKITA LANDRY, YANN CHEMLA, University of Illinois at Urbana-Champaign, MICHAEL STRANO, Massachusetts Institute of Technology, TAEKJIP HA, University of Illinois at Urbana-Champaign — We have developed an experimental platform to control and modify the DNA on a DNA-Single Walled Nanotube (SWNT) complex for the purpose of detecting labeled and unlabeled protein-DNA interactions via visible fluorescence. By exploiting the distance-dependent photophysical interaction between organic fluorophores and the surface of a SWNT as the sensing mechanism, fluorophore-conjugated DNA-SWNTs are immobilized and observed using single molecule-total internal reflection microscopy. By analyzing the number of molecules, photobleaching steps and the absolute size of the observed DNA-SWNTs, we have confirmed the presence of a duplex, partial duplex and single-strand DNA scaffold on the SWNT surface using both nucleic acids and proteins as probes. Our approach offers multiple experimental schemes to extend the current use of carbon nanotubes for applications involving the interaction with biologically relevant molecules.

4:54PM D20.00013 Selective Intracellular Activation by Designing pH-Sensitive and Tunable Fluorescent Nanoparticle , KEJIN ZHOU, YIGUANG WANG, XIAONAN HUANG, MILAN POUDEL, GANG HUANG, KATE LUBY-PHELPS, JINMING GAO — Integration of nanotechnology with molecular biology and medical imaging has propelled the development of various nanoscopic imaging probes and targeted therapeutics. Despite great advances, it remains a formidable challenge to create highly biointeractive nanosystems that can respond to subtle changes in physiological stimuli (e.g. pH, enzymes) to achieve desired biological specificity. Here we report a set of robust, pH-activatable micelle nanoprobes with tunable pH transitions in the physiological range. These nanoprobes have a fast fluorescence response ($<$5 ms), up to 55-fold increase of emission intensity between OFF and ON states, and only require $<$0.25 pH unit for activation (vs. 2 pH unit for small molecular dyes). Nanoprobes with different transition pH can be selectively activated in specific endocytic compartments such as early endosomes or lysosomes. This capability allows for the development of pH-activatable imaging probes or nanocarriers that can target specific subcellular organelles for therapy.

5:06PM D20.00014 Formation of Lipid Bilayer Membrane including Ion Channels on Graphene , JUNG YOON CHOI, KYUNG EUN BYUN, SEON NAMGUNG, Seoul National University, HEEJUN YANG, JINSEONG HEO, HYUN-JONG CHUNG, SUNAE SEO, Samsung Advanced Institute of Tech., SEUNGHUN HONG, Seoul National University — Lipid bilayer membrane on a solid electrode has been extensively utilized to study membrane proteins. Recently, graphene has drawn an attention as a transparent and high conductive electrode compatible with biological systems. Herein, we report the successful formation of lipid membrane including ion channels on graphene. In this method, graphene was functionalized by biocompatible molecular layers and utilized as a substrate to support lipid bilayer membrane including ion channels. The functionality of ion channels incorporated in the lipid bilayer membrane was studied via the electrochemical impedance spectroscopy. This lipid membrane-coated graphene structure can be a versatile platform for various applications such as bio-sensing and in vitro drug screening.

5:18PM D20.00015 Aptamer sandwich-based carbon nanotube sensors for single-carbon-atomicresolution detection of non-polar small molecular species , JOOHYUNG LEE, Department of Physics and Astronomy, Seoul National University, Seoul, Korea, MINJOUNG JO, JI-YOUNG AHN, SOYOUN KIM, Department of Biomedical Technology, Dongguk University, Seoul, Korea, TAE HYUN KIM, Department of Chemistry, Soonchunhyang University, Asan, Chungnam, Korea, DONG-KI LEE, Department of Chemistry, Sungkyunkwan University, Suwon, Korea, SEUNGHUN HONG, Department of Biophysics and Chemical Biology, Seoul National University, Seoul, Korea — Portable sensor platforms are crucial for the on-site monitoring of disease-related metabolites, environmental pollutants and food toxicants. However, it is still difficult to build highly-sensitive and selective sensor platforms for small molecular detection. We developed an aptamer sandwich-based carbon nanotube sensor, where aptamers were utilized to capture target molecules as well as to enhance the sensor signals. Using this strategy, we successfully demonstrated the detection of non-polar bisphenol A molecules with a picomolar sensitivity and single-carbon-atomic resolution. Furthermore, by modifying the labeling aptamer with additional biotin, we enhanced the detection limit of our sensors for one hundred times. These results overcome the fundamental limitation of general FET-based sensors and should make a major breakthrough in various applications such as environmental protection and food safety.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D21 GIMS: Focus Session: Novel Instrumentation & Measurements for Biomedical Research D161

2:30PM D21.00001 Physical principles of genomic regulation through cellular nanoscale structure and implications for initiation of carcinogenesis , VADIM BACKMAN, Northwestern University — Although compelling evidence suggests that cellular nanoarchitecture and nanoscale environment where molecular interactions take place would be expected to significantly affect macromolecular processes, biological ramifications of cellular nanoscale organization have been largely unexplored. This understanding has been hampered in part by the diffraction limited resolution of optical microscopy. The talk will discuss a novel optical microscopy technique, partial wave spectroscopic (PWS) microscopy, that is capable of quantifying statistical properties of cell structure at the nanoscale. Animal and human studies demonstrated that an alteration in the statistical properties of the nanoscale mass density distribution in the cell nucleus (e.g. nuclear nanoarchitecture) is one of the earliest and ubiquitous events in carcinogenesis and precedes any other known morphological changes at larger length scales (e.g. microarchitecture). The talk will also discuss the physical principles of how the alteration in nuclear nanoarchitecture may modulate genomic processes and, in particular, gene transcription.

Work done in collaboration with Hariharan Subramanian, Prabhakar Pradhan, Dhwanil Damania, Lusik Cherkezyan, Yolanda Stypula, Jun Soo Kim, Igal Szleifer, Northwestern University, Evanston, IL, Hemant K. Roy, Northshore University HealthSystems, Evanston, IL

3:06PM D21.00002 3D Cell Culture Imaging with Digital Holographic Microscopy[1] , THOMAS DIMIDUK, Harvard University, KENDRA NYBERG, University of Oregon, DARIELA ALMEDA, Harvard University, EKATERINA KOSHELVA, University of Chigago, RYAN MCGORTY, DAVID KAZ, EMILY GARDEL, DEBRA AUGUSTE, VINOTHAN MANOHARAN, Harvard University — Cells in higher organisms naturally exist in a three dimensional (3D) structure, a fact sometimes ignored by in vitro biological research. Confinement to a two dimensional culture imposes significant deviations from the native 3D state. One of the biggest obstacles to wider use of 3D cultures is the difficulty of 3D imaging. The confocal microscope, the dominant 3D imaging instrument, is expensive, bulky, and light-intensive; live cells can be observed for only a short time before they suffer photodamage. We present an alternative 3D imaging techinque, digital holographic microscopy, which can capture 3D information with axial resolution better than $2\mu m$ in a $100\mu m$ deep volume. Capturing a 3D image requires only a single camera exposure with a sub-millisecond laser pulse, allowing us to image cell cultures using five orders of magnitude less light energy than with confocal. This can be done with hardware costing $\sim \$1000$. We use the instrument to image growth of MCF7 breast cancer cells and p. pastoras yeast.

[1]We acknowledge support from NSF GRFP.

3:18PM D21.00003 Carbogen Enhanced Femto Oximetry Breast Cancer Diagnosis Method with High Specificity , BOGDAN C. MAGLICH, California Science and Engineering Corp., J.K. SHULTIS, C.J. SOLOMON, Kansas State University — As large malignant tumors are oxygen deficient (hypoxic), cancer could be diagnosed *in vivo* and online, by non-invasive measurement of oxygen difference between tumor and adjacent tissue. Computer simulations of noninvasive diagnosis by Femto Oximetry (FO) of hypoxia in 1 cm tumor in 10 cm breast shows that background γ's from non hypoxic tissue will mask hypoxia. To amplify the hypoxic-to-normal O difference, air breathing will be replaced with carbogen (O_2 95%, CO_2 5%) using vasco-constrictive property whereby carbogen breathing increases O in normal tissue, while not in malignant hypoxic tumors. 90% hypoxia will be detectable by FO with specificity 99%. Our method will be tested on R3230 tumors in Fischer rats at UCI.

3:30PM D21.00004 Fractal Analysis of Optical Coherence Tomography of Normal and Malignant Breast Tissue , AMANDA C. SULLIVAN, JOHN P. HUNT, AMY L. OLDENBURG, University of North Carolina at Chapel Hill — Optical coherence tomography (OCT) provides real-time imaging of tissue several mean free photon paths into tissue by heterodyne detection of backscattered light. OCT can potentially be used to rapidly assess tumor margins during breast cancer resection, however, currently it is difficult to differentiate between normal and malignant tissues with OCT. Because cancer is characterized morphologically by increasing disorder, we investigated the fractal dimension of OCT images of normal and cancerous breast tissue. 3D OCT images of 44 specimens were collected, then tissues were histologically processed to independently determine distinct regions of adipose, stroma and cancer. The fractal dimension of each tissue type was then calculated with a one-dimensional box-counting algorithm applied to the OCT axial scans. We found that the fractal dimensions of stromal tissues were significantly higher than those of cancer ($P<10^{-6}$), while those of adipose tissue were significantly lower than those of cancer ($P<10^{-4}$).

3:42PM D21.00005 A new algorithm for detection of apnea in infants in neonatal intensive care units[1] , HOSHIK LEE, College of William and Mary, BROOKE VERGALES, ALIX PAGET-BROWN, CRAIG RUSIN, RANDALL MOORMAN, JOHN KATTWINKEL, University of Virginia, JOHN DELOS, College of William and Mary — Apnea is a very common problem for premature infants: apnea of prematurity (AOP) occurs in $> 50\%$ of babies whose birth weight is less than 1500 g, and AOP is found in almost all babies who are $< 1000\,\mathrm{g}$ at birth. Current respiration detectors often fail to detect apnea, and also give many false alarms. We have created a new algorithm for detection of apnea. Respiration is monitored by continuous measurement of chest impedance (CI). However, the pulsing of the heart also causes fluctuations in CI. We developed a new adaptive filtering system to remove heart activity from CI, thereby giving much more reliable measurements of respiration. The new approach is to rescale the impedance measurement to heartbeat-time, sampling 30 times per interbeat interval. We take the Fourier transform of the rescaled signal, bandstop filter at 1 per beat to remove fluctuations due to heartbeats, and then take the inverse transform. The filtered signal retains all properties except the impedance changes due to cardiac filling and emptying. We convert the variance of CI into an estimated likelihood of apnea.

[1]This work is supported by NICHD 5RCZHD064488

3:54PM D21.00006 The Suppression of Dominant Acoustic Frequencies in MRI[1] , XINGXIAN SHOU, ROBERT BROWN, Case Western Reserve University — Patient discomfort and brain imaging distortion are serious MRI acoustic noise problems arising from the rapid switching on and off of gradient coils in the presence of the strong Larmor magnetic field. A study is made of dominant frequencies in the acoustic noise spectrum and, motivated by both spring and string ideas, we propose the cancellation of selected frequencies by appropriate gradient pulse sequence design. From both simulations and experiments, vibrations resulting from an impulsive force associated with a ramping up of a gradient pulse are shown to be cancelled upon the application of another impulsive force coming from the appropriately timed ramping down of that pulse. A method for the suppression of multiple-frequency contributions involving a series of gradient pulses with variable timings is developed and confirmed by experiment. Whether we refer to reduction in terms of dB (about 30-40 dB per peak), or to the verdict of a listener, the conclusion is that a marked reduction in sound can be achieved when at least three of the dominant frequency peaks are suppressed. A variety of pulse profiles and timing combinations can be used to attenuate important contributions to the acoustic spectrum.

[1]Supported by the Ohio Third Frontier Program.

4:06PM D21.00007 Linewidth Narrowing for ^{31}Phosphorus MRI of Bones , MERIDETH FREY, SEAN BARRETT, Yale University Physics Dept. — Bone is a particularly challenging tissue to study with conventional MRI given the relatively low water density and wider linewidths of its solid components.[1] Recent fundamental research in quantum computing gave rise to a new NMR pulse sequence that can be used to narrow the broad NMR spectrum of solids.[2] Here we narrow the spectrum of the ^{31}P in natural bone mineral (by a factor of up to 1600x). This technique offers a new route to do high spatial resolution, 3D ^{31}P MRI of bone which complements conventional MRI and x-ray based techniques to study bone physiology and structure. Thus far we have used our pulse sequence to do high spatial resolution (sub-250 μm)^3 3D ^{31}P MRI of *ex vivo* dry bovine cortical bones, wet procine rib bones, and wet rabbit femoral bones at 4T. We have also explored the use of compressive sampling[3] to push imaging time down to less than two hours without distracting artifacts.

[1]F. W. Wehrli, J. MRI **25**, 390 (2007); S. Anumula et al., Bone **42**, 405 (2008); D. Idiyatullin et al., J. Mag Res **193**, 267 (2008); E.E. Sigmund et al., NMR Biomed **22**, 436 (2009); Y. Wu et al., J. MRI **31**, 954 (2010)
[2]Y. Dong et al. Phys. Rev. Lett. **100**: 247601 (2008); D. Li et al. Phys. Rev. B **77**: 214306 (2008)
[3]M. Lustig et al., Mag Res Med **58**, 1182 (2007)

4:18PM D21.00008 Linewidth narrowing for ^{31}Phosphorus MRI of cell membranes , SEAN BARRETT, MERIDETH FREY, Yale University Physics Dept., JOSEPH MADRI, MICHAEL MICHAUD, Yale Medical School — Most ^{31}P Magnetic Resonance Spectroscopy studies of tissues try to avoid contamination by a relatively large, but broad, spectral feature attributed to cell membrane phospholipids[1]. MRI using this broad ^{31}P membrane spectrum is not even attempted, since the spatial resolution and signal-to-noise would be poor, relative to conventional MRI using the narrow ^{1}H water spectrum. This long-standing barrier has been overcome by a novel pulse sequence, recently discovered in fundamental quantum computation research[2], which narrows the broad ^{31}P spectrum by $\sim$1000$\times$. Applying time-dependent gradients in synch with a repeating pulse block enables a new route to high spatial resolution, 3D ^{31}P MRI of the soft solid components of cells and tissues. So far, intact and sectioned samples of *ex vivo* fixed mouse organs have been imaged, with (sub-mm)^3 voxels. Extending the reach of MRI to broad spectra in natural and artificial tissues opens a new window into cells, enabling progress in biomedical research.

[1]W.J. Thoma et al., J. MR **61**, 141 (1985); E.J. Murphy et al., MR Med **12**, 282 (1989); R. McNamara et al., NMR Biomed **7**, 237 (1994).
[2]Y. Dong et al. Phys. Rev. Lett. **100**, 247601 (2008); D. Li et al. Phys. Rev. B **77**, 214306 (2008).

4:30PM D21.00009 Producing >60,000-fold room-temperature ^{89}Y NMR signal enhancement[1] , LLOYD LUMATA, ASHISH JINDAL, MATTHEW MERRITT, CRAIG MALLOY, A. DEAN SHERRY, ZOLTAN KOVACS, UT Southwestern Medical Center — ^{89}Y in chelated form is potentially valuable in medical imaging because its chemical shift is sensitive to local factors in tumors such as pH. However, ^{89}Y has a low gyromagnetic ratio γ_n thus its NMR signal is hampered by low thermal polarization. Here we show that we can enhance the room-temperature NMR signal of ^{89}Y up to 65,000 times the thermal signal, which corresponds to 10 % nuclear polarization, via fast dissolution dynamic nuclear polarization (DNP). The relatively long spin-lattice relaxation time T_1 ($\sim$500 s) of ^{89}Y translates to a long polarization lifetime. The ^{89}Y NMR enhancement is optimized by varying the glassing matrices and paramagnetic agents as well as doping the samples with a gadolinium relaxation agent. Co-polarization of ^{89}Y-DOTA with a ^{13}C sample shows that both nuclear spin species acquire the same spin temperature T_s, consistent with thermal mixing mechanism of DNP. The high room-temperature NMR signal enhancement places ^{89}Y, one of the most challenging nuclei to detect by NMR, in the list of viable magnetic resonance imaging (MRI) agents when hyperpolarized under optimized conditions.

[1]This work is supported in part by the National Institutes of Health grant numbers 1R21EB009147-01 and RR02584.

4:42PM D21.00010 Raman spectroscopy as a diagnostic tool to detect head and neck squamous cell carcinoma in archived tissues , SUNEETHA DEVPURA, Wayne State University, SEEMA SETHI, Pathology, Karmanos Cancer Institute, JAGDISH S. THAKUR, Wayne State University, VAMAN M. NAIK, U of Michigan-Dearborn, RATNA NAIK, Wayne State University — Recently, many spectroscopic techniques are being tried for diagnostic applications. Among them Raman spectroscopy is one of the powerful non-invasive techniques which can differentiate between different biomolecular compositions of tissues on the basis of their vibrational spectra and hence can become an efficient diagnostic tool for detection of cancers. This technique has not yet been explored to study the head and neck squamous cell carcinoma (HNSCC) for archived tissues; here we report its results on HNSCC. Raman spectra were collected from three regions; normal, carcinoma in situ, and carcinoma. The Raman data was analyzed with chemometric methods of principal component analysis (PCA) and discriminant function analysis (DFA). Our preliminary results show that PCA and DFA analysis of Raman spectra can successfully distinguish the pathological states in archived HNSCC tissues. However, large Raman data set from many tissue sections is needed to validate these findings.

4:54PM D21.00011 Optical measurements of mechanical resonances in biological tissues via magnetic nanoparticle interrogation , VASILICA CRECEA, STEVEN ADIE, University of Illinois at Urbana-Champaign, AMY OLDENBURG, University of North Carolina at Chapel Hill, RENU JOHN, Indian Institute of Technology - Hyderabad, STEPHEN BOPPART, University of Illinois at Urbana-Champaign — We present a real-time phase-resolved optical coherence tomography-based technique that interrogates the mechanical properties of tissue phantoms with different elasticities as well as healthy and cancerous rat tissues, via the interaction of high susceptibility iron oxide nanoparticles that reside inside the samples and an external magnetic field. A chirped magnetic field selects the region of natural resonance in the probed samples as evidenced by scatterer displacements measured with nanometer-level sensitivity. This methodology, entitled magnetomotive optical coherence elastography (MM-OCE), which exploits frequency dependent viscoelastic response in biological media, has potential for detecting tissue pathologies.

5:06PM D21.00012 Imaging the Vector Magnetic Field of Magnetospirillum Gryphiswaldense by Optically Detected Magnetic Resonance using Nitrogen-Vacancy Centers in Diamond[1] , RICHELLE M. TEELING, YOUNG WOO JUNG, INHEE LEE, JUSTIN NORTH, ROBIN NAKKULA, ROHAN ADUR, EZEKIEL JOHNSTON-HALPERIN, MICHAEL G. POIRIER, P. CHRIS HAMMEL, The Ohio State University — Nitrogen vacancy centers in diamond are single-spin systems that are stable under ambient conditions with strong optical spin transitions, making them optimal for room-temperature detection of nanoscale magnetic fields using optically detected magnetic resonance (ODMR). We use these ensembles of diamond spins as a scanned probe magnetometer to map the field emitted by Magnetospirillum Gryphiswaldense, in vivo. These bacteria mineralize nanoscale magnetite particles in their internal vesicles. Imaging these living bacteria cells will serve as a strong foundation for the application of our ODMR technique to the medical field, where the bacteria can be used to synthesize functionalized magnetic particles which can be used as biomarkers and targeted drug-delivery systems.

[1]Funding Provided by the Center for Emergent Materials at the Ohio State University, an NSF MRSEC (Award Number DMR-0820414)

5:18PM D21.00013 Sub-Nanoparticle Femto Atometry: Measurement of Genome Lengths of Mammalian Tissues , CHRIS DRUEY, BOGDAN C. MAGLICH, ANNA Z. RADOVIC, California Science & Engineering Corp. — Measurement of porcine and bovine genome length, giga nucleotide base pairs, Gbp, was made by irradiating each tissue for 30' with neutrons of femto DeBroglie $\lambda \sim 10^{-15}$ m, which, unlike nanoparticles, interact only locally with atomic nuclei in nucleotide. O and C atoms were counted via γ rays emitted from (n, n' γ) reaction. By irradiating free dA, dC and T nucleotides for 30' we got response constant: (1,450 $\pm$ 44) γ/O. From 2 measurements we obtained 2.59 $\pm$ .05 and 3.19 $\pm$ .06 Gbp for porcine and bovine, respectively, consistent with 2.7 and 3 Gbp (errors not quoted) obtained by genome sequencing method that took 6 years each.

Monday, March 21, 2011 2:30PM - 5:30PM –
Session D22 DCMP: Metal Insulator Transition in VO2 D163

2:30PM D22.00001 The band structure of VO2 measured by angle-resolved photoemission[1] , LUCA MORESCHINI, Advanced Light Source, YOUNG JUN CHANG, ALS and Fritz-Haber Institut, DAVIDE INNOCENTI, ALS and University of Rome-Tor Vergata, ANDREW L. WALTER, ALS and FHI, YOUNG SU KIM, GEOFFREY GAINES, AARON BOSTWICK, JONATHAN DENLINGER, ELI ROTENBERG, ALS — The origin of the 340K metal-insulator transition (MIT) in VO2 is still under debate. the main reason is that no direct experimental verifications of the electronic structure of VO2 exist up to this point. The quality of the available single crystals is not sufficient for ARPES measurements, so that photoemission is limited to angle-integrated mode. New opportunities are offered by oxide films, on which data of equal or even higher quality have been reported (Saeki *et al.*, PRB 2009). WIth the *in situ* pulsed-laser-deposition (PLD) system available on beamline 7.0.1 at the Advanced Light Source we have grown VO2(001) films on a TiO2 substrate and measured the Fermi surface of the metallic phase. These results will permit a direct comparison with the existing band calculations and open the way to the study of the MIT as a function, e.g., of film thickness or electron doping with Cr.

[1]Work supported by U.S. DOE (DE-AC02-05CH11231 for ALS), the Max Planck Society, and the Swiss National Science Foundation (PBELP2- 125484).

2:42PM D22.00002 Electronic structure of strained vanadium dioxide thin films using soft X-ray spectroscopy , JUDE LAVEROCK, LOUIS PIPER, ANDREW PRESTON, BO CHEN, JAMES MCNULTY, KEVIN SMITH, Boston University, SALINPORN KITTIWATANAKUL, JIWEI LU, STUART WOLF, University of Virginia — Despite over five decades of intense investigation, the origin of the metal-insulator transition (MIT) in VO_2 still presents a challenge to explain. Whether the lattice (Peierls physics) or electron-electron correlations (Mott-Hubbard physics) are responsible for the MIT has been hotly debated; more recently, the general consensus has favored a co-operative description, in which both structural and correlation effects are important and sympathetic to the transition. Key to understanding such a co-operative picture has been the behavior of VO_2 under doping and strain. Here, we report recent soft X-ray measurements of strained VO_2 thin films grown on TiO_2(001) and (110) substrates. We employ X-ray absorption spectroscopy and X-ray emission spectroscopy to probe the changes in both the *unoccupied* and *occupied* partial density of states across the MIT, observing distinct changes in the V $3d$-O $2p$ hybridization. Additionally, the location in energy of the unoccupied $d_{\|}$ state in the insulating phase is found to be dependent on the lattice strain, in agreement with the predictions of recent dynamical mean-field theory calculations. Finally, our results are discussed in the context of the origin of the MIT in VO_2.

2:54PM D22.00003 Scanning Photocurrent Microscopy of VO_2 Nanobeams , CHRISTOPHER MILLER, MARK TRIPLETT, JOEL LAMMATAO, University of California, Davis, KEVIN WANG, DERRICK FU, JUNQIAO WU, University of California, Berkeley, DONG YU, University of California, Davis — Vanadium dioxide (VO_2) is a strongly correlated material that displays a near-room temperature metal-to-insulator transition ($\sim 68^oC$). This transition can be explored at the single domain level in single crystalline VO_2 nanobeams, where the material dimension is smaller than the characteristic domain size. Here we investigate the metal-insulator phase transition and its domain wall physics in single VO_2 nanobeam devices through scanning photocurrent microscopy. This technique, which measures the photocurrent as a function of the local photo-injection position, allows us to determine the band bending direction and the height of the Schottky barriers at each domain wall. Our results may shed light on the charge dynamics in strongly correlated materials and the metal-insulator phase transition mechanism.

3:06PM D22.00004 Conductivity anisotropy in strained VO_2 thin films, probed by THz Time Domain Spectroscopy[1] , MENGKUN LIU, mengkun@buphy.bu.edu, ELSA ABREU, JIWEI LU, KEVIN WEST, SALINPORT KITTIWATANAKUL, WENJING YIN, STUART WOLF, RICHARD AVERITT, 1DEPARTMENT OF PHYSICS, BOSTON UNIVERSITY, BOSTON MA COLLABORATION, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING, UNIVERSITY OF VIRGINIA, CHARLOTTESVILLE VA COLLABORATION, DEPARTMENT OF PHYSICS, UNIVERSITY OF VIRGINIA, CHARLOTTESVILLE VA COLLABORATION — We used THz time domain spectroscopy to measure the temperature and polarization dependent far-infrared conductivity of high quality strained VO_2 thin films epitaxially grown on (100) TiO_2 substrates. A large conductivity anisotropy is observed in the metallic phase of our VO_2 films with the conductivity along the rutile axis ∼30 times larger than the orthogonal direction. The MIT temperature also exhibits anisotropy with a value of 360K along the rutile c axis and 340K along the perpendicular direction. Our results are consistent with substrate induced strain modulation of the energy and bandwidth associated with the vanadium 3d orbitals.

[1]We would like to acknowledge sup- port from DOE-BES for this work under grant DE-FG02- 09ER46643, DE-FG02-00ER45799, and ETRI.

3:18PM D22.00005 X-ray induced photoconductivity in Vanadium Dioxide samples , SEBASTIAN DIETZE, JYOTI MOHANTY, MOSES MARSH, JONG WOO KIM, KEVIN WEST, IVAN K. SCHULLER, OLEG G. SHPYRKO, Department of Physics University of California, San Diego — Vanadium Dioxide (VO2) goes through a first-order phase transition at approximately 340K, exhibiting both an insulator to metal transition (IMT) and a structural phase transition (SPT), with a monoclinic (M1) insulating phase at low temperatures and a rutile (R) metallic phase at high temperatures. We show an anomalous behavior of x-ray induced persistent photoconductivity (PPC) well below the temperature induced phase transition in VO2 devices. We present conductivity and X-ray Diffraction (XRD) measurements, revealing a large enhancement of conductivity due to photo-induced carriers. Moreover, with the addition of nominal electric fields, we are able to fully transition into the rutile metallic phase at room temperature. This effect is completely reversible, allowing the monoclinic insulating phase to be recovered via annealing.

3:30PM D22.00006 Electric field-induced breakdown of the Mott insulating state in V2O3 nanostructures , JUSTIN BROCKMAN, Stanford University, LI GAO, NAGAPHANI AETUKURI, BRIAN HUGHES, CHARLES RETTNER, MAHESH SAMANT, KEVIN ROCHE, STUART PARKIN, IBM Almaden Research Center — The origin of the electric field-induced breakdown of the Mott insulating state in vanadium sesquioxide (V2O3) nanostructures is of considerable interest. We have prepared high quality, epitaxial films of V2O3 on (0001)-oriented sapphire substrates by oxygen plasma-assisted thermal evaporation. Lateral, two-terminal nanostructures were patterned by electron beam lithography. The nanostructures displayed strong metal-to-insulator transitions upon cooling to below ∼150K. Modest voltages applied across the devices drive the films into a conducting state. We discuss the role of temperature, applied voltage, device size, and potential Joule heating effects on the switching process, as well as implications for the underlying mechanism involved.

3:42PM D22.00007 Gatability of vanadium dioxide single crystal nanobeams and hydrogen doping[1] , JIANG WEI, HENG JI, DOUGLAS NATELSON, Rice University — Vanadium dioxide is famous for its dramatic metal insulator transition, exhibiting up to 4 or 5 orders magnitude change in conductivity. It is also known to be nongatable, although in the insulating phase it behaves like a semiconductor with 0.5-0.7 eV energy gap. With no sign of gating effects using conventional dielectric materials, such as SiO_2, Al_2O_3 and HfO_2, ionic liquids were used as the gating medium. Ionic liquids form electric double layers (EDL) and could possibly exert an electric field as high as 10^9V/m on the interface of ionic liquid and single-crystal vanadium dioxide nanobeam. No gating effect was observed in the vanadium dioxide device. On the other hand, we found that under positive gate voltage the hydrogen ions originating from trace amounts of water diffuse into the vanadium dioxide crystal, acting as dopants. By controlling the gate voltage and temperature, the insulating phase's conductivity can be reversibly increased up to 2-3 orders magnitude by this process.

[1]Supported by Robert A.Welch Foundation and Department of Energy award DE-FG02-06ER46337.

3:54PM D22.00008 Dependence of VO_2 thin-film metal-insulator transition on its intrinsic impurities , CHANGHONG CHEN[1], YONG ZHAO, ZHAOYANG FAN, Nano Tech Center and Department of Electrical and Computer Engineering, Texas Tech University — We present variation in strain, metal-insulator transition temperature (T_{MIT}), activation energy (ΔE_a), and charge carrier type in the insulating phase of (011) preferred polycrystalline (Poly-) and multidomain (020) epitaxial (Epi-) VO_2 films grown at different temperature (T_S), to produce variable intrinsic impurities. Both the Poly- and Epi-VO_2behave n-type conductivity when grown at relative low T_S. As T_S increases, acceptor density of impurity increases to alter conductivity from n- to p-type in the Poly-VO_2, while conductive n-type still keeps in the Epi-VO_2 with increased donor density. Moreover, the strain along monoclinic a_m axis dramatically reverses from tensile to compressive in both the Poly- (848 K< T_S <873 K) and Epi-VO_2(873 K< T_S <898 K), and eventually tend to relaxation again in the Poly-VO_2($T_S \geq$898 K) in particular. Consequently, T_{MIT} decreases with increasing the carrier density independent of the conductive type, and low-temperature ΔE_a is associated with the strain. The larger strain leads to higher ΔE_a, while the relaxed strain produces saturated or the minimum ΔE_a in the Poly- or Epi-VO_2.

[1]Wuhan National Laboratory for Optoelectronics, Huazhong University of Science and Technology

4:06PM D22.00009 Manipulation of avalanche characteristics in nanoscaled VO_2 devices[1] , SIMING WANG, KEVIN G. WEST, IVAN K. SCHULLER, Department of Physics and Center for Advanced Nanoscience, University of California San Diego, La Jolla CA 92093 — The temperature driven metal insulator transition (MIT) in nanoscaled VO_2 devices occurs through a series of resistance jumps ranging over two decades in magnitude. A power law distribution of the jump sizes, demonstrates that the transition is caused by avalanches across the percolation transition. We investigate the effect of a DC write current on the intrinsic behavior of the MIT transition in nanoscaled VO_2 devices. We find an increase in the maximum resistance jump size by as much as a factor of 10x after application of a DC write current at room temperature. Interestingly, we find no significant changes in the exponent of the power law distribution as a function of an applied DC write current. The observations suggest that the DC current changes the intrinsic properties of the VO_2 thin film and may be related to spatial confinement which leads to an increase in the maximum resistance jump size.[2]

[1]Work supported by US-DOE.

[2]Hong-Ying Zhai, J.X. Ma, D.T. Gillaspie, X.G. Zhang, T.Z. Ward, E.W. Plummer, and J. Shen, Phys. Rev. Lett. **97** 167201 (2006).

4:18PM D22.00010 stoichiometry engineering of metal-insulator transition in suspended single crystalline vanadium dioxide nanobeams , SHIXIONG ZHANG, IN SOO KIM, LINCOLN J. LAUHON, Department of Materials Science and Engineering, Northwestern University — While the metal-insulator transition (MIT) in VO2 bulk and thin films has been investigated for several decades, recent studies of nanobeams have provided new opportunities to investigate and manipulate the metal-insulator transition and structural domain formation in a correlated manner. We will describe the electrical and structural characterization of suspended single crystal VO2 nanobeams grown/annealed under various conditions. Annealing nanobeams under reducing conditions led to the stabilization of single-crystal rutile nanobeams at room temperature, in some cases suppressing the MIT temperature from 340 K down to below 100 K. Re-annealing under oxidizing conditions led to a recovery of the transition temperature for stoichiometric VO2. Furthermore, growth under oxidizing conditions produced the Mott insulator M2 phase and an intermediate M3. Systematic annealing studies enabled the generation of a pseudo-phase diagram with dimensions of stoichiometry and temperature. The temperature dependence of the electrical resistivity of rutile nanobeams above the transition temperature will also be discussed.

4:30PM D22.00011 Tungsten as a substitutional dopant and its effect on ultrafast switching of vanadium dioxide , JOYEETA NAG, KANNATASSEN APPAVOO, Vanderbilt University, WEIDONG LUO, Lawrence Berkeley National Laboratory and Oak Ridge National Laboratory, GERD DUSCHER, Univeristy of Tennessee, Knoxville and Oak Ridge National Laboratory, SOKRATES PANTELIDES, Vanderbilt University and Oak Ridge National Laboratory, RICHARD HAGLUND, Vanderbilt University — VO_2 undergoes a metal-insulator transition (MIT) at 340K accompanied by a structural change from monoclinic (M1) to tetragonal (R). We have grown W-doped VO_2 films on glass and epitaxially on sapphire substrates and have characterized them by SEM, white light transmission, RBS, XRD, and Z-STEM. These provide direct experimental evidence that W acts as a substitutional dopant in the VO_2 lattice in addition to lowering the transition temperature. From GGA+U, DFT-based simulations we have also calculated the formation energy of substitutional W in VO_2, and relative stability of M1 and R phases before and after doping. Ultrafast pump-probe measurements at 800nm with varying pump fluences show that doped VO_2 switches at substantially lower fluences than undoped VO_2, indicating that the W dopant provides additional conduction-band electrons, thus altering the photo-induced dynamics of the phase transition.

4:42PM D22.00012 Control of the metal-insulator transition in vanadium dioxide nanobeams[1] , JAE HYUNG PARK, SERKAN KASIRGA, University of Washington, JIANG WEI, Rice University, NICHOLAS NOLL, VINCENT ROMA, DAVID H. COBDEN, University of Washington, DEPARTMENT OF PHYSICS TEAM — Single-crystal nanobeams of vanadium dioxide, which are smaller than the characteristic domain size, exhibit a more reproducible and controllable metal-insulator transition (at around 67 degrees C) than bulk samples. We are exploiting this fact to perform systematic studies of the intrinsic properties of the phases involved, the phase transition, and the interphase wall, as well as to control the transition temperature. For these purposes it is necessary to have high quality crystals and to apply uniform strain. We are therefore investigating and improving the procedure of VO2 small-crystal growth by vapor phase transport, while developing experimental techniques in which thin nanobeams can be suspended across adjustable-widths gaps on silicon structures. The latter will enable application of strain purely along the tetragonal c-axis, to tune the transition, while simultaneously carrying out transport, optical and scattering measurements.

[1]The work is sponsored by the Department of Energy (BES contract number DE-SC0002197) and the Army Research Office (contract number 956073-PH).

4:54PM D22.00013 Electrical properties of vanadium dioxide devices for micro-electronic applications making use of metal-insulator phase transitions[1] , KOEN MARTENS, IULIANA P. RADU, KULeuven - IMEC, SOFIE MERTENS, CHRISTOPH ADELMANN, XIAOPING SHI, HILDE TIELENS, MARC SCHAEKERS, CEDRIC HUYGHEBAERT, SVEN VAN ELSHOCHT, IMEC, STEFAN DE GENDT, MARC HEYNS, KULeuven - IMEC, JORGE A KITTL, IMEC — In principle the metal-to-insulator transition offers prospects for use in an electronic switch. This study investigates the properties of VO_2 test devices to evaluate VO_2's potential use in micro-electronic applications such as a memory, two-terminal selector or transistor device. Vanadium dioxide thin films were produced by thermal oxidation of vanadium and the physical properties of these layers were investigated. Electrical properties of concentric two-terminal vanadium dioxide structures will be discussed such as current-voltage behavior, switching behavior and contact formation to VO_2 with different metals and implications such as Fermi-level pinning and Schottky-type behavior for different metals.

[1]The FWO is acknowledged.

5:06PM D22.00014 Metal-insulator transition mechanism in VO2 under electric bias , YONG ZHAO, JI HAO[1], CHANGHONG CHEN, ZHAOYANG FAN, Nano Tech Center and Department of Electrical and Computer Engineering, Texas Tech University — It is in controversy if metal-insulator phase transition (MIT) of VO_2 can be triggered by electric field/current. In this work, a series of two terminal devices with different gap length, width, and multiple-channel configurations were fabricated on epitaxially grown VO_2 thin films, to study its MIT mechanism under the electric bias. Micro-Raman spectroscopy was used to differentiate the rutile metallic phase from the monoclinic insulator phase. Voltage-current measurements indicated that a temperature-dependent critical current density (J_c) is required to induce MIT. Under the electric bias, the phase transition was observed to be a percolation process until a clear current path (or filament) is formed between the electrodes. Afterwards the pure metallic phase was identified along the current path, while outside of it become pure insulator phase. As current varies, current path width is proportionally changed to keep a constant current density. These observations indicate that a J_c is necessary to maintain the metallic phase current path. Contributions of the current effect and Joule heat effect to the phase transition were discussed.

[1]Wuhan National Laboratory for Optoelectronics, Huazhong University of Science and Technology

5:18PM D22.00015 Electric-field-driven phase transition in vanadium dioxide , B. WU, LPEM, ESPCI-ParisTech-CNRS-UPMC, 10 rue Vauquelin, Paris 05, France / National Laboratory for Superconductivity, IOP, CAS, Beijing 100190, P.R.China, A. ZIMMERS, H. AUBIN, LPEM, ESPCI-ParisTech-CNRS-UPMC, 10 rue Vauquelin, Paris 05, France, R. GOSH, Y. LIU, R. LOPEZ, Department of Physics and Astronomy, University of North Carolina at Chapel Hill, Chapel Hill, North Carolina 27599, USA — In recent years, various strongly correlated materials have shown sharp switching from insulator to metallic state in their I(V) transport curves. Determining if this is purely an out of equilibrium phenomena (due to the strong electric field applied throughout the sample) or simply a Joule heating issue is still an open question. To address this issue, we have first measured local I(V) curves in vanadium dioxide (VO_2) Mott insulator at various temperatures using a conducting AFM setup and determined the voltage threshold of the insulator to metal switching. By lifting the tip above the surface (>35nm), we have then measured the purely electrostatic force between the tip and sample surface as the voltage between these two was increased. In a very narrow temperature range (below 360K), a tip height range (below 60nm) and a voltage applied range (above 8V), we observed switching in the electrostatic force (telegraphic noise vs. time and vs. voltage). This purely electric field effect shows that the switching phenomenon is still present even without Joule heating in VO_2.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D23 DMP: Focus Session: Search for New Superconductors I: Exploring Emergent Phases D165

2:30PM D23.00001 Phase Transitions in CuAs-based $K_xSr_{1-x}Cu_4As_2$ System , BING LV, BERND LORENZ, MELISSA GOOCH, FENG CHEN, LIANGZI DENG, CHING-WU CHU[1], Dept. of Physics and TcSUH, University of Houston — Inspired by the superconductivity with a $T_c \sim 3.5$ K reported by Han et al. in Cu-based $LiCu_2P_2$, the Cu-based compound $SrCu_4As_2$, which has a more complex CuAs layers structure sandwiched by Sr layers, was synthesized and characterized. The magnetoresistance measurements show two anomalies around ∼140K and ∼60K, respectively, which is also consistent with the results of specific heat measurement. Systematically studies of K-doping into $SrCu_4As_2$ system are carefully investigated at ambient and high pressures and no superconductivity has been found in the $K_xSr_{1-x}Cu_4As_2$ system down to 2K, although superconductivity might occur at lower temperature in this system. The overall pressure and doping effects on the magnetic and transport properties of the compounds will be presented and discussed.

[1]also at: Lawrence Berkeley National Laboratory

2:42PM D23.00002 Synthesis and Characterization of ACu_4Pn_2, with A = alkaline and Pn = As and Sb , L.Z. DENG, BING LV, Y.Y. XUE, C.W. CHU[1], Department of Physics and TcSUH, University of Houston — A large number of the Cu-based layer compounds have been known to exist since the 1970's: some display structures similar to the Fe-based pnictide superconductors, such as the 111 and 122 phases. Unfortunately, other than their structures, reports on their physical properties are generally sparse. Only recently observation of superconductivity with a $T_c \sim 3.5$ K was reported by Han et al. in $LiCu_2P_2$ that displays a 122 structure. It was suggested that a more complex layer structure in pnictides may favor higher T_c as in the case of cuprates. We have therefore examined systematically ACu_4Pn_2 (142), with A = alkaline and Pn = pnictigen which has a more complicated layer substructure than the 1111, 111, 122 or 11 homologues. We have synthesized ACu_4Pn_2, with A = Li, Na, K, Rb and Cs and Pn = As and Sb, some of which were made for the first time. The magnetic, electrical, calorimetric and thermal electric properties were determined at ambient pressure and compared. High pressure was also applied to some of the compounds. The results will be presented and discussed.

[1]Also at: Lawrence Berkeley National Laboratory

2:54PM D23.00003 Superconductivity and Competing Ordered Phase in RuPn (Pn = As, P) , DAIGOROU HIRAI, TOMOHIRO TAKAYAMA, Dept. of Advanced Materials, Univ. of Tokyo, DAISUKE HASHIZUME, AYAKO YAMAMOTO, Riken, HIDENORI TAKAGI, Dept. of Advanced Materials, Univ. of Tokyo — Unconventional superconductivity likely manifests itself when some competing electronic phases are suppressed down to zero temperature such as cuprates and iron-pnictide superconductors. Therefore, the correlated metallic state neighboring a competing electronic ordering can be a promising playground for unconventional superconductivity. Here we report superconductivity emerging adjacent to electronically ordered phases of RuPn (Pn = As, P). We found that RuAs(P) exhibits phase transitions at 240 (265) K, which is discerned as a drop of magnetic susceptibility or a resistivity upturn. Such anomalies can be suppressed by substituting Rh to the Ru site. Accompanied by the disappearance of the electronic order, superconductivity was found to emerge below 1.8 K and 3.8 K for RuAs and RuP, respectively. The superconductivity in Rh substituted RuPn, which neighbors a competing electronic order, might exhibit an exotic pairing state as seen in the unconventional superconductors known to date.

3:06PM D23.00004 Towards New and Higher Temperature Superconductors via Theory Assisted Synthesis[1] , MEIGAN ARONSON, Stony Brook University and Brookhaven National Laboratory — We discuss here a new methodology where electronic structure calculations are integrated with the synthesis of new superconducting materials, with the objective to design and realize new lamellar superconductors with high onset temperatures, and to rigorously test the apparent association of high temperature superconductivity with electron delocalization transitions occurring at quantum critical points. Since lamellar superconductors like the cuprates and iron pnictides are comprised of functional layers where superconductivity resides and charge reservoir layers that determine the electron count in the functional layers, we will use realistic electronic structure calculations to assess which transition metal monopnictides are closest to electron delocalization, and hence optimal for superconductivity. Optical conductivity and photoemission measurements will be used to compare the real and calculated electronic structures. We report initial results on electron and hole doped LaMnPO.

[1]This research is carried out in collaboration with G. Kotliar, D. Basov, and H. Tjeng under the auspices of an NSSEFF fellowship administered by the AFOSR.

3:42PM D23.00005 Gap physics of the doped semiconductor (Ca,F):LaMnPO[1] , J.W. SIMONSON, M.C. ARONSON, Physics and Astronomy Dept., Stony Brook University — Single crystals of $Ca_xLa_{1-x}MnPO$ and $LaMnPO_{1-y}F_y$ (x = 0 to 0.50, y = 0 to 0.40) were synthesized to study the effect of Ca and F doping on LaMnPO, which is isostructural with several recently discovered Fe-based superconductors. The inclusion of F into the lattice was confirmed with single crystal XRD, showing a systematic reduction in unit cell volume with dopant content, in agreement with published accounts of similar compounds. Little change from undoped LaMnPO was observed in the resistivity of Ca doped crystals, while doping with successively higher concentrations of F yielded a systematic enhancement of conductivity. Nonetheless, all resistivity measurements were semiconducting, suggesting that E_F remains pinned within the gap regardless of dopant concentration. Activated behavior was observed, with activation energies falling below 100 meV, substantially less than the 1 eV optical gap. At low temperatures, the resistivity of all compositions exhibited temperature dependence in accord with variable range hopping, suggesting that transport is dominated by disordered and localized states at the Fermi level.

[1]Research supported by a DOD National Security Science and Engineering Fellowship via the AFOSR

3:54PM D23.00006 Properties of layered iron oxychalcogenides with checkerboard structure[1] , LIANG L. ZHAO, DANIEL WARD, DOUGLAS NATELSON, EMILIA MOROSAN, Department of Physics and Astronomy, Rice University, Houston TX 77005 — The layered iron oxychalcogenides $La_2O_3Fe_2X_2$ (X = S, Se) have a unique checkerboard-like Fe_2OX_2 sublattice. Their Mott insulating behavior makes them promising candidates for novel superconductors. In this talk, we present results on the isostructural $A_2F_2Fe_2OS_2$ (A = Sr, Ba) compounds. Both pure and doped samples are characterized by magnetization, resistivity, heat capacity and Raman spectroscopy measurements. In addition to the previously reported antiferromagnetic transition around $T_N \approx 100$ K, we observed another phase transition in the ordered state, as well as a possible structural phase transition near room temperature. A change in the excitation gap at the high temperature (structural) phase transition is indicated by the temperature dependent resistivity.

[1]This work is supported by AFOSR-MURI

4:06PM D23.00007 Development of high-temperature solutions for the crystal growth of chalcogenide and pnictide bearing compounds[1] , XIAO LIN, RONGWEI HU, SERGEY BUD'KO, PAUL CANFIELD, Iowa State University/Ames Lab — With the discovery of superconductivity in the FeAs and FeSe/S based materials and proposed topological insulators in a variety of Te and Se based compounds the need to develop crystal growth techniques that readily incorporate and simultaneously control volatile (and often toxic) elements is of growing importance. In this talk we will review our initial efforts to develop versatile solution growth techniques for single crystal growth of P, As, S, Se and/or Te containing compounds. We will present our results on our use of S-bearing solutions to grow binary and ternary sulphides as well as the development of hybrid solutions the components of which each allow for the incorporation of hard to dissolve elements.

[1]Work was supported by AFOSR-MURI grant #FA9550-09-1-0603.

4:18PM D23.00008 ABSTRACT WITHDRAWN –

4:30PM D23.00009 Bulk superconductivity in intercalated M_xZrTe_3 (M=Cu, Ni) , XIANGDE ZHU, HECHANG LEI, CEDOMIR PETROVIC, Brookhaven National Laboratory — We report the bulk superconductivity of 3d transition metal (e.g. Cu, Ni) intercalated $ZrTe_3$ single crystals, M_xZrTe_3 (M=Cu, Ni). ZrTe3 shows charge density wave (CDW) transition at T_{CDW}=63K and the CDW nesting vector q_{CDW}=(1/14,0,1/3) (reciprocal space). It is metallic below 300K with an anomaly due to CDW transition and becomes filamentary superconductor below 2 K. The derived superconducting parameters indicate that M_xZrTe_3 are bulk type-II superconductors and can be depicted in the framework of Bardeen-Cooper-Schrieffer (BCS) scenario. Intercalation depresses the CDW transition and enhances the superconductivity.

4:42PM D23.00010 New layered oxuchalcogenide $La_2O_2Mn_2OSe_2$, HECHANG LEI, CEDOMIR PETROVIC, Brookhaven National Laboratory — We report a new $La_2O_2Mn_2OSe_2$ and investigate its physical properties. It is a member of $Ln_2O_2Tm_2OCh_2$ (Ln= rare earth, Tm=Fe, Co, and Ch=S, Se). The structure of these compounds can be described as an alternate stacking of fluorite type $[Ln_2O_2]^{2+}$ or $[A_2F_2]^{2+}$ layers and anti-CuO_2-type $[Tm_2OCh_2]^{2-}$ layers (anti-perovskite type). $La_2O_2Mn_2OSe_2$ is the first manganese-base compound with anti-CuO_2-type layers. It is a ferromagnetic (FM) Mott insulator exhibiting several successive magnetic transitions. The magnetic properties are different from other compounds with this structure.

4:54PM D23.00011 Physical Properties of $CaFe_4As_3$ Single Crystals , AMAR KARKI, YIMIN XIONG, JIANNENG LI, SHANE STADLER, GREGORY MCCANDLESS, JULIA CHAN, RONGYING JIN, Louisiana State University — New compound $CaFe_4As_3$ crystallizes in an orthorhombic structure with Fe_2As_2 layers aligned along b direction but a rectangular cross-section in *ac* plane. The needle-shaped $CaFe_4As_3$ single crystals were grown and are found to undergo two successive phase transitions occurring at $T_1 \sim 90$ K and $T_2 \sim 27$ K, respectively. At T_1 the electrical resistivity increases and magnetic susceptibility decreases in both parallel and perpendicular to b directions consistent with the scenario of spin-density-wave formation. At T_2, resistivity decreases sharply at T_2 with hysteresis while magnetic susceptibility increases along either b direction or *ac* plane. The underlying physics will be discussed by taking into account other physical properties.

5:06PM D23.00012 Superconductivity in SnO: a Nonmagnetic Analogue to Fe-based Superconductors , DANIEL KHOMSKII, M.K. FORTHAUS, K. SENGUPTA, O. HEYER, Koeln University, Germany, N.E. CHRISTENSEN, A. SVANE, Aarus University, Denmark, K. SYASSEN, Max-Plank-Institut fuer Festkoerperforschung, Stuttgart, Germany, T. LORENZ, M.M. ABD-ELMEGUID, Koeln University, Germany — We found that under pressure SnO with α-PbO structure, the same structure as in many Fe-based superconductors, e.g. β-FeSe, undergoes a transition to a superconducting state for $p \geq 6$ GPa with a maximum T_c of 1.4 K at $p = 9.3$ GPa. The pressure dependence of T_c reveals a dome-like shape and superconductivity disappears for $p > 16$ GPa. It is further shown from band structure calculations that SnO under pressure exhibits a Fermi surface topology similar to that reported for some Fe-based superconductors and that the nesting between the hole and electron pockets correlates with the change of T_c as a function of pressure. M.K. Forthaus et al., Phys.Rev.Lett. **105**, 15701 (2010)

5:18PM D23.00013 Development of iron pnictides with very thick perovskite-type blocking layers , HIRAKU OGINO, SHINYA SATO, NAOTO KAWAGUCHI, YASUAKI SHIMIZU, KENJI MACHIDA, AKIYASU YAMAMOTO, KOHJI KISHIO, JUN-ICHI SHIMOYAMA — Recently we have discovered several new layered iron pnictides having extremely thick blocking layers [1]. These compounds have up to 5 sheets of perovskite-type layers between iron pnictide layers. Similar to LiFeAs, these compounds showed bulk superconductivity without intensive carrier doping, and the Tc of the compounds are 40 K-class. On the other hand, the relationship between Tc and the iron-plane interlayer distance suggested that Tc of the iron based superconductor is basically determined by the local structure of Fe2As2 layer. It is thought that there is still considerable room for the development of new layered iron pnictide compounds, due to the structural and chemical flexibility of the blocking layer. However, the results suggest that optimization of the local structure of Fe2As2 layers and the dimensionality of the crystal structure may not lead to further enhancement of Tc. Their structural features as well as physical properties will be presented.

[1] H. Ogino et al., APL 97 (2010) 072506

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D24 DCOMP: Focus Session: Quantum Transport Simulations and Computational Electronics – Nanostructures D167

2:30PM D24.00001 Transient response of a quantum point contact due to the coupling with reservoirs[1]

, BOZIDAR NOVAKOVIC, IRENA KNEZEVIC, University of Wisconsin-Madison — Transient response is important for better understanding of the DC and AC response of open quantum systems connected to large charge reservoirs. In this study we calculate the transient response of a quantum point contact (QPC) due to its coupling with reservoirs. The QPC, an open system, is modeled by a solution to the coupled, two-dimensional Schrödinger and Poisson equations using a discrete subset of the normal modes basis. The normal modes are projected onto the traveling-wave solutions that match the incoming reservoir plane waves. The occupation of the open system states carries the information about the time evolution and is calculated by solving a coarse-grained quantum master equation with suitably defined open system/contact interaction Hamiltonians. The final electronic transient response is obtained by enforcing the current continuity across the open system/contacts boundaries through a time-dependent reservoir drift wavevector. We investigate the transient current response to a voltage step and its dependence on the gate bias and relaxation time in the contacts.

[1]This work has been supported by the NSF, award ECCS-0547415.

2:42PM D24.00002 Open boundary-conditions using empirical pseudopotentials in quantum transport[1]

, BO FU, MASSIMO FISCHETTI, The University of Texas at Dallas — As device dimensions approach the 10 nm length-scale, the study of electronic transport requires the knowledge of an accurate band structure and of transport equations transcending the semiclassical Boltzmann picture. Having as our ultimate goal the study of dissipative quantum transport using the Pauli Master Equation, in this talk we address the numerical issue of how to formulate and implement numerically the open-boundary-condition Schrödinger equation within an empirical-pseudopotential full- band framework. Results regarding ballistic transport in Si nanowires will be presented.

[1]SRC

2:54PM D24.00003 Quantum Transport in Crossbar Devices

, BRANDON COOK, PETER DIGNARD, KALMAN VARGA, Vanderbilt Univeristy — Electronic devices with crossbar geometries have recently been fabricated with nanoscale features (Zhong. et al, Science Vol. 302). Consisting of a two dimensional grid of wires, devices have been formed with a variety of components including carbon nanotubes and semiconductor nanowires. These devices are assumed to operate classically, but as the dimensions of the device shrink consideration of quantum effects becomes necessary. We consider a single junction between two wires up to a four by four grid of wires. Through a series of calculations with atomistic first-principles, tight-binding and analytic models of multi-terminal devices we demonstrate the presence of unique behavior, such as interference effects, not present in classical models. It is expected that exploitation of these effects will useful in the creation of circuit components.

3:06PM D24.00004 Empirical Pseudopotential Approach to Semiclassical and Quantum Electronic Transport in Nanometer-scale Structures

, MASSIMO FISCHETTI, University of Texas at Dallas — The study of electronic transport in semiconductor structures requires an accurate knowledge of the kinematics ($i.e.$, band structure) and of the dynamics ($i.e.$, transport equations and collision processes). As the VLSI technology looks at various sub-10 nm structures as alternatives to the traditional Si CMOS, neither the conventional bulk band structure of the semiconductor nor the semiclassical (Boltzmann) transport equations can be used with confidence to treat the kinematics and dynamics of electronic transport, the former because of size-dependent (quantum confinement) and interface/surface dependent band structure effects; the latter because of the possibility of quantum interference effects at this length scale. Here we will show that empirical pseudopotentials – obtained from the literature and adjusted to yield correct workfunctions, band-alignment, and strain effects – can be used to obtain a sufficiently accurate (as compared to first-principle results) band structure of several systems of technological interest ($e.g.$, thin Si and Ge layers, III-V hetero-layers, nanowires, graphene nanoribbons and C nanotubes). Using this information, semiclassical transport is studied using a Monte Carlo technique and calculating the scattering rates consistently with the band structure information. In some cases, such as in considering scattering with interface and line-edge roughness, the pseudopotential themselves can be used to obtain accurate scattering potentials. The case of high-field transport in Si inversion layers is discussed, showing how the band-structure near the X symmetry point induces a lower saturated electron velocity. Finally, we discuss the wave equation and open boundary conditions which must be employed to handle ballistic quantum transport accounting for the full band structure. Dissipative transport is discussed in the context of a Master equation approach, illustrating this approach with examples ranging from double-gate FETs to Si nanowires.

3:42PM D24.00005 Self-Consistent Monte Carlo Study of the Coulomb Interaction under Nano-Scale Device Structures[1]

, NOBUYUKI SANO, University of Tsukuba — It has been pointed that the Coulomb interaction between the electrons is expected to be of crucial importance to predict reliable device characteristics. In particular, the device performance is greatly degraded due to the plasmon excitation represented by dynamical potential fluctuations in high-doped source and drain regions by the channel electrons. We employ the self-consistent 3D Monte Carlo (MC) simulations, which could reproduce both the correct mobility under various electron concentrations and the collective plasma waves, to study the physical impact of dynamical potential fluctuations on device performance under the Double-gate MOSFETs. The average force experienced by an electron due to the Coulomb interaction inside the device is evaluated by performing the self-consistent MC simulations and the fixed-potential MC simulations without the Coulomb interaction. Also, the band-tailing associated with the local potential fluctuations in high-doped source region is quantitatively evaluated and it is found that the band-tailing becomes strongly dependent of position in real space even inside the uniform source region.

[1]This work was partially supported by Grants-in-Aid for Scientific Research B (No. 2160160) from the Ministry of Education, Culture, Sports, Science and Technology in Japan.

3:54PM D24.00006 Oxygen vacancy mediated dielectric breakdown in ultrathin high-k gate dielectric stacks

, BLANKA MAGYARI-KOPE, YOSHIO NISHI, Stanford University — The reliability of the high-k gate stack becomes a significant challenge with the continuous scaling of the metal-oxide-semiconductor-field-effect-transistors, due to deposition techniques of ultrathin oxides and defects in the gate stack. One of the key problems associated with ultrathin oxide layers is the degradation of the gate oxides under electrical stress, due to traps generated by oxygen vacancies present in these materials. First principles methods based on density functional theory combined with non-equilibrium Green's function calculations are employed to calculate the tunneling current through ultrathin oxide layers of HfO_2 and SiO_2 in a gate stack structure with TiN metal electrode. Model systems that incorporate the atomistic description of a conductive filament formation due to ordering of oxygen vacancies in the oxide layers and the oxide-oxide interface of the gate stack were investigated. The microscopic effects of defects ordering on the electronic transport through the gate oxides are analyzed and discussed.

4:06PM D24.00007 Electron-phonon coupling in semiconductors and their nanostructures: effect on transport properties , JELENA SJAKSTE, PAOLA GAVA, NATHALIE VAST, Ecole Polytechnique, Laboratoire des Solides Irradiés, CEA-DSM-DRECAM, CNRS, 91128 Palaiseau, France, VALERIY TYUTEREV, Tomsk State Pedagogical University, Tomks, Russia — Parameter-free description of the electron-phonon coupling is crucial for the simulation of the electron and thermal transport in materials, especially nanostructured ones. Recently, we have developed an *ab initio* approach which allows to calculate the electron-phonon constants and scattering times for collisions of carriers in the conduction band with short-wavelength phonons [1,2]. We will present our results on the electron-short-wavelength phonon interaction in silicon, which enables us, on one hand, to shed new light on the transitions between shallow donor levels in doped Si [2], and, on the other hand, to improve the description of its electronic mobility [3]. Finally, we will discuss the effect of the material nanostructuring on the electron-phonon coupling constants, e.g. in semiconducting superlattices.

[1] J. Sjakste, N. Vast, V. Tyuterev, Phys. Rev. Lett. 99, 236405 (2007).
[2] V. Tyuterev, J. Sjakste, N. Vast, Phys. Rev. B 81, 245212 (2010)
[3] Z. Wang, S. Wang, S. Obukhov, N. Vast, J. Sjakste, V. Tyuterev, N. Mingo, submitted (2010)

4:18PM D24.00008 Ballistic Spin Field Effect Transistor Based on Silicon Nanowires[1] , DMITRI OSINTSEV, VIKTOR SVERDLOV, ZLATAN STANOJEVIC, SIEGFRIED SELBERHERR, Institute for Microelectronics, TU Wien — We investigate the properties of ballistic spin field-effect transistors build on silicon nanowires. An accurate description of the conduction band based on the $\mathbf{k}\cdot\mathbf{p}$ model is necessary in thin and narrow silicon nanostructures. The subband effective mass and subband splitting dependence on the nanowire dimensions is analyzed and used in the transport calculations. The spin transistor is formed by sandwiching the nanowire between two ferromagnetic metallic contacts. Delta-function barriers at the interfaces between the contacts and the silicon channel are introduced. The major contribution to the electric field-dependent spin-orbit interaction in confined silicon systems is due to the interface-induced inversion asymmetry which is of the Dresselhaus type [1]. We study the current and conductance through the system for the contacts being in parallel and anti-parallel configurations. Differences between the [100] and [110] orientated structures are investigated in details.

[1] M.O. Nestoklon *et al., Phys.Rev.B* **77**, 155328 (2008); M. Prada *et al.*, cond-mat 0908.2417.

[1]This work is supported by the European Research Council through the grant #247056 MOSILSPIN

4:30PM D24.00009 Junctionless nanowire field-effect transistor versus inversion mode devices , BART SORÉE, IMEC, Kapeldreef 75, B-3001 Leuven, Belgium. Universiteit Antwerpen, Physics department, Groenenborgerlaan 171, B-2020 Wilrijk, Belgium, ANH-TUAN PHAM, DRIES SELS, AN DE KEERSGIETER, WIM MAGNUS — Several years ago, a novel device concept was proposed : the nanowire (NW) iJFET [1]. Today, this device concept is being explored by several research teams [1-3] and is also known as the pinch-off FET (POFET) or junctionless transistor. The most important advantage of the junctionless transistor is the uniform doping throughout source, channel and drain which greatly simplifies its fabrication. We have performed modeling and simulations to compare the performance of the junctionless pinch-off FET with that of inversion mode devices. In order to make the comparison, we address the regime of thick and long nanowires through analytical modeling of the current- voltage characteristics, while for long and thin nanowires we perform dissipative transport modelling to obtain the low-field mobility. Finally, ballistic transport modelling is performed using the sub band decomposition method for ultra- short nanowires.

[1] B. Sorée, et al., Journal of Computational Electronics, vol.7, issue 3, 380-383 2008.
[2] B. Sorée, et al., Nanoelectronics days 2010, Aachen, Germany.
[3] J.-P. Colinge, et al., Nature Nanotechnology 5, 225-229, 2010

4:42PM D24.00010 Gap suppression and delocalization of 1D electron gas driven by a strong AC electric field , KATHLEEN E. HAMILTON, LEONID P. PRYADKO, UCR — We will argue that a strong AC electric field can coherently suppress a band gap in a high-mobility one-dimensional wire. At half-filling, the expected effect is delocalization of the carriers, in contrast to Stark localization at low frequencies, or Dynamical Destruction of Tunneling at frequencies exceeding the bandwidth. Another effect of the gap suppression is the doubling of the Bloch oscillations' period. We support these expectations with numerical simulations of the non-linear current response for several model systems driven by a combined high and low-frequency electric field.

4:54PM D24.00011 Modeling of Phonon-assisted Zener Tunneling in Indirect Semiconductors , WILLIAM VANDENBERGHE, K.U.Leuven / imec, BART SORÉE, imec, MASSIMO FISCHETTI, U.T.Dallas, WIM MAGNUS, Univ. Antwerpen / imec, GUIDO GROESENEKEN, K.U.Leuven / imec — With the scaling in the semiconductor device dimensions, Zener tunneling has become an important source of leakage in conventional MOSFET devices but it could also provide drive current for a novel type of tunnel transistor. A good understanding of the process of Zener tunneling is therefore required and present-day one-dimensional semi-classical models fall short of explaining tunneling in devices with potential profiles with a pronounced two-dimensional shape. We have developed a formalism to calculate the phonon-assisted current under a given three dimensional external potential profile. The current is calculated from the transition probability for an electron to go from the valence to the conduction band. The transition probability is determined from the spectral functions corresponding to the valence and the conduction band. In the presence of a one-dimensional uniform low electric field, the Kane model is recovered. An example of the formalism is given for the case of an abrupt p-n diode and compared with existing semi-classical models. It is seen that the uniform field model is actually better than the WKB model but that none of the semi-classical models give good results at low bias conditions.

5:06PM D24.00012 Zener Tunneling: Correspondence between Quantum and Semi-Classical Formalisms , KARTIK GANAPATHI, SAYEEF SALAHUDDIN, University of California Berkeley — The resurgence of interest in band-to-band tunneling has been due to its usefulness in overcoming the 60 mV/decade limit in turn-on characteristics of a MOSFET thereby providing path for lowering the operating power. The expression due to *Kane*, for calculating transmission coefficient and current due to Zener tunneling in a $p-n$ diode, has been extensively used over the years for explaining experimental tunneling characteristics. While this closed form expression relates tunneling probability with simple quantities like bandgap, effective mass, electric field etc., being a formula based on semi-classical approximation, it is valid strictly in the low-field regime. With finite size effects playing significant role in ultra small device dimensions, this approximation breaks down and one needs to have a full quantum mechanical treatment of the tunneling problem with a realistic band-structure. We report a numerical simulation of this problem within the NEGF formalism with a tight-binding Hamiltonian wherein the extent of validity of Kane's formula is examined. We also discuss how Kane's parameters should be altered and interpreted in high field region. The results are compared with experimental data in two different systems – InAs $p^+ - n^+$ and GaN/AlGaN heterojunction tunnel diodes.

5:18PM D24.00013 Simulation of nanoscale four-probe resistance measurements under finite bias voltages , ASAKO TERASAWA, KEIJI TOBIMATSU, TOMOFUMI TADA, TAKAHIRO YAMAMOTO, SATOSHI WATANABE, Dept. of Materials Engineering, The Univ. of Tokyo — To understand the interesting features in nanoscale four-probe measurements such as the negative value and the oscillation of four-probe resistance [1], we investigate the behavior of nanoscale four-probe resistance theoretically [2-3]. In the present work, we examine the effect of bias voltage on four-probe resistance in nanoscale four-probe systems. For a set bias voltage between current probes, we first estimate the voltage between voltage probes when no current flows between them from the four-probe and two-probe resistances at the zero-bias limit, assuming the linear response. Then we calculate the dependence of currents in the voltage probes on the bias voltage applied to the current probes with applying the voltage thus estimated between the voltage probes. The calculated currents in the voltage probes have nonzero but much smaller values compared with those in current probes, and show the non-linear dependence on the bias voltage. This result indicates assumption of linear response is not valid for the bias voltage of the order of a tenth V, and that currents and voltages should be determined self-consistently to estimate four-probe resistance. [1] B. Gao et al., Phys. Rev. Lett. 95, 196802 (2005). [2] A. Terasawa et al., Phys. Rev. B 79, 195436 (2009). [3] A. Terasawa et. al., New J. Phys. 12, 083017 (2010).

Monday, March 21, 2011 2:30PM - 5:18PM –
Session D25 DCMP: Superconductivity: Vortex Phenomena I D166

2:30PM D25.00001 Anomalous field-symmetric Nernst signal in striped cuprate $La_{2-x}Ba_xCuO_4$[1] , N. PHUAN ONG, LU LI[2], Princeton University, J. M. TRANQUADA, GENDA GU, Brookhaven National Lab — Starting at the structural transition temperature $T_{d2} = 54$ K, the striped cuprate $La_{2-x}Ba_xCuO_4$ ($x = \frac{1}{8}$) displays a remarkable cascade of transitions[1] at the characteristic temperatures $T_{d2} > T_1^{**} > T_{BKT} > T_c$, before settling down to 3D superconductivity with long-range coherence at T_c= 5 K. The Nernst signal e_N and thermopower S have been investigated in detail in these multiple states. As in pure LaSrCuO, the Nernst coefficient $N = lim_{B\to 0} e_N/B$ (initially negative) acquires a positive vortex contribution at 120 K that grows rapidly. However, here, N saturates in the interval T_{d2} (54 K) $\rightarrow T_1^{**}$ (34 K). As the vortex liquid becomes increasingly stabilized below T_1^{**}, N resumes increasing at an even steeper rate. Surprisingly, below 34 K, e_N acquires a B-symmetric component that is very large and oscillatory in B. We have excluded S and quasiparticles as the source of the anomalous term. We will discuss various origins including the possibility of vortex formation mechanisms that break time-reversal invariance.
1) J. M. Tranquada *et al.*, Phys. Rev. B 78, 174529 (2008).

[1]Supported by NSF-DMR 0819860 (at Princeton) and US DOE Contract No. DE-AC02-98CH10886 (at BNL).
[2]Current address: MIT

2:42PM D25.00002 Torque measurements in underdoped $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$ single crystals[1] , T. HU, Kent State University, Kent, Ohio, USA and University of California, Davis, CA, USA, H. XIAO, Kent State University, Kent, Ohio, USA and Institute of Physics, Beijing, China, P. GYAWALI, Kent State University, Kent, Ohio, USA, H.H. WEN, Institute of Physics, Beijing, China, C.C. ALMASAN, Kent State University, Kent, Ohio, USA — We report in-plane and out-of-plane angular-dependent torque measurements on underdoped $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$ single crystals both below and above the zero-field superconducting transition temperature $T_c(0)$ and in applied magnetic fields H up to 14 T. The out-of-plane torque data show that a diamagnetic signal persists into the normal state, which is consistent with previous reports on $Bi_2Sr_2Ca_2CuO_{8+\delta}$. These data also reveal that the vortex matter in the superconducting state has lower dimensionality compared to the one in the normal state. Furthermore, in-plane torque measurements show that the presence of vortices above $T_c(0)$ destroys the phase coherence of the Cooper pairs.

[1]This research was supported by the National Science Foundation under Grant No. DMR-1006606 at KSU. TH acknowledge the support of ICAM Branches Cost Sharing Fund from the Institute for Complex Adaptive Matter.

2:54PM D25.00003 Generics of the diamagnetism, Nernst signal, and finite size effects in superconductors above the transition temperature , S. WEYENETH, T. SCHNEIDER, Physics Institute, University of Zurich, CH-8057 Zurich, Switzerland — Various superconductors exhibit peculiar features above the transition temperature T_c. In particular the observation of a large Nernst signal N and a remarkable diamagnetism above T_c in cuprate and conventional superconductors attracted considerable attention. Noting that in these materials the spatial extent of the homogeneous domains is limited, we explore the relevance of a zero dimensional (0D)-model, neglecting thermal fluctuations, to describe the isothermal magnetization curves $m_{\rm d}(H)$ in various superconductors above T_c. It is shown that for cuprates as well as for Pb nanoparticles, both, the full 0D-model as well as its Gaussian approximation, mimic the essential features of the magnetization curves above T_c rather well. Furthermore, the isothermal Nernst signal of a superconducting $Nb_{0.15}Si_{0.85}$ film is fully consistent with this scenario. Accordingly, the observed diamagnetism above T_c in Pb nanoparticles, in the cuprates $La_{1.91}Sr_{0.09}CuO_4$ and $BiSr_2Ca_2CuO_{8-\delta}$, as well as the Nernst signal in $Nb_{0.15}Si_{0.85}$ films, are all in excellent agreement with the scaling properties emerging from the here discussed 0D-model. Therefore, singlet Cooper pairs subjected to orbital pair breaking in a 0D-system are the main source of the observed diamagnetism and Nernst signal in an extended temperature window above T_c.

3:06PM D25.00004 Effects of Vortex Charge Explored by NMR Spectroscopy in $Bi_2Sr_2CaCu_2O_{8+\delta}$, ANDREW MOUNCE, S. OH, Northwestern University, S. MUKHOPADHYAY, W.P. HALPERIN, A.P. REYES, P.L. KUHNS, K. FUJITA, M. ISHIKADO, S. UCHIDA — We measure nuclear magnetic resonance (NMR) spectra for various dopings of $Bi_2Sr_2CaCu_2O_{8+y}$ to determine the variations of local magnetic fields generated by the vortex lattice at low temperatures. With increasing the external magnetic field H_0, the local field variations decrease to values lower than expected by Ginzburg-Landau calculations for an Abrikosov vortex lattice.[1] Taking into account charge accumulation in vortex cores, which has been predicted by theory[2] and suggested by experiment,[3] we are able to identify the amount of charge needed to disturb the vortex lattice and decrease local field variations as in the observed spectra. The amount of charge is found to be $\sim 2\text{x}10^{-3}$e and doping dependent in line with theoretical predictions.[2] This work is supported by DOE/BES: DE-FG02-05ER46248 and the NHMFL by NSF and the State of Florida.

[1]Brandt, E. H., Phys. Rev. Lett. **66**, 3213-3216 (1991).
[2]Khomskii, D. I. & Freimuth, A. Phys. Rev. Lett. **75**, 1384-1386 (1995).
[3]Kumagai, *et al.* Phys. Rev. B **63**, 144502 (2001).

3:18PM D25.00005 Vortex dynamics in ferromagnetic / high T_c superconducting heterostructures , N. HABERKORN, J. KIM, M. MIURA, B. MAIOROV, P. DOWDEN, L. CIVALE, Superconductivity Technology Center, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — In this work we explore the influence of the ferromagnetic landscape generated by magnetic phase separation in manganites on the vortex pinning of HTS/FM heterostructures. We have grown $Gd_{2/3}Ca_{1/3}MnO_3$(GCMO), $Y_{2/3}Ca_{1/3}MnO_3$(YCMO) and YBCO films, as well as GCMO/YBCO and YCMO/YBCO bilayers by Pulsed Laser Deposition. GCMO is a ferrimagnetic material with Curie temperature of $\sim$ 80 K and a compensation temperature of 15 K, whereas YCMO is ferromagnetic with Curie temperature $\sim$ 80 K. In both materials the saturation magnetization is smaller than the value expected from ferrimagnetic and ferromagnetic order, suggesting phase separation with small ferromagnetic domains. The magnetic domain size as a function of temperature for the magnetic films was investigated using magnetic force microscopy (MFM). We will present a comparison of the vortex pinning and dynamics in the YBCO single layers and the GCMO/YBCO and YCMO/YBCO bilayers that allows us to identify the temperature and field regimes where magnetic pinning is effective.

3:30PM D25.00006 Hysteretic magneto-transport of a High-T_c superconducting/ferromagnetic multilayer with tunable magnetic domain structure , JAVIER E. VILLEGAS, CRISTINA VISANI, PETER J. METAXAS, AURELIE COLLAUDIN, BAPTISTE CALVET, ROZENN BERNARD, JAVIER BRIATICO, CYRILE DERANLOT, KARIM BOUZEHOUANE, Unite Mixte de Physique CNRS/Thales, 1 avenue A. Fresnel, 91767 Palaiseau, and Universite Paris Sud 11, 91405 Orsay, France — The magneto-transport of a hybrid heterostructure combining a $YBaCuO_{7-\delta}$ thin film and a Co/Pt superlattice shows an unusual hysteretic behavior. Depending on the angle between the external applied field and the film plane, and on the magnetic history, either a increase or a decrease of the mixed-state resistance is observed. The combination of magneto-transport, magnetic force microscopy and anomalous Hall effect measurements allows us to correlate these effects to the magnetic domain structures in the Co/Pt superlattice. We unequivocally prove that the hysteretic magneto-transport is induced by the stray magnetic fields from tunable magnetic domain structures, which may induce vortices or produce vortex pinning, leading to the increase/decrease of the mixed-state resistance. Work supported by French ANR "Superhybrids-II" and RTRA "Supraspin" grants.

3:42PM D25.00007 Vortex/Domain Coupling in Superconducting Films on Ferromagnetic Substrates with Different Domain Structures , VITALII VLASKO-VLASOV, ULRICH WELP, DANIEL ROSENMANN, WAI KWOK, Argonne National Laboratory, Argonne, IL, ALEXANDER BUZDIN, University of Bordeaux, France, ALEXANDER MELNIKOV, Institute Ior Physics of Microstructures RAS, Russia, LYUDMILA USPENSKAYA, Institute of Solid State Physics RAS, Russia, VINCENT FRATELLO, Integrated Photonics, Hillsborough, NJ — In this work we address engineering of magnetic pinning in the superconducting/ferromagnetic hybrids. Using direct magneto-optical observations effects of interactions between superconducting vortices in Nb film and magnetization in domains of substituted iron garnet films are studied. Two garnet films with perpendicular anisotropy but different thickness-to-domain width ratios and one showing the reorientation from the in-plane to the normal easy axis are used as substrates. All three samples demonstrate strong domain/vortex coupling and reveal high pinning by domain walls, which persists up to temperatures close to the superconducting Tc. In turn, vortex motion modifies domain structures of garnets at T$<$Tc resulting in the alignment and strong contraction of wide domains but smaller width changes of narrow domains. A model is proposed explaining the results of our observations. This work was supported by DOE-BES under Contract No. DE-AC02-06CH11357.

3:54PM D25.00008 Matching field effects in high-T_c superconductors with self-assembled columnar defects , J.W. SINCLAIR, University of Tennessee, Y.L. ZUEV, Oak Ridge National Laboratory, J.R. THOMPSON, University of Tennessee, Knoxville, D.K. CHRISTEN, C. CANTONI, S.-H. WEE, A. GOYAL, Oak Ridge National Laboratory, C. VARANASI, Univ of Dayton/Air Force Research Lab — Columnar defects (CDs) in a superconductor provide angularly selective vortex pinning, where the density of CDs provides a natural scale for the magnetic field, the "matching field." While dramatic changes in the critical current density J_c might be expected when the vortex density exceeds the CD density, observations of this phenomena has been elusive in systems with chemically produced, self-assembled CDs of $BaSnO_3$, $BaZrO_3$, $SrZrO_3$, etc. Here we describe studies of two $RBa_2Cu_3O_{\sim 7}$ systems containing these self-avoiding CDs, using either contact free magnetic or transport measurements. In magnetic measurements on a material with measured areal CD of $\sim$2.5 T, the J_c decreased abruptly when the applied field H exceeded this level; this feature was observed over a wide temperature range, from 77 to $\sim$ 40 K. All these features disappeared when the field was tilted away from the CD orientation. Research at ORNL sponsored by US DOE.

4:06PM D25.00009 Superconducting vortex dynamics on asymmetric arrays with symmetric pinning centers[1] , JOSE L. VICENT, Universidad Complutense, 28040 Madrid, DAVID PEREZ DE LARA, IMDEA-Nanociencia, 28049 Madrid and Universidad Complutense, 28040 Madrid, ALEJANDRO ALIJA, Universidad Oviedo, 33007 Oviedo, ELVIRA M. GONZALEZ, Universidad Complutense, 28040 Madrid, MARIA VELEZ, JOSE I. MARTIN, Universidad Oviedo, 33007 Oviedo — Arrays of Ni nanodots embedded in Nb superconducting films have been fabricated by sputtering and electron beam lithography techniques. The arrays are periodic triangular lattices of circular Ni dots arranged in a kagomé-like pattern with broken reflection symmetry. DC magnetoresistance shows several fractional matching field minima below the first matching field for vortex motion parallel and perpendicular to the array reflection symmetry. AC magnetoresistance shows reversal ratchet effect when the vortex lattice moves parallel to the array reflection symmetry. These effects could be understood taking into account the vortex lattice density.

[1]Work supported by Spanish MICINN and CAM.

4:18PM D25.00010 Enhanced superconducting vortex pinning in the Corbino geometry[1] , YANIV ROSEN, IVAN K. SCHULLER, Department of Physics and Center for Advanced Nanoscience, University of California San Diego, La Jolla CA 92093 — We probed a dynamic system of superconducting vortices with an artificial pinning landscape in the Corbino geometry. Current was applied from the center of the disc and propagated radially outward to produce a circular force with a strength proportional to 1/r on the vortices. This caused a shearing force on the vortex lattice and was studied with varying current densities and temperature. Matching minima in the magnetoresistance curves were still observed under the Corbino conditions for the square lattice pinning site geometry. Surprisingly the even numbered matching fields show enhanced pinning compared to the odd matching fields. Other interesting temperature and current density dependencies will also be discussed.

[1]This work was supported by the US-NSF.

4:30PM D25.00011 Proximity Effects and Vortex Dynamics in Nanostructured Superconductors , SERENA ELEY, NADYA MASON, Department of Physics and Materials Research Laboratory, University of Illinois Urbana-Champaign — We report transport measurements on triangular arrays of proximity-coupled superconducting islands placed on normal-metal substrates. The superconducting islands are well-understood coherent systems with long-range electron interactions, while the intervening normal metal channels introduce known dissipation into the system. We show how by changing the island spacing, we can tune characteristics such as the critical temperature and field. The arrays undergo a Kosterlitz-Thouless vortex-unbinding phase transition at zero-field, and we observe frustration-induced magnetoresistance oscillations at finite fields. We also observe unusual cusp-like behavior in resistance vs temperature at finite magnetic fields

4:42PM D25.00012 Vortex-induced dissipation in current-biased superconducting nanowires , LEV BULAEVSKII, MATTHIAS GRAF, CRISTIAN BATISTA, Los Alamos National Laboratory, VLADIMIR KOGAN, Ames Lab and Iowa State Univ. — We study the dissipation due to vortex crossings in thin current-biased superconducting films with thickness on the order of the coherence length, and with width much narrower than the magnetic Pearl length in thin films. We find that for technologically relevant thin and narrow films or nanowires with width much larger than the coherence length, the barrier for phase slips by creation of temporary normal regions across the entire film width is too big. Thus phase slips become highly improbable. Instead, we propose the process of a vortex crossing the strip from one edge to the other, perpendicular to the bias current, as the dominant mechanism for generalized phase slips resulting in detectable voltage pulses. We derive phase-current relations and predict the amplitude and duration of voltage pulses induced by vortex motion due to thermal fluctuations and bias current. The consequnces for the current-voltage characteristics and the fundamental limitations for dark counts in superconducting nanowire single-photon detectors are discussed.

4:54PM D25.00013 Synthesis and vortex dynamics of high-Tc superconducting nanoribbons with a periodic array of holes , QIONG LUO, MICHAEL LATIMER, ZHILI XIAO, Northern Illinois University, LEI FANG, WAI-KWONG KWOK, Argonne National Lab — We fabricated nanoribbons of high-temperature superconductors YBCO-123 and BSCCO-2212. Experimental procedures for growing, manipulating and characterizing the nanoribbons will be presented. Furthermore, we introduced regular arrays of nanoscale holes into these nanoribbons through focused-ion-beam (FIB) milling to study the effects of periodic pinning on vortex dynamics. Resistive measurements reveal vortex matching effect and striking feature in the volage-current behavior associated with various driven regimes of the vortex matter related to vortex dynamics phase transitions

5:06PM D25.00014 Strong pinning of vortex lines by nanoparticles[1] , ALEXEI KOSHELEV, Materials Science Division, Argonne National Laboratory, ALEJANDRO KOLTON, Centro Atomico Bariloche and Instituto Balseiro, Argentina — Pinning of vortex lines by array of nanoparticles embedded inside superconductors became the most efficient practical way to achieve high critical currents. In this situation pinning occurs via trapping of the vortex-line segments and the critical current is determined by the typical length of trapped segment. To verify analytical estimates and develop a quantitative description of strong pinning, we use large-scale numerical simulations. We study the dependence of the critical force on the density of pins in the regime of independently pinned lines, statistical properties of trapped lines, and suppression of the apparent critical force by thermal fluctuations.

[1]This work is supported by the Center for Emergent Superconductivity funded by the U.S. DOE, Office of Science, under Award No. DE-AC0298CH1088.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D26 DCOMP DMP: Focus Session: Iron Based Superconductors – Electronic Structure

D162/164

2:30PM D26.00001 Confronting LDA+DMFT results with experiments in the iron pnictide families , GABRIEL KOTLIAR, Rutgers University — The normal state electronic structure of the pnictides is an important challenge to electronic structure theory . Optical conductivity experiments are indicative of electronic electron correlations (with mass renormalizations of the order of three). Neutron scattering experiments have features characteristic of both itinerant and localized electrons. High energy spectroscopies indicate the absence of satellite peaks. In this talk, we will show how LDA+DMFT allows us to reconcile these apparently inconsistent facts, and trace them to the unique chemical ingredients of these compounds: the iron Hunds rule coupling and the hybridization with very broad arsenide bands. Quantitative results for the different iron pnictide families will be presented and the factors that govern the strength of the correlations in this family of compounds will be discussed.

3:06PM D26.00002 Electronic structure of iron-pnictide superconductors: just scratching the surface , ERIK VAN HEUMEN, University of Amsterdam, J. VUORINEN, Tampere University, K. KOEPERNIK, IFW Dresden, F. MASSEE, Y. HUANG, J.B. GOEDKOOP, University of Amsterdam, M. LINDROOS, Tampere University, M. SHI, PSI, K. HAULE, Rutgers University, J. VAN DEN BRINK, IFW Dresden, M.S. GOLDEN, University of Amsterdam — Angle resolved photoemission (ARPES) and scanning tunneling microscopy (STM) are important tools in the study of iron-pnictide high T_c superconductors. These techniques are surface sensitive and one has to ensure that the electronic structure probed in an experiment corresponds to the bulk electronic structure. Using a combination of experimental techniques (STM, ARPES, LEED) and theoretical calculations (LEED simulations, DFT), I will show that the surface structure of $BaFe_{2-x}Co_xAs_2$ is both reconstructed and distorted. LEED data combined with simulations is used to solve the real surface and sub-surface structure. The impact of the surface on the electronic structure is then determined by comparing DFT slab calculations, based on the real surface structure, with ARPES experiments. The presence of surface states gives a natural explanation for the large k-space broadening observed in these materials. Having identified the surface states and bulk bands, I will address the more fundamental questions with regard to the electronic structure and its role in the mechanism of high temperature superconductivity.

3:18PM D26.00003 The superconducting phase and electronic excitations of (Rb,Cs)Fe_2As_2 , J. KANTER, Lab. for Solid State Physics, ETH Zurich, CH-8093 Zurich, Z. SHERMADINI, R. KHASANOV, A. AMATO, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland, Z. BUKOWSKI, B. BATLOGG, Lab. for Solid State Physics, ETH Zurich, CH-8093 Zurich — We present specific heat, transport and Muon-Spin Rotation (μSR) results on (Rb,Cs)Fe_2As_2. $RbFe_2As_2$ was only recently found to be superconducting below 2.6 K by Bukowski et al. Compared to the related $BaFe_2As_2$ the electron density is lower and no magnetic order is observed. For the superconducting phase the superfluid density was calculated from μSR data. The temperature dependence of the superfluid density and the magnetic penetration depth is well described by a multi-gap scenario. In addition the electronic contribution the specific heat was studied for different compositions and magnetic fields and reveals a high value for the Sommerfeld coefficient γ.

3:30PM D26.00004 Revealing the degree of magnetic frustration in iron pnictides , CHENG-CHIEN CHEN, Stanford University, RYAN APPLEGATE, University of California at Davis, BRIAN MORITZ, THOMAS DEVEREAUX, SIMES, SLAC National Accelerator Laboratory, RAJIV SINGH, University of California at Davis — Proposed theories for collinear antiferromagnetism in iron pnictides vary greatly in the amount of magnetic frustration and proximity to a quantum critical point. We discuss how imaging the magnetic fields around a non-magnetic impurity can quantify the degree of magnetic frustration and thereby distinguish various theoretical proposals. It is found that in a frustrated J1-J2 model a non-magnetic impurity strongly reduces its neighboring local moments, and overturned dynamical spins appear close to zero energy. In contrast, the spatially anisotropic J1a-J1b-J2 model produces enhanced local moments on sites neighboring the impurity. In both cases, the disturbance in the magnon local density of states exhibits an anisotropic stripe pattern. These predictions can be tested by experiments such NMR or spin-resolved STM measurements. The results can elucidate the role of frustration in antiferromagnets and help narrow the possible models for the iron-pnictide superconductors.

3:42PM D26.00005 Theory for Magnetism and Triplet Superconductivity in LiFeAs[1]

, MARIA DAGHOFER, IFW Dresden, PHILIP BRYDON, CARSTEN TIMM, TU Dresden, JEROEN VAN DEN BRINK, IFW Dresden — Superconducting pnictides are widely found to feature spin-singlet pairing in the vicinity of an antiferromagnetic phase, for which nesting between electron and hole Fermi surfaces is crucial. LiFeAs differs from the other pnictides by (i) poor nesting properties and (ii) unusually shallow hole pockets. Investigating magnetic and pairing instabilities in an electronic model that incorporates these differences, we find antiferromagnetic order to be absent. Instead we observe almost ferromagnetic fluctuations which drive an instability toward spin-triplet p-wave superconductivity.
P.M.R. Brydon, M. Daghofer, C. Timm, and J. van den Brink, arXiv:1009.3104

[1]Support from the DFG under the priority program 1458 and the Emmy-Noether program

3:54PM D26.00006 Unified Picture for Magnetic Correlations in Iron-Based Superconductors

, WEI-GUO YIN, CHI-CHENG LEE, WEI KU, Brookhaven National Laboratory — The spin-density-wave mechanism due to Fermi surface nesting is widely used to describe magnetism in the parent compounds of iron-based superconductors; however, the field is puzzled by the different magnetic structure of FeTe, which apparently has similar Fermi-surface topology. Here we propose [1] an orbital-degenerate double-exchange model which includes both itinerant electrons and localized spins. The physical properties of the model are governed by the competition between the antiferromagnetic superexchange and Hund's rule coupling. We show that the strength of the effective Hund's rule coupling term strongly depends on the anion height from the iron plane, leading to the collinear (C-type) magnetic order with the ferro-orbital order in iron pnictides and the bicollinear (E-type) magnetic order without orbital ordering in FeTe. This shows that the magnetism in iron-based superconductors can be described in a unified picture and may have a universal origin for all of the materials. Our results reveal the crucial role of Hund's rule coupling for the strongly correlated nature of the system and suggest exploring the interplay of the spin, orbital, charge, and lattice degrees of freedom in promoting high-temperature superconductivity. Work supported by US DOE.
[1] W.-G. Yin, C.-C. Lee, and W. Ku, PRL 105, 107004 (2010).

4:06PM D26.00007 Electronic specific heat of the iron chalcogenide superconductor $Fe(Te_{0.55}Se_{0.45})$

, JIN HU, TIJIANG LIU, BIN QIAN, ZHIQIANG MAO, Department of Physics and Engineering Physics, Tulane University — We report specific heat studies of superconducting $Fe(Te_{0.55}Se_{0.45})$[1]. We have obtained the electronic specific heat by subtracting the phonon contribution evaluated from the normalization of the phonon specific heat of a non-superconducting reference sample $(Fe_{0.9}Cu_{0.1})(Te_{0.55}Se_{0.45})$. Our results show that the superconducting ground state is accompanied by unpaired quasiparticles, as in FeAs superconductors, with γ_0~2.3 mJ/mol K^2. The temperature dependence of the electronic specific heat $C_{es}(T)/T$ can be well fitted using either a single s-wave gap model with $2\Delta = 5.2\ k_BT_c$ or a two-gap model with $2\Delta_1/k_BT_c = 5.8$ and $2\Delta_2/k_BT_c = 4.0$; the two-gap model fitting is slightly better than the single gap fitting. Such large gaps, together with a large specific heat jump $\Delta C(T_c)/T_c$ ~57.3 mJ/mol K^2, suggest a strong-coupling superconducting state. While $C_{es}(T)/T$ exhibits isotropic s-wave gap behavior, the magnetic field-induced change in the electronic specific heat $\Delta\gamma(H)$ exhibits sublinear field dependence, implying the superconducting pairing in iron chalcogenide superconductors also involves a multiple band effect, as seen in pnictide superconductors. [1] M. H. Fang, H. M. Pham, B. Qian, T. J. Liu, E. K. Vehstedt, Y. Liu, L. Spinu, and Z. Q. Mao, Superconductivity close to magnetic instability in $Fe(Se_{1-x}Te_x)_{0.82}$, Phys. Rev. B 78, 224503 (2008).

4:18PM D26.00008 Electronic correlations and superconducting response in the optical properties of $FeTe_{0.55}Se_{0.45}$[1]

, C.C. HOMES, A. AKRAP, J.S. WEN, Z.J. XU, Z.W. LIN, Q. LI, G.D. GU, Condensed Matter Physics and Materials Science Dept., Brookhaven National Laboratory, Upton, New York — The in-plane complex optical properties of the iron-chalcogenide superconductor $FeTe_{0.55}Se_{0.45}$ have been determined above and below $T_c = 14$ K. At room temperature the conductivity is described by a weakly-interacting Fermi liquid with $\omega_{p,D} \simeq 7200$ cm^{-1} and $1/\tau_D \simeq 414$ cm^{-1}. Below 100 K the conductivity is no longer described by the Drude model. Adopting the generalized Drude model reveals that $1/\tau(\omega) \propto \omega$ in the terahertz region just above T_c, signaling the increasingly correlated nature of this material.[2] For $T \ll T_c$ the superconducting plasma frequency $\omega_{p,S} \simeq 3000$ cm^{-1} ($\lambda_{eff} \simeq 5300$ Å); $\omega^2_{p,S}/\omega^2_{p,D} \ll 1$ indicating that this material is not in the clean limit. Allowing $\sigma_{dc} \equiv \sigma_1(\omega \to 0)$, then $\sigma_{dc}(T \simeq T_c) \simeq 3500 \pm 400\ \Omega^{-1}$cm^{-1} and the superfluid density $\rho_{s0} \equiv \omega^2_{p,S} \simeq 9 \pm 1 \times 10^6$ cm^{-2} places material close to the scaling line $\rho_{s0}/8 \simeq 8.1\,\sigma_{dc}T_c$ for a BCS dirty-limit superconductor. Below T_c the optical conductivity reveals two energy scales for the superconductivity at $\Delta_1(0) \simeq 2.5$ meV and $\Delta_2(0) \simeq 5.1$ meV, consistent with the $s^{\pm}$ model.

[1]Supported by the DOE under Contract No. DE-AC02-98CH10886.
[2]C. C. Homes *et al.*, Phys. Rev. B **81**, 180508(R) (2010).

4:30PM D26.00009 Microwave surface impedance measurements of LiFeAs and LiFe(As,P) single crystals

, Y. IMAI, H. TAKAHASHI, T. OKADA, A. MAEDA, Dept. of Basic science, the University of Tokyo, K. KITAGAWA, K. MATSUBAYASHI, M. TAKIGAWA, Y. UWATOKO, ISSP, the University of Tokyo, N. NAKAI, Y. NAGAI, M. MACHIDA, Japan Atomic Energy Agency — We report results of microwave surface impedance measurements in LiFeAs and LiFe(As,P) single crystals [1]. These crystals were grown by self-flux method. The surface impedances of crystals were measured by a cavity perturbation technique. The in-plane penetration depth calculated from the surface reactance shows an exponential temperature dependence at low temperatures in both of LiFeAs and LiFe(As,P). This indicates that these materials do not have any nodes in the superconducting gap. The temperature dependence of the superfluid density indicates that LiFeAs and LiFe(As,P) are multi-gap superconductors with at least two isotropic gaps. In addition, the real part of complex conductivity exhibits an enhancement below T_c, which is different from the so-called coherence peak. This is due to the rapid increase of the relaxation time of the quasiparticle below T_c. We believe that this enhancement is rather common to all superconductors where an inelastic scattering is dominant above T_c, irrespective of the strength of the electron correlation.

[1] Y. Imai *et al.*, J. Phys. Soc. Jpn, *in-press*.(arXiv: 1009.4628.)

4:42PM D26.00010 Electromagnetic response of Fe(Se,Te) in the superconducting sate

, A. MAEDA, H. TAKAHASHI, D. NAKAMURA, T. AKIIKE, F. NABESHIMA, Y. IMAI, Department of Basic Sciences, University of Tokyo, S. KOMIYA, I. TSUKADA, Central Research Institue of Electric and Power Industry (CRIEPI) — We investigate the electromagnetic response of Fe(Se,Te) from microwave to THz region, with special interests in the superconducting state. Samples were epitaxial thin films or bulk single crystals, depending on the technique of measurements. The results obtained are the followings. (1) Temperature dependence of the penetration depth was almost flat, with a very small contribution of T^2, suggesting nodeless gap plus some disorder induced pair breaking. (2) Temperature dependence of superfluid density is rather different from that of, eg, LiFeAs, suggesting weak interband scattering. (3) Quasiparticle (QP) conductivity, $\sigma(\omega, T)$ shows a broad peak below T_c. Both of temperature dependence and frequency dependence show that this peak is not the coherence peak in conventional s-wave superconductors, but is due to the enhancement of the QP scattering time. These strongly suggest that the symmetry of superconducting wave function is sign-changed s-wave. (4) Sharp peak around T_c was invisible in $\sigma(T)$, suggesting very small superconductivity fluctuation. (5) Conductivity spectra ($\sigma(\omega)$) suggest that the superconducting gap, 2Δ is 1.2 meV, leading to $2\Delta/k_BT_c$ is 1.37. We will discuss possible reasons for the small gap value.

4:54PM D26.00011 Iron isotope effect on the superconducting transition temperature and the crystal structure of $FeSe_{1-x}$, MARKUS BENDELE, Physik-Institut der Universität Zürich, RUSTEM KHASANOV, KAZIMIERZ CONDER, EKATERINA POMJAKUSHINA, VLADIMIR POMJAKUSHIN, Paul Scherrer Institute, ANNETTE BUSSMANN-HOLDER, Max-Planck-Institut für Festkörperforschung, HUGO KELLER, Physik-Institut der Universität Zürich — The Fe isotope effect (Fe-IE) on the transition temperature Tc and the crystal structure was studied in the Fe chalcogenide superconductor $FeSe_{1-x}$ by means of magnetization and neutron powder diffraction (NPD). The substitution of natural Fe (containing $\simeq 92\%$ of ^{56}Fe) by its lighter ^{54}Fe isotope leads to a shift in T_c of 0.22(5) K corresponding to an Fe-IE exponent of $\alpha_{\rm Fe} = 0.81(15)$. Simultaneously, a small structural change with isotope substitution is observed by NPD. This may help to clarify the currently controversal results of the Fe-IE. Upon correcting the isotope effect exponent for these structural effects, an almost unique value of $\alpha \sim 0.35 - 0.4$ is observed for at least three different families of Fe-based HTS.

5:06PM D26.00012 Magnetism of SmFeAsO1-xFx[1] , YOICHI KAMIHARA, Keio Univ., YASUHIRO KOBAYASHI, SHINJI KITAO, Kyoto Univ., YOSHITAKA YODA, JASRI, MAKOTO SETO, Kyoto Univ., HIDEO HOSONO, Tokyo Institute of Technology, JST TRIP COLLABORATION, JST CREST COLLABORATION — Magnetic properties of superconducting $SmFeAsO_{1-x}F_x$ are demonstrated by ^{57}Fe Mossbauer spectroscopy (MS) and ^{149}Sm Nuclear resonant forward scattering (NRFS). Polycrystalline $SmFeAsO_{1-x}F_x$ samples were synthesized using two-step solid state reaction described elsewhere. [New J. Phys. 12, 033005 (2010).] Purity of samples was checked by X-ray diffraction patterns using Cu K-alpha radiation. Resistivity and magnetization measurements, as well as by ^{57}Fe MS and ^{149}Sm NRFS spectroscopy, at various temperatures were performed to define superconducting, magnetic ordering temperatures. [Phys. Rev. B 78, 184512 (2008) & J. Phys. Soc. Japan 77, 103706 (2008).] A magnetic phase diagram we have proposed is closer to that by Hess et al [Europhys. Lett. 87, 17005 (2009).]; that is long-range AF ordering of Fe (a static magnetism) does not persist in the superconducting regime. Such a relation between spin dynamics and SC is a common feature among $LnFeAsO_{1-x}F_x$ (Ln = La, Ce, Pr, Nd, and Sm). Our results indicate that the relation between the static magnetism and T_c of $LnFeAsO_{1-x}F_x$ shows similar topology to that of copper-based high-Tc superconductors. [Phys. Rev. B 42, 7981 (1990).]

[1]One (Y. K) of us was financially supported by the Keio Leading-edge Laboratory of Science and Technology (KLL).

5:18PM D26.00013 Surface geometric and electronic structures of $A(Fe, Co)_2As_2$ (A=Ba,Ca) , GUORONG LI, V.B. NASCIMENTO, XIAOBO HE, AMAR B. KARKI, JIANDI ZHANG, RONGYING JIN, Dept. of Physics, Louisiana State University, Baton Rouge, LA 70802, USA, A.S. SEFAT, M.A. MCGUIRE, B.C. SALES, Materials Science & Technology Division, ORNL, Oak Ridge, TN 37831, USA, D. MANDRUS, Dept. of Materials Science & Engineering, The University of Tennessee, Knoxville, TN, 37996, USA, WARD PLUMMER, Depart. of Physics, Louisiana State University, Baton Rouge, LA 70802, USA — We utilize Low Energy Electron Diffraction (LEED) to determine the surface structure combined with real-space scanning tunneling microcopy/spectroscopy (STM/STS), to investigate the local geometric and electronic structures at the (001) surface of the compounds of AFe_2As_2 (A= Ba, Ca). In general two competing surface reconstructions are observed with either a 1x2 or a $(\sqrt{2}\times\sqrt{2})R45^\circ$ (tetragonal notation) structure. The $(\sqrt{2}\times\sqrt{2})R45^\circ$ structure corresponds to the 1x1 orthorhombic phase. While the $(\sqrt{2}\times\sqrt{2})R45^\circ$ phase always present for A=Ba, the 1x2 structure dominates for A=Ca. We will discuss the detailed structural change with Co doping, thermal cycling, contamination, electron beam induced damage, and cleaving temperature. Specifically, 1x2 phase is sensitive to the thermal processing, with indications of a temperature dependence phase transition. *Supported by NSF DMR-1002622

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D27 GQI: Focus Session: Superconducting Qubits - Gates and Algorithms C155

2:30PM D27.00001 Scaling Superconducting Qubits with the ResQu Architecture , JOHN MARTINIS, University of California at Santa Barbara — This abstract not available.

3:06PM D27.00002 Quantum Logic Gates for Coupled Superconducting Resonators , FREDERICK STRAUCH, Williams College — Superconducting resonators are a promising element for many applications in quantum information processing, such as memory, state transfer, and qubit-qubit coupling. Here I introduce a new application—multi-level quantum logic using superpositions of Fock states. A circuit-QED implementation of single and coupled-resonator gates will be presented and theoretically analyzed. This scheme, using experimentally demonstrated interactions, will be compared with traditional qubit operations.

3:18PM D27.00003 Two-qubit gates and coupling with low-impedance flux qubits , JERRY CHOW, ANTONIO CORCOLES, CHAD RIGETTI, JIM ROZEN, GEORGE KEEFE, MARY-BETH ROTHWELL, JOHN ROHRS, MARK BORSTELMANN, DAVID DIVINCENZO, MARK KETCHEN, MATTHIAS STEFFEN, IBM Research — We experimentally demonstrate the coupling of two low-impedance flux qubits mediated via a transmission line resonator. We explore the viability of experimental coupling protocols which involve selective microwave driving on the qubits independently as well as fast frequency tuning through on-chip flux-bias. Pulse-shaping techniques for single-qubit and two-qubit gates are employed for reducing unwanted leakage and phase errors. A joint readout through the transmission line resonator is used for characterizing single-qubit and two-qubit states.

3:30PM D27.00004 ABSTRACT WITHDRAWN –

3:42PM D27.00005 Entangling ISWAP gate using frequency shifted anharmonic qubits , FELIX MOTZOI, JAY GAMBETTA, SETH MERKEL, AMIRA ELTONY, FRANK WILHELM, University of Waterloo — In this talk, we examine the coupling between frequency separated qubits, typical of superconducting implementations. We show how to correct for errors coming from finite turn-on time (corresponding to bringing the qubits into resonance) as well as leakage error (corresponding to exciting population out of the qubit manifold), namely by bringing the qubits in and out of resonance repeatedly to cancel out the unwanted parts of the Hamiltonian. The gates presented are smooth and robust and represent a whole class of analytic and numeric solutions for the evolution of the composite system.

3:54PM D27.00006 Analytic control methods for high fidelity unitary operations in a weakly nonlinear oscillator , SETH MERKEL, JAYDE GAMBETTA, FELIX MOTZOI, FRANK WILHELM, University of Waterloo — In qubits made from a weakly anharmonic oscillator the leading source of error at short gate times is leakage of population out of the two dimensional Hilbert space that forms the qubit. In this talk we explore a general technique based on an adiabatic expansion to find pulse shapes that correct this type of error. This leads to a family of solutions that can be further refined based on what is feasible for a particular application. This set of pulses contains and improves upon the previously developed DRAG solution [F. Motzoi, et. al., Phys. Rev. Lett. 103, 110501 (2009)] and can be further generalized to more complicated systems with additional leakage channels.

4:06PM D27.00007 CNOT gate for superconducting qubits biased at their symmetry points , SAHEL ASHHAB, FRANCO NORI, Advanced Science Institute, RIKEN, Wako-shi, Japan, PIETER DE GROOT, KEES HARMANS, HANS MOOIJ, Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands, JÜRGEN LISENFELD, Karlsruher Institute of Technology, Germany, ADRIAN LUPASCU, Institute for Quantum Computing, University of Waterloo, Canada — A number of different techniques have been proposed and demonstrated in the past few years for implementing two-qubit gates in a system of two coupled superconducting qubits biased at their symmetry points. Most of these techniques implement the iSWAP gate. I will discuss a new technique that implements the CNOT gate. The two qubits are driven at the frequency of the target qubit, and the amplitudes applied to the two qubits are chosen such that the target qubit undergoes Rabi oscillations for only one of the two possible states of the control qubit. As a result a CNOT gate can be implemented.

4:18PM D27.00008 Controlled-NOT logic gate based on conditional spectroscopy , MICHAEL GELLER, JOYDIP GHOSH, University of Georgia, Athens — A controlled-NOT logic gate based on conditional rotation of a target qubit by applying a microwave pulse of appropriate frequency has been demonstrated experimentally for a pair of superconducting flux qubits [Plantenberg et. al., Nature 447, 836 (2007)] . Here we discuss a related construction appropriate for coupled phase qubits or a phase qubit coupled to a resonator. Our results show that an intrinsic fidelity of more than 99% is achievable in about 45ns.

4:30PM D27.00009 Quantum Logic Gates for the Rezqu Architecture , JOYDIP GHOSH, MICHAEL GELLER, University of Georgia, Athens — A promising quantum computing architecture has been recently proposed by the UCSB superconducting quantum computation group. In this architecture, n phase qubits are capacitively coupled to individual memory resonators as well as a common bus. In this talk we discuss the design of quantum logic gates for this architecture and discuss the intrinsic fidelities.

4:42PM D27.00010 Idling error and SWAP/MOVE operation in RezQu architecture for phase qubits[1] , ANDREI GALIAUTDINOV, ALEXANDER KOROTKOV, University of California - Riverside — We analyze several basic operations in the RezQu architecture for superconducting phase qubits recently proposed by John Martinis, concentrating on the idling error, generation of single-excitation states, and the single-excitation transfer (which we call MOVE) between a phase qubit and its memory. We show that the idling error is negligible, being proportional to the sixth power of the coupling strength. We also show that in the rotating wave approximation the MOVE operation, which is simpler than the usual SWAP, can be realized perfectly using a tune/detune pulse with four adjustable parameters. The pulse consists of the front ramp (with proper shaping), a constant near-resonant overshoot, and an arbitrary rear ramp.

[1]This work was supported by NSA and IARPA under ARO grant No. W911NF-10-1-0334.

4:54PM D27.00011 Experimental demonstration of quantum algorithms on a 4-qubit/5-resonator quantum microprocessor utilizing superconducting qubits in the RezQu architecture , ERIK LUCERO, RAMI BARENDS, RADOSLAW BIALCZAK, YU CHEN, JULIAN KELLY, MIKE LENANDER, MATTEO MARIANTONI, ANTHONY MEGRANT, AARON O'CONNELL, PETER O'MALLEY, DANIEL SANK, AMIT VAINSENCHER, HAUHOA WANG, JAMES WENNER, TED WHITE, YI YIN, JIAN ZHAO, ANDREW CLELAND, JOHN MARTINIS — We present our newly designed and fabricated 4-qubit/5-resonator quantum microprocessor composed of "off-the-shelf" qubit and resonator components in the RezQu ("rez-(,)kyoo") architecture. The RezQu architecture uses resonators with qubits in the zero state to turn off stray coupling. Each qubit is coupled to a $\lambda/4$ memory resonator and coupling between the qubits is mediated by a common $\lambda/2$ resonator bus. Eight microwave lines drive the individual qubits, memory resonators, and coupling resonator. We demonstrate control over the quantum microprocessor via small scale quantum algorithms that require executing high- fidelity single qubit gates, quantum Fourier transform, Toffoli, CNOT, and other entangling gates.

5:06PM D27.00012 Efficient Toffoli Gate in Circuit Quantum Electrodynamics[1] , MATTHEW REED, Department of Applied Physics and Physics, Yale University, New Haven, Connecticut 06520, USA, LEONARDO DICARLO, Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands, LUYAN SUN, LUIGI FRUNZIO, ROBERT SCHOELKOPF, Department of Applied Physics and Physics, Yale University, New Haven, Connecticut 06520, USA — The fidelity of quantum gates in circuit quantum electrodynamics is typically limited by qubit decoherence.As such, significant improvements can be realized by shortening gate duration [1, 2]. Thethree-qubit Toffoli gate, also called thecontrolled-controlled NOT, is an important operation in basic quantum error correction.We report a scheme for a Toffoli gate that exploits interactions with non-computational excited states of transmon qubits which can be executed faster than an equivalent construction using one- and two-qubit gates. The application of this gate to efficient measurement-free quantum error correction will be discussed.

[1] DiCarlo, et al. Nature 467, 574 (2010).
[2] Chow, et al. Phys. Rev. Lett. 102, 090502 (2009).

[1]Research supported by NSF, NSA, and ARO.

5:18PM D27.00013 Progress towards a microwave-based high-fidelity Toffoli gate with superconducting qubits , CHAD RIGETTI, JERRY CHOW, ANTONIO CORCOLES, JIM ROZEN, GEORGE KEEFE, MARY BETH ROTHWELL, JACK ROHRS, MARK BORSTELMANN, DAVID DIVINCENZO, MARK KETCHEN, MATTHIAS STEFFEN, IBM Research — We describe recent progress at IBM towards a microwave-based implementation of the Toffoli gate using three capacitively shunted flux qubits dispersively coupled to a resonator. We discuss the device architecture and the microwave protocol, along with expected limits to gate fidelity and scaling.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D28 DMP: Focus Session: Graphene Growth, Characterization, and Devices: Metal Substrates C156

2:30PM D28.00001 Theory of the Growth of Epitaxial Graphene on Close-Packed Metals , ANDREW ZANGWILL, School of Physics, Georgia Institute of Technology, Atlanta, GA 30332, DIMITRI VVEDENSKY, Blackett Laboratory, Imperial College, London SW7 2BZ, UNITED KINGDOM — We present a simple rate theory of epitaxial graphene growth on close-packed metals. Motivated by recent low-energy electron microscopy experiments [E. Loginova, N.C.Bartelt, P.J. Feibelman, and K.F. McCarty, New Journal of Physics, **10**, 093026 (2008)], our theory supposes that graphene islands grow predominantly by the addition of five-atom clusters, rather than solely by the capture of diffusing carbon atoms. With suitably chosen kinetic parameters, we find quantitative agreement with (i) the measured time-evolution of the adatom density and (ii) the measured temperature-dependence of the adatom density at the onset of nucleation by assuming that the smallest stable precursor to graphene growth is an immobile island composed of six five-atom clusters.

2:42PM D28.00002 Graphene Growth on Cu Surface: A Theoretical Study[1] , ZHENYU LI, PING WU, WENHUA ZHANG, JINLONG YANG, J. G. HOU, University of Science and Technology of China, THE ELECTRONIC STURCTURE TEAM AT USTC TEAM — Graphene is an important material with many unique properties and a great application potential. A promising way to produce wafer-size graphene is chemical vapor deposition (CVD) on metal surfaces. To improve sample quality, it is important to understand the atomic details during graphene CVD growth. In this talk, some relevant elementary processes on Cu surface have been studied from first principles. Although diffusion of atomic carbon on Cu (111) surface is almost barrierless, coalescence of carbon atoms on the surface is found to be hampered by an intermediate bridging-metal structure. The fact which makes things more complicated is that thermodynamic analysis indicates that the main species on the Cu surface during graphene growth is not the simplest atomic carbon. Therefore, CxHy species should be explicitly considered for initial stage growth of graphene on Cu surface.

[1]Partially supported by NSFC (20933006, 20803071, and 50721091), by MOE (FANEDD-2007B23 and NCET-08-0521), and by MOST(2006CB922004)

2:54PM D28.00003 Graphene Made Easy: A Simple Method to Grow Large-Area Single-Layer Graphene on Copper Foils , S. GADIPELLI, UPENN/NIST, I. CALIZO, NIST, J. FORD, UPENN/NIST, G. CHENG, A. H. WALKER, NIST, T. YILDIRIM[1], NIST/UPENN — In order to realize the remarkable properties of graphene in practical devices, an easy, scalable, and inexpensive synthesis method is necessary. Currently the most promising approach is through chemical vapor deposition (CVD). However, this method requires expensive CVD furnaces and flow controllers, as well as a large amount of explosive gases (H_2 and CH_4). Consequently, it is desirable to establish alternative methods to grow large-area, single-layer graphene that are simple and that can be carried out in an ordinary research laboratory. In this talk, we will discuss our systematic study of the parameters that are critical for high-quality, single-layer graphene formation. Our results not only shed light on the graphene growth mechanism, but have also yielded a straightforward synthesis method that requires neither H_2/CH_4 nor any special CVD equipment. We have prepared graphene samples at the inch scale that have been characterized by Raman spectroscopy, optical transmittance, and sheet resistance measurements. Our method is simple, safe, and economical and will be of value to both fundamental researchers and nanodevice engineers.

[1]Contact author: taner@nist.gov, http://www.ncnr.nist.gov/staff/taner

3:06PM D28.00004 Graphene on metals - structure and properties , JOOST WINTTERLIN, University of Munich — The "metal route" to graphene, i.e., the epitaxial growth of graphene on a metal surface by chemical vapor deposition (CVD) of hydrocarbon molecules and the following transfer of the graphene film to an insulating support, has recently made great progress [see, e.g., S. Bae et al., Nature Nanotechnol. 5, 574 (2010)]. However, structurally and from their charge carrier mobilities, metal-grown graphene samples have not yet reached the quality of exfoliated graphene, most likely resulting from uncontrolled processes during the CVD. In order to better understand how graphene interacts with metal surfaces we have performed a series of surface science studies. As experimental techniques we have applied STM, ARPES, LEED, and SXRD, mainly on Ru(0001)/graphene, and we have performed extensive DFT analyses. We find a short metal-graphene separation, a strong deformation of the graphene, a lifting of the Dirac point, and shifts of the electronic bands. The structural and electronic properties evidence surprisingly strong interactions of the graphene with the Ru surface which are probably prototypical for other metals such as Co, Ni, and Pd. A second group of metals, namely Ir, Pt, Cu, Ag, and Au, only show weak interactions. In situ STM experiments at high temperatures (between 380 and 780 C) show that the usual "carpet mode" by which graphene grows across steps of the metal surface [P. W. Sutter et al., Nature Mater. 7, 406 (2008)] can lead to defects. However, the growth mode changes at high temperatures and low pressures of the hydrocarbon precursor, partially a result of the relatively high Ru-graphene interactions. They lead to a faceting of the surface, and one can grow extremely large single-crystalline graphene films on single terraces in this way.

3:42PM D28.00005 Second-layer graphene growth from below on metals[1] , SHU NIE, ELENA STARODUB, NORMAN BARTELT, KEVIN MCCARTY, Sandia National Laboratories — Once a metal substrate is covered by the first graphene layer, CVD processes slow greatly. However, C dissolved in the metal can still segregate to the surface under the first graphene layer. To determine whether these C atoms nucleate a new layer below or above the first layer, we examine growth on Ir(111), where one-layer graphene has several discrete in-plane orientations relative to substrate directions. LEED reveals that the 1st and 2nd graphene layers are not always rotationally aligned in-plane. This misalignment allows determining which sheets are on the top and the bottom by varying the electron energy and thus the escape depth. We first use LEEM to determine the spatial distribution of rotational domains in a single-layer film. We then cool and observe 2nd layer growth. We find that the top sheet of the bilayer has the exact same domain structure as the initially grown single layer. Thus, new layers are added from below. In this mechanism the nucleation and growth of the 2nd layer strongly depends on the difficulty in debonding the 1st layer from the substrate.

[1]Supported by BES/USDOE under Contract #DE-AC04-94AL85000.

3:54PM D28.00006 Low Temperature Graphene Growth by Down-Stream Chemical Vapor Deposition[1] , LOLA BROWN, MARK LEVENDORF, CHAD HUNTER, JIWOONG PARK, Cornell University — Integration of high quality graphene directly onto the surface of metal provides a novel way of controlling the functionality of metal surfaces. This can be used to control the chemical and physical surface interactions and enhance energy transfer through the surfaces, thus allowing for new sensors, flexible electronic devices and better electrodes for organic photovoltaics. However, the implementation of a pristine graphene layer in patterned devices is currently limited, due to the high temperature growth ($\sim$1000 C) and contamination of the graphene surfaces during transfer. This work presents graphene grown at low temperatures (below 750 C) using down-stream chemical vapor deposition (DS-CVD), where a metallic growth substrate is positioned down-stream from the CVD furnace "hot zone". High quality graphene is produced using long growth times ($\sim$ 60 minutes) and low gas flow rates. We study graphene quality and grain structure using Raman spectroscopy and dark-field transmission electron microscopy (DF-TEM). We demonstrate the strength of this technique by growing graphene on thin and micro patterned copper films, and three dimensional structures.

[1]L.B. is supported by a Fulbright fellowship.

4:06PM D28.00007 Evolution of graphene islands growing on Cu foils[1] , JOSEPH WOFFORD, University of California at Berkeley and Lawrence Berkeley National Laboratory, SHU NIE, NORMAN BARTELT, KEVIN MCCARTY, Sandia National Laboratories, OSCAR DUBON, University of California at Berkeley and Lawrence Berkeley National Laboratory — Using low-energy electron microscopy we investigate, in real time, the growth of graphene monolayers on Cu foils. Graphene islands evolve from an initially compact form into an increasingly ramified, four-lobed shape, reflecting the symmetry of the (100)-textured Cu surface. Diffraction analysis reveals that each lobe is an individual graphene domain, differentiated by a rotation about the film normal, making the islands polycrystalline. An inspection of the morphological evolution of the graphene lobes shows the growth fronts posses an angularly dependent velocity, which is consistent with a growth mode dominated by edge kinetics. The fast growth direction of each lobe tends to align with the <001> in-plane directions of the Cu surface but not with a high symmetry direction of the graphene lattice. Finally, the implications of this unexpected growth mechanism on the formation of high-quality graphene films on Cu foils are evaluated.

[1]Supported by BES/USDOE under contracts #DE-AC04-94AL85000 and #DE-AC02-05CH11231.

4:18PM D28.00008 Characterization of Graphene Films Grown on Cu-Ni Foil by XPS[1]

, P. TYAGI, R.L. MOORE, Z.R. ROBINSON, C.A. VENTRICE, JR., Univ. at Albany, D.D. MOODY, W. PRIYANTHA, R. DROOPAD, Texas State Univ., C. MAGNUSON, D. MUNSON, S. CHEN, R.S. RUOFF, Univ. of Texas — Monolayer graphene films can be grown on Cu substrates by the catalytic decomposition of methane molecules. The solubility of carbon in Cu is negligible at the growth temperatures typically used for graphene growth, which results in the formation of films that self-terminate at a monolayer. In an attempt to enhance the catalytic activity of the surface, use of Cu-Ni alloy foils has been investigated. Growth is performed in a CVD system at a temperature of 1000 $^\circ$C with pure CH_4. To determine the graphene coverage and the surface alloy composition during the different phases of growth, XPS measurements have been performed on the Cu-Ni foils before anneal, after anneal in H_2, and after growth of graphene. Analysis of the C-1s core emission for graphene/Cu is used as reference for monolayer growth. Before anneal, the measurements indicate that the surface is Ni-rich and heavily oxidized. After annealing in H_2, only a small amount of oxide remained and the Cu:Ni alloy fraction was similar to the bulk. After growth of the graphene overlayers, only trace amounts of oxygen are present, indicating uniform graphene growth.

[1]Support from the NSF (1006350 and 1006411) is appreciated.

4:30PM D28.00009 Effects of heat-treatment and hydrogen adsorption on Graphene grown on Cu foil

, JONGWEON CHO, LI GAO, Center for Nanoscale Materials, Argonne National Laboratory, JIFA TIAN, HELIN CAO, Department of Physics, Purdue University, QINGKAI YU, Center for Advanced Materials, University of Houston, JEFFREY GUEST, Center for Nanoscale Materials, Argonne National Laboratory, YONG CHEN, Department of Physics, Purdue University, NATHAN GUISINGER, Center for Nanoscale Materials, Argonne National Laboratory — Graphene has recently been a subject of intense research efforts due to its remarkable physical properties as an ideal two-dimensional material. While numerous different methods for graphene synthesis are being explored, CVD-grown graphene on Cu foil presents the possibility of a large-scale and high-quality synthesis of graphene. [1] To improve the quality of graphene films on Cu foil prepared by CVD and better understand its microscopic growth, atomic-scale characterization becomes of great importance. We have investigated the effects of thermal annealing and hydrogen adsorption/desorption on *ex-situ* CVD-grown monolayer graphene on polycrystalline Cu foil at the atomic-scale using ultrahigh vacuum scanning tunneling microscopy, and we will report on these studies.

[1] Li et al, Science **324**, 1312 (2009).

4:42PM D28.00010 Imaging Grains and Grain Boundaries in Single-Layer CVD Graphene

, P.Y. HUANG, A.M. VAN DER ZANDE, C.S. RUIZ-VARGAS, W.S. WHITNEY, M.P. LEVENDORF, Y. ZHU, J. PARK, P.L. MCEUEN, D.A. MULLER, Cornell University — Single-layer graphene can be produced by chemical vapor deposition (CVD) on copper substrates on up to meter scales [1, 2], making their polycrystallinity [3,4] almost unavoidable. By combining aberration-corrected scanning transmission electron microscopy and dark-field transmission electron microscopy, we image graphene grains and grain boundaries across five orders of magnitude. Atomic-resolution images of graphene grain boundaries reveal that different grains stitch together predominantly via pentagon-heptagon pairs. We use diffraction-filtered imaging to map the shape and orientation of several hundred grains and boundaries. These images reveal an intricate patchwork of grains with structural details depending strongly on growth conditions. These imaging techniques will enable studies on the structure, properties, and control of graphene grains and grain boundaries.

[1] X. Li et al., Science 324, 1312 (2009).
[2] S. Bae et al., Nature Nanotechnol. 5, 574 (2010).
[3] J. M. Wofford, et al.,Nano Lett., (2010).
[4] P.Y. Huang et al., arXiv:1009.4714, (2010).

4:54PM D28.00011 Analysis of Substrate Grain Size and Orientation on the Growth of Graphene Films[1]

, Z.R. ROBINSON, P. TYAGI, T.M. MURRAY, C.A. VENTRICE, JR., CNSE, Univ. at Albany, C. MAGNUSON, D. MUNSON, S. CHEN, R.S. RUOFF, Dept. of Mech. Engr., Univ. of Texas — Graphene growth on Cu foils by catalytic decomposition of methane forms predominately single layer graphene films due to the low solubility of C in Cu. One of the key issues for the use of CVD graphene in device applications is the influence of defects on the transport properties of the graphene. For instance, growth on foil substrates is expected to result in multi-domain graphene growth because of the presence of randomly oriented grains within the foil. Therefore, the size and orientation of the grains within the metal foil should strongly influence the defect density of the graphene. To study this effect, we have initiated a study of the influence of pre-growth anneal time and H_2 pressure on the grain size and structure of Cu and Cu-Ni foil substrates. Preliminary measurements of the grain size have been performed with SEM and AFM. These results show a typical lateral dimension of $\sim$100 μm for an anneal time of 30 min in 40 mTorr of H_2 at 1000 $^\circ$C. Measurements are currently being performed with electron backscatter diffraction to determine the crystallographic orientation within each grain.

[1]Support from the NSF (1006350 and 1006411) is appreciated.

5:06PM D28.00012 Alloy substrates: towards precise control of thickness and quality of multilayer graphene growth

, SHANSHAN CHEN, Univ. of Texas at Austin, WEIWEI CAI, Xiamen University, RICHARD D. PINER, Univ. of Texas at Austin, XUESONG LI, IBM, YANWU ZHU, RODNEY S. RUOFF, Univ. of Texas at Austin — Graphene has gained a lot of attention due to its remarkable properties, such as high electron hole mobility, high current carrying capability and high mechanical robustness. It has been further demonstrated that the properties of graphene materials depend on the number of graphene layers present. As a result, it is highly desirable to develop reliable synthesis techniques to synthesize few- or multi-layered high quality large area graphene materials. Here we report a facile method to grow few-layer graphene films using an alloy substrate by chemical vapor deposition. The thickness and quality of the graphene and graphite films can be controlled using CVD with methane and hydrogen gas as precursors, by varying the deposition temperature and cooling rate. The optical and electrical properties of the graphene/graphite films were studied as a function of their thickness.

5:18PM D28.00013 Improving Polycrystalline Copper Surface by Hydrogen Etching for Graphene Growth[1]

, MERVE ARSEVEN, Advanced Materials Research Group, Nanotechnology and Nanomedicine Department, TAYFUN VURAL, Biopolymeric Systems Research Group, Chemistry Department, ENGIN OZDAS, Advanced Materials Research Group, Physics Department, Hacettepe University, Turkey — Growth of high quality, large scale pattern of graphene is the main important phenomenon to use this material in novel technological applications. CVD methods can provide an effective way to produce graphene, however, require a rigid stable substrate at high temperature processes [1]. Besides, the substrate that can be used in these processes must have low solubility of carbon to obtain mono or few layers of graphene, and be able to provide bigger grains for a large-scale growth [2]. Polycrystalline copper foil is an appropriate candidate to achieve these attributions in case of reducing the pinhole and defect density, and increase the grain size. In this study, we investigate the effect of hydrogen partial pressure, heating rate, annealing temperature and duration on the etching process to optimize the surface. Surface roughness analyses are performed by AFM, and grain size distributions are determined by the analyses of optical microscope images. [1] Sukang Bae *et al.*, Nature Nanotechnology **5**, 574, 2010. [1] Xuesong Li *et al.*, Science **324**, 1312, 2009.

[1]Supported by HU Research Council Grant 08A602010 and 07A601007.

Monday, March 21, 2011 2:30PM - 5:30PM –
Session D29 GQI: Quantum Computing and Simulation I C148

2:30PM D29.00001 Scalable Quantum Computing Over the Rainbow , OLIVIER PFISTER, University of Virginia, NICOLAS C. MENICUCCI, Perimeter Institute, Waterloo, Canada, STEVEN T. FLAMMIA, IQI, Caltech — The physical implementation of nontrivial quantum computing is an experimental challenge due to decoherence and the need for scalability. Recently we proved a novel theoretical scheme for realizing a scalable quantum register of very large size, entangled in a cluster state, in the optical frequency comb (OFC) defined by the eigenmodes of a single optical parametric oscillator (OPO). The classical OFC is well known as implemented by the femtosecond, carrier-envelope-phase- and mode-locked lasers which have redefined frequency metrology in recent years. The quantum OFC is a set of harmonic oscillators, or Qmodes, whose amplitude and phase quadratures are continuous variables, the manipulation of which is a mature field for one or two Qmodes. We have shown that the nonlinear optical medium of a single OPO can be engineered, in a sophisticated but already demonstrated manner, so as to entangle in constant time the OPO's OFC into a finitely squeezed, Gaussian cluster state suitable for universal quantum computing over continuous variables. Here we summarize our theoretical result and survey the ongoing experimental efforts in this direction.

2:42PM D29.00002 Implementing quantum gates through scattering between a static and a flying qubit , GUILLERMO CORDOURIER-MARURI, Cinvestav, Department of Applied Physics, Cordemex 97310, Merida, Mexico, FRANCESCO CICCARELLO, Universit'a degli Studi di Palermo, CNISM, I-90128 Palermo, Italy, YASSER OMAR, Universidade Tecnica de Lisboa, P-1200-781 Lisbon, Portugal, MICHELANGELO Z, Universit'a degli Studi di Palermo, Palermo, Italy, ROMEO DE COSS, Cinvestav, Department of Applied Physics, Cordemex 97310, Mérida, Mexico, SOUGATO BOSE, UCL, Department of Physics and Astronomy, London WC1E 6BT, UK — We investigate whether a two-qubit quantum gate can be implemented in a scattering process involving a flying and a static qubit. We focus on a paradigmatic setup made out of a mobile particle and a quantum impurity, whose respective spin degrees of freedom couple to each other during a one-dimensional scattering process. A condition for the occurrence of quantum gates is derived in terms of spin-dependent transmission coefficients. This can be fulfilled through the insertion of an additional narrow potential barrier. Under resonance conditions this procedure enables a gate only for Heisenberg interactions and fails for an XY interaction. We show the existence of parameter regimes for which gates able to establish a maximum amount of entanglement can be implemented. The gates are found to be robust to variations of the optimal parameters.

2:54PM D29.00003 The 2D AKLT state is a universal quantum computational resource , TZU-CHIEH WEI, University of British Columbia, IAN AFFLECK, ROBERT RAUSSENDORF, University of British Columbia — We demonstrate that the two-dimensional AKLT state on a honeycomb lattice is a universal resource for measurement-based quantum computation. Our argument proceeds by reduction of the AKLT state to a 2D cluster state, which is already known to be universal, and consists of two steps. First, we devise a local POVM by which the AKLT state is mapped to a random 2D graph state. Second, we show by Monte Carlo simulations that the connectivity properties of these random graphs are governed by percolation, and that typical graphs are in the connected phase. The corresponding graph states can then be transformed to 2D cluster states.

3:06PM D29.00004 Robust benchmarking of quantum processes , EASWAR MAGESAN, JAY GAMBETTA, JOSEPH EMERSON, Institute for Quantum Computing, University of Waterloo — Fault-tolerant threshold theorems show that as long as the noise affecting a quantum system is below some threshold, reliable quantum computation can take place. As a result, methods for noise characterization are of great interest in quantum information theory. Unfortunately, methods for complete noise characterization scale exponentially in the number of qubits comprising the system. This non-scalability highlights the importance of developing mathematical methods for scalable partial characterization of the noise affecting a quantum system. We discuss a randomized benchmarking protocol that provides fitting models for the fidelity decay of the noisy gates used in quantum information processing. We show that when the average variation of the noise is not too large the first order model gives a robust estimate of both the average error affecting the gate set and the gate-dependence of the noise. We also show that the protocol is scalable in the number of qubits comprising the system. The protocol allows the noise to be both time and gate-dependent, and takes into account state preparation and measurement errors.

3:18PM D29.00005 Universal Quantum Computation within the Bose-Hubbard Model[1] , MICHAEL S. UNDERWOOD, DAVID L. FEDER, Institute for Quantum Information Science at the University of Calgary — We present a novel scheme for universal quantum computation based on spinless bosons hopping on a two-dimensional lattice with on-site interactions. Our setup is comprised of a $2 \times n$ lattice for an n-qubit system; the two rows correspond to the computational basis states, and a boson in each column encodes a qubit. The system is initialized with n bosons occupying the n sites of the $|0\rangle$ row, and the lattice deep enough to prevent tunneling. Arbitrary single-qubit X rotations are implemented by tuning the tunneling strength between the $|0\rangle$ and $|1\rangle$ sites of the appropriate column, and Z rotations by applying a local potential to the $|1\rangle$ site. Entanglement is generated by hopping between the $|1\rangle$ sites of adjacent qubits; by tuning the on-site interaction strength of the bosons, a non-trivial controlled phase is acquired if these two qubits are in the state $|11\rangle$. Because the quantum information is encoded entirely in the lattice positions of the bosons, the encoded qubits are inherently robust against decoherence. An implementation in terms of ultracold atoms in optical lattices is suggested.

[1]This work was supported by NSERC and iCORE.

3:30PM D29.00006 Optimal Trajectories for Quantum Adiabatic Factoring , JORDAN KYRIAKIDIS, ROBERT ARCHIBALD, Dalhousie Univeristy, WILLIAM MACREADY, D-Wave Systems, Inc. — We show how a classical multiplication circuit can be expressed as an optimization problem. The circuit can then be effectively run backwards by fixing the output states in the optimization problem and determining the corresponding input states, thereby factoring the output state. This can in turn be expressed as a problem in adiabatic quantum computing. We show by solving a coupled set of Euler-Lagrange equations how (locally) optimal trajectories from initial to final Hamiltonians can be found whose efficacy vastly exceeds that of the usual linear scaling trajectory. Explicit examples will be given for factoring 6-bit integers.

3:42PM D29.00007 Deterministic Random-Length Computation with Weakly Entangled Cluster States , ADAM G. D'SOUZA, DAVID L. FEDER, Institute for Quantum Information Science, University of Calgary — Universal quantum computation can be accomplished via single-qubit measurements on a highly entangled resource state, together with classical feedforward of the measurement results. The best-known example of such a resource state is the cluster state, on which judiciously chosen single-qubit measurements can be used to simulate an arbitrary quantum circuit with a number of measurements that is linear in the number of gates. We examine the power of the orbit of the cluster states under GL(2,C), also known as the SLOCC equivalence class of the cluster state, as a resource for deterministic universal computation. We find that, under certain circumstances, these states do indeed constitute resources for such computations, but of random length.

3:54PM D29.00008 Logical operator tradeoff for local quantum codes[1] , JEONGWAN HAAH, JOHN PRESKILL, IQI, Caltech — We study the structure of logical operators in local D-dimensional quantum codes, considering both subsystem codes with geometrically local gauge generators and codes defined by geometrically local commuting projectors. We show that if the code distance is d, then any logical operator can be supported on a set of specified geometry containing $\tilde{d}$ qubits, where $\tilde{d}d^{1/(D-1)} = O(n)$ and n is the code length. Our results place limitations on partially self-correcting quantum memories, in which at least some logical operators are protected by energy barriers that grow with system size. We also show that two-dimensional codes defined by local commuting projectors admit logical "string" operators and are not self correcting.

[1]NSF PHY-0803371, DOE DE-FG03-92-ER40701, NSA/ARO W911NF-09-1-0442, and KFAS

4:06PM D29.00009 ABSTRACT WITHDRAWN –

4:18PM D29.00010 Simulating Concordant Computations , BRYAN EASTIN, Northrop Grumman — A quantum state is called concordant if it has zero quantum discord with respect to any part. By extension, a concordant computation is one such that the state of the computer, at each time step, is concordant. In this talk, I describe a classical algorithm that, given a product state as input, permits the efficient simulation of any concordant quantum computation having a conventional form and composed of gates acting on two or fewer qubits. This shows that such a quantum computation must generate quantum discord if it is to efficiently solve a problem that requires super-polynomial time classically. While I employ the restriction to two-qubit gates sparingly, a crucial component of the simulation algorithm appears not to be extensible to gates acting on higher-dimensional systems.

4:30PM D29.00011 Photonic Phase Gate via an Exchange of Fermionic Spin Waves in a Spin Chain , ALEXEY GORSHKOV, California Institute of Technology, USA, JOHANNES OTTERBACH, Universitat Kaiserslautern, Germany, EUGENE DEMLER, Harvard University, USA, MICHAEL FLEISCHHAUER, Universitat Kaiserslautern, Germany, MIKHAIL LUKIN, Harvard University, USA — We propose a new protocol for implementing the two-qubit photonic phase gate. In our approach, the π phase is acquired by mapping two single photons into atomic excitations with fermionic character and exchanging their positions. The fermionic excitations are realized as spin waves in a spin chain, while photon storage techniques provide the interface between the photons and the spin waves. Possible imperfections and experimental systems suitable for implementing the gate are discussed. [Reference: Phys. Rev. Lett. 105, 060502 (2010)]

4:42PM D29.00012 Scalable Neutral Atom Quantum Computer with Interaction on Demand[1] , MIKIO NAKAHARA, ELHAM HOSSEINI LAPASAR, KENICHI KASAMATSU, TETSUO OHMI, YASUSHI KONDO, Department of Physics, Kinki University — We propose a scalable neutral atom quantum computer with an on- demand interaction. Artificial lattice of near field optical traps is employed to trap atom qubits. Interactions between atoms can be turned off if the atoms are separated by a high enough potential barrier so that the size of the atomic wave function is much less than the interatomic distance. One-qubit gate operation is implemented by a gate control laser beam which is attached to an individual atom. Two-qubit gate operation between a particular pair of atoms is introduced by leaving these atoms in an optical lattice and making them collide so that a particular two-qubit state acquires a dynamical phase. Our proposal is feasible within existing technology developed in cold atom gas, MEMS, nanolithography, and various areas in optics.

[1]Work partially supported by "Open Research Center" Project for Private Universities: matching fund subsidy from MEXT, Japan.

4:54PM D29.00013 General-Purpose Quantum Simulation with Prethreshold Superconducting Qubits , EMILY PRITCHETT, IQC Waterloo, COLIN BENJAMIN, University of Georgia, ANDREI GALIAUTDINOV, UC Riverside, MICHAEL GELLER, ANDREW SORNBORGER, PHILLIP STANCIL, University of Georgia, JOHN MARTINIS, UC Santa Barbara — We introduce a protocol for the fast simulation of n-dimensional quantum systems on n-qubit quantum computers with tunable couplings. A mapping is given between the control parameters of the quantum computer and the matrix elements of an n- dimensional real (but otherwise arbitrary) Hamiltonian that is simulated in the n- dimensional *single-excitation subspace* of the quantum simulator. A time- dependent energy/time rescaling minimizes the simulation time on hardware having a fixed coherence time. We demonstrate how three tunably coupled superconducting phase qubits can simulate a three-channel molecular collision using this protocol. The method makes a class of general-purpose time-dependent quantum simulation practical with today's sub-thershold-fidelity qubits.

5:06PM D29.00014 Currently Realizable Quantum Error Detection/Correction Algorithms for Superconducting Qubits[1] , KYLE KEANE, Department of Physics and Astronomy, University of California, Riverside, ALEXANDER N. KOROTKOV, Department of Electrical Engineering, University of California, Riverside — We investigate the efficiency of simple quantum error correction/detection codes for zero-temperature energy relaxation. We show that standard repetitive codes are not effective for error correction of energy relaxation, but can be efficiently used for quantum error detection. Moreover, only two qubits are necessary for this purpose, in contrast to the minimum of three qubits needed for conventional error correction. We propose and analyze specific two-qubit algorithms for superconducting phase qubits, which are currently realizable and can demonstrate quantum error detection; each algorithm can also be used for quantum error correction of a specific known error. In particular, we analyze needed requirements on experimental parameters and calculate the expected fidelities for these experimental protocols.

[1]This work was supported by NSA and IARPA under ARO grant No. W911NF-10-1-0334.

5:18PM D29.00015 Interface between Topological and Superconducting Qubits[1] , LIANG JIANG, California Institute of Technology, CHARLES KANE, University of Pennsylvania, JOHN PRESKILL, California Institute of Technology — We propose and analyze an interface between a topological qubit and a superconducting flux qubit. In our scheme, the interaction between Majorana fermions in a topological insulator is coherently controlled by a superconducting phase that depends on the quantum state of the flux qubit. A controlled phase gate, achieved by pulsing this interaction on and off, can transfer quantum information between the topological qubit and the superconducting qubit.

[1]This work was supported by the Sherman Fairchild Foundation, by NSF grants DMR-0906175 and PHY-0803371, by DOE grant DE-FG03-92-ER40701, and by NSA/ARO grant W911NF-09-1-0442.

Monday, March 21, 2011 2:30PM - 5:06PM –

Session D30 DCMP: Graphene: Hydrogenation and Defects C147/154

2:30PM D30.00001 Thermal conductivity of partially hydrogenated graphene , JEONG YUN KIM, JEFFREY GROSSMAN, Massachusetts Institute of Technology — Graphene superlattices made with partial hydrogenation are of great interest and have been explored recently due to the enhanced tunability of electronic properties as a function of the hydrogenation pattern. However, the thermal transport properties of such materials have received little attention. In this work, we investigate the effects of 2D periodic patterns of hydrogen atoms on the thermal conductivity of partially hydrogenated graphene using classical molecular dynamics simulations and an Einstein relation. Our calculations show that the thermal conductivity of partially hydrogenated graphene varies substantially as a function of hydrogen coverage, periodicity, edge shape, and width of hydrogenated region compared to the bare graphene region. In addition, we show that the use of patterned 2D shapes of hydrogenation on graphene could lead substantially lower thermal conductivities that may be of interest for thermoelectric applications.

2:42PM D30.00002 Thermoelectric Properties of Hydrogenated Graphene , RUWANTHA JAYASINGHA, KASUN FERNANDO, CHRISTOF KEEBAUGH, ROBERT STALLARD, GAMINI SUMANASEKERA, University of Louisville, Louisville, KY 40292 — We have studied the temperature dependence of thermopower (S) and 4-probe resistance (R) of large area Graphene subjected to various degree of hydrogenation. Graphene samples with electrical contacts mounted within a quartz reactor was placed inside a custom made inductively coupled plasma coil and hydrogen gas was introduced to a pressure of $\sim$ 10 Torr. Samples were placed well away from the plasma and both S and R were monitored *in –situ* during the hydrogenation. At desired level of hydrogenation the plasma was turned off and the sample was cooled down to $\sim$140 K by lowering the reactor into a liquid nitrogen dewar and both R(T) and S(T) were measured. Both S(T) and R(T) show metal to insulator transition characteristics during the progressive hydrogenation. Both epitaxially grown Graphene on Si-terminated face of SiC and Graphene grown by chemical vapor deposition and transferred on to quartz substrate were studied. The CVD grown sample was found to be p-type under ambient condition but could be tuned to n-type after high temperature annealing at 550 K in a vacuum of 2x10^{-7}Torr. In contrast, epitaxial sample was n-type under ambient conditions. However, the hydrogenation was performed on both samples under degassed conditions.

2:54PM D30.00003 The Influence of Hydrogenation on the Hall Effect in Exfoliated Mono- and Multi-layer Graphene , Y. MO, J.D. JONES, P.E. ECTON, M. MANESHIAN, W.D. HOFFMAN, A.V. JESSEPH, N. SHEPHERD, G.F. VERBECK, J.M. PEREZ, University of North Texas, Z. YE, G. ZHAO, Southern University and A&M College — Graphene samples exfoliated from highly ordered pyrolytic graphite are deposited using the standard scotch-tape method on 300nm thick SiO_2 covered and slightly conductive Si substrates. Devices with 4 silver electrode pads on the graphene samples for Hall effect measurements are made with simple evaporation procedures by using transmission electron microscopy grids as masks. At room temperature, we measure the Hall effect of mono- and multi-layer graphene before and after plasma hydrogenation. During plasma hydrogenation, the sample substrates are biased at +150 V to attract electrons in the plasma for hydrogenation and push away ions in the plasma avoiding possible damage to the graphene. We also measure the Hall effect after annealing the samples at 200 $^\circ$C and vacuum of 10^{-6} torr for an hour. Micro-Raman is employed to monitor the quality and change of the graphene at each process step. We compare the Hall effect results for pristine, hydrogenated, and annealed mono- and multi- layer graphene samples.

3:06PM D30.00004 Density of states of a graphene in the presence of strong point defects , BOR-LUEN HUANG, MING-CHE CHANG, Department of Physics, National Taiwan Normal University, CHUNG-YU MOU, Department of Physics, National Tsing Hua University — The density of states near zero energy in a graphene due to strong point defects with random positions are computed. Instead of focusing on density of states directly, we analyze eigenfunctions of inverse T-matrix in the unitary limit. Based on numerical simulations, we find that the squared magnitudes of eigenfunctions for the inverse T-matrix show random-walk behavior on defect positions. As a result, squared magnitudes of eigenfunctions have equal a priori probabilities, which further implies that the density of states is characterized by the well-known Thomas-Porter type distribution. The numerical findings of Thomas-Porter type distribution is further derived in the saddle-point limit of the corresponding replica field theory of inverse T-matrix. Furthermore, the influences of the Thomas-Porter distribution on magnetic and transport properties of a graphene, due to its divergence near zero energy, are also examined.

3:18PM D30.00005 Tuning graphene's electronic structure via unbalanced disordered sublattices and defect superlattices , FRANCOIS VARCHON, AURÉLIEN LHERBIER, JEAN-CHRISTOPHE CHARLIER, UCL IMCN/NAPS — Graphene, a single carbon plane arranged on a honeycomb lattice, has received a lot of attention in the last few years due to its very appealing physical properties as the room temperature quantum hall effect, a large coherence length or a high electronic mobility. These basic properties hold a high application potential for graphene in nanoelectronics. Nevertheless the future of this field strongly depends on the possibility to control the electronic properties of this material. On the basis of extensive tight-binding and ab initio calculations, we demonstrate the possibility to tune graphene's electronic structure via realistic atomic defects (epoxide and hydroxyl groups chemisorbed on graphene). For example we report on the bandgap opening in graphene monolayer induced by unbalanced disordered sublattices. Our findings show that the bandgap width depends on the nature, the concentration and the distribution (random, semi-random, periodic) of the impurities. We also perform an indepth study about the special case of periodic distribution of atomic defects. We demonstrate the existence of three different families of defect superlattices which conduct to specific band structures and therefore could lead to different electronic and transport properties [1].

[1] A. Lherbier, F. Varchon, J.-C. Charlier (in preparation)

3:30PM D30.00006 Numerical study of impurity effects in Graphene[1] , ZHOU LI, FRANK MARSIGLIO, Dept. of Physics, University of Alberta, STEPAN GRINEK, JIE CHEN, Dept. of ECE, University of Alberta — It is known that long-range Coulomb impurities could induce a novel supercritical regime in gapped graphene [1]. For short range impurities, the electron wave function is less localized near the band edge and thus numerical results may depend on the size and boundary conditions of the simulated graphene. For six attractive impurities forming a quantum well with radius=a(a is the distance between two nearest neighbor atoms in graphene), we found that the bound states will not merge into the continuum. The results from a finite size exact diagonalization with open boundary conditions agree well with that from an infinite size study based on Green's functions. Also an efficient numerical approach based on kernel polynomial methods [2] will be adopted to evaluate the Green's function accurately in the regime with strong interference effects and compared to T-matrix results.

[1] V.M. Pereira et.al, Phys. Rev. B, 78, 8, 2008, pp. 085101.
[2] L.Covaci et.al, Phys. Rev. Lett. 105, 167006 (2010)

[1]This work was supported in part by the Natural Sciences and Engineering Research Council of Canada (NSERC), by ICORE (Alberta), by Alberta Ingenuity, and by CIfAR.

3:42PM D30.00007 Plasma Hydrogenation of n-Layer Graphene , J.D. JONES, W.D. HOFFMAN, A.V. JESSEPH, C.J. MORRIS, G.F. VERBECK, J.M. PEREZ, University of North Texas — We propose a new mechanism for the hydrogenation of mono-, bi-, and tri-layer graphene samples using an H_2 plasma. We find that hydrogenation occurs as a result of electron irradiation of H_2O adsorbates on the sample rather than H species from within the plasma. We propose that the mechanism is electron-impact fragmentation of the H_2O adsorbates occurring naturally above and below the sample. The stability of the hydrogenation increases with the incident electron energy, allowing for hydrogenated samples that are stable at temperatures $>$ 200 $^\circ$C. We also observe fully hydrogenated bi- and tri-layer graphene, which may be evidence for new materials, diamane and *triamane*. Diamane, a two atom thick layer of hydrogenated diamond, is predicted to have a band gap of 3.12 eV and be stronger than graphane, hydrogenated graphene.

3:54PM D30.00008 ABSTRACT WITHDRAWN –

4:06PM D30.00009 Oxygen reduction activity of BN decorated bulk defects in graphene , SHYAM KATTEL, BORIS KIEFER, Physics Department, New Mexico State University, PLAMEN ATANASSOV, Chemical and Nuclearing Department, University of New Mexico — We use Density-Functional-Theory to investigate the interaction between O_2 and H_2O_2 with co-doped bulk BN defects in graphene. The results show that the mixed defects are thermodynamically stable in contrast to the nitrogen only defects that need a transition metal for stabilization. The interaction between O_2 and H_2O_2 and the BN defects are found to be very different: O_2 is adsorbed as a molecule on boron with a bond length increase of $\sim$20%. H_2O_2, on the other hand, is predicted to adsorb dissociatively to form $B(OH)_2$. The predicted binding energy (BE) of O_2 is similar to the N only defects. This observation suggests that BN defects promote the reduction of O_2 to H_2O_2. However, we also found that the binding energy per OH is $\sim$75% higher than the corresponding BE for the N only defect. Thus, restoring the catalytic site through OH removal is more difficult as compared to the N only defect. This implies that bulk BN defects are most likely less active than N only defects and edge BN defects which enhance ORR.

4:18PM D30.00010 Effect of Laser Irradiation on Structural and Electronic Properties of Single-layer and Bi-layer Graphene , PUBUDU GALWADUGE, JOSEPH LAMBERT, ROBERTO RAMOS, Drexel University — Graphene is a two-dimensional crystal with remarkable electronic properties which have made it a component of interest in fabricating chemical sensors, superconducting devices and room-temperature transistors. Fabrication and metrology techniques typically use energetic beams such as lasers which are likely to induce unintentional changes in graphene. We report results of Time-Resolved Raman Spectroscopy experiments that investigate the effect of low,medium, and high power laser irradiation on the structural and electronic properties of single-layer and bi-layer graphene. We have irradiated graphene using a 514.5nm laser at power levels of 1.8mW, 9mW and 18mW. Changes in electronic and structural properties were observed by observing the time evolution of the Raman D and G bands. Under irradiation at 1.8mW and 9mW, single layer graphene flakes show changes in charge carrier concentration. Under irradiation at 18mW,single layer graphene shows signs of defect formation and breakdown into nano-crystalline graphene. Bi-layer graphene shows no measurable changes in the Raman D and G bands under irradiation at 9mW.

4:30PM D30.00011 Effect of irradiation by electron-beam and oxygen plasma on graphene studied with Raman spectroscopy and electronic transport , ROMANEH JALILIAN, NaugaNeedles, ISAAC CHILDRES, LUIS A. JAUREGUI, Purdue University, MICHAEL FOXE, Penn State, JIFA TIAN, Purdue University, IGOR JOVANOVIC, Penn State, YONG P. CHEN, Purdue University — We report a study of the effects of electron-beam irradiation and oxygen plasma etching on graphene and graphene field-effect transistors (GFET). For both types of exposure, Raman spectra show a characteristic evolution with increasing irradiation-induced disorder. Electron-beam exposure causes a down-shifting in the charge-neutral point (CNP), interpreted as due to a hole-doping in the substrate. Oxygen plasma etching causes an up-shifting of the CNP, interpreted as due to hole-doping molecules adsorbed on the plasma-induced defects. Both types of exposure decrease the carrier mobilities and minimum conductivity of graphene. Additionally, weak localization and the quantum Hall effect are characterized in exposed devices. Our findings are valuable for understanding the effects of irradiation damage on graphene and the physics of disordered graphene through artificially generated defects.

4:42PM D30.00012 Stability and Mobility of Vacancy Defects in Monolayer Graphene[1] , WEI CHEN, U of Tennessee-Knoxville, HAIPING LAN, PING CUI, JINLONG YANG, U of Sci. and Tech. of China, ZHENYU ZHANG, Oak Ridge National Lab, U of Tennessee-Knoxville, U of Sci. and Tech. of China — Using DFTB and first-principle calculations, we study the stability and mobility of vacancy defects in graphene. First, we calculate the formation energy of vacancy defects of varying sizes in different supercells, including its dependence on the Brillouin zone sampling. We find a large difference, of 1eV, in the formation energy between the value with only Gamma-point sampling and that with more symmetrical k-point sampling in the 3N*3N (N=2,3,4) supercells. This variance is attributed to significant contributions of the electronic states around the Dirac points. We then explore the mobility of the vacancy defects, including single atom vacancy, trivacancy, and tetravacancy. We find that both trivacancy and tetravacancy have relatively small activation energies for migration via a Stone-Wales transformation of the edge atoms. These results will be compared with recent experimental observations.

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

4:54PM D30.00013 Controllable defect healing and N-doping of graphene by CO and NO molecules[1] , BIN WANG, Department of Physics and Astronomy, Vanderbilt University, SOKRATES PANTELIDES, Department of Physics and Astronomy, Vanderbilt University and Oak Ridge National Laboratory — Controllable defect healing and N-doping in graphene would be very valuable for potential device applications. Here we report first-principles molecular dynamic simulations that suggest a procedure with fast dynamics and low thermal budget. Vacancies can be healed by sequential exposure to CO and NO molecules. A CO molecule gets adsorbed at a vacancy site and a NO molecule subsequently removes the extra O by forming NO_2. Controllable N-doping can be achieved by sequential vacancy creation (e.g. by electron beam) and subsequent exposure to NO molecules at room temperature. A combination of CO and NO molecules can potentially provide simultaneous healing and doping at a desirable ratio. The proposed strategy introduces no extra defects and is promising for graphene-based materials in radiation environments.

[1]This work was supported by DTRA Grant No. HDTRA1-10-1-0016 and the William A. and Nancy F. McMinn Endowment at Vanderbilt University. The calculations were performed at ORNL's Center for Computational Sciences.

Monday, March 21, 2011 2:30PM - 5:18PM –

Session D31 DMP: Focus Session: van der Waals Bonding in Advanced Materials: Applications to Advanced and Functional Materials C145

2:30PM D31.00001 Rotational and vibrational excitations of van der Waals bonded hydrogen in nanoporous materials: calibrating first-principle calculations with experiments[1] , LINGZHU KONG, Princeton University — The adsorption of H_2 within a metal-organic framework is studied via van der Waals density-functional calculations and maximally-localized-Wannier- function analysis. The calculated low-lying vibrational and rotational energy states as well as the adsorption sites are consistent with experiments. The induced dipole due to H_2 bond stretching and its quantum mechanic matrix element is found to be accurately given by a first-principles driven approximation. The resulting calculations of IR intensity explain the experimentally mysteriously missing primary line for para hydrogen. The strengths and positions of lines in the complex spectra of rotational-vibrational transitions are in reasonable agreement with experiment, and a selection rule is obtained.

[1]This work was performed under the supervision of Prof. David C. Langreth and supported by grant DOE-DE-FG02-08ER46491.

3:06PM D31.00002 CO2 Binding in Zeolitic Imidazolate Frameworks from First Principles Calculations , KEITH RAY, DAVID OLMSTED, NING HE, YAO HOUNDONOUGBO, BRIAN LAIRD, MARK ASTA — Zeolitic Imidazolate Frameworks (ZIFs) are excellent candidate carbon capture materials owing to their high surface area, selectivity, and stability. In this work we use electronic-structure based methods to investigate the binding of CO2 in a set of ZIFs that share the same topology but feature different functionalized linkers [1]. Since a large portion of the CO2 binding comes from van der Waals (vdW) forces, we explore several different schemes for incorporating these contributions into ab-initio density-functional-theory (DFT) including vdW-DFT [2]. The results are combined with those of classical simulation studies to allow comparisons between calculations and experimentally measured values of the heat of adsorption and adsorption isotherms [1]. This research is supported by the Energy Frontier Research Center "Molecularly Engineered Energy Materials," funded by the US Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001342.
[1] W. Morris, B. Leung, H. Furukawa, O. K. Yaghi, N. He, H. Hayashi, Y. Houndonougbo, M. Asta, B. B. Laird, and O. M. Yaghi, J. AM. CHEM. SOC. 132, 11006-11008 (2010)
[2] M. Dion, H. Rydberg, E. Schroder, D. C. Langreth, and B. I. Lundqvist, Phys. Rev. Let. 92, 246401 (2004)

3:18PM D31.00003 The Importance of van der Waals Interactions in the Stability of the Phases of $Mg(BH_4)_2$, BRIAN KOLB, Wake Forest University, ANDRZEJ BIL, ALEKSEY KOLMOGOROV, University of Oxford, TIMO THONHAUSER, Wake Forest University — As hydrogen gains attention as a potential replacement for fossil fuels, materials to store hydrogen safely and efficiently are becoming increasingly important. Metal borohydrides are attracting much attention for this role and, in particular, $Mg(BH_4)_2$ is a promising candidate for hydrogen storage because of its relatively high hydrogen content (over 12 wt%) and the abundance of its constituent elements. This system has been investigated previously, both experimentally and via density functional theory (DFT) studies. These two approaches give conflicting results, however, regarding the identity of the low-temperature ground-state. In this work, we investigate the impact of van der Waals (vdW) interactions on the stability of various phases of $Mg(BH_4)_2$. vdW interactions are included both through the fully self-consistent vdW-DF approach as well as the semi-empical PBE-D/PBE-D* approach. Our results settle the longstanding discrepancy between theory and experiment, as we find inclusion of vdW interactions stabilizes the experimentally determined ground-state structure at low temperature, relative to those predicted by previous DFT studies.

3:30PM D31.00004 Influence of van der Waals contact forces on the deformation mechanics of thin flexible membranes assembled from metallic or semiconducting single-wall carbon nanotubes[1] , ERIK K. HOBBIE, JOHN HARRIS, SWATHI IYER, NDSU, JI YEON HUH, JEFFREY A. FAGAN, STEVEN D. HUDSON, CHRISTOPHER M. STAFFORD, NIST — Thin membranes of single-wall carbon nanotubes (SWCNTs) assembled from either metallic or semiconducting SWCNTs are subjected to the compressive strains imposed by a stretched elastic substrate, and the mechanical characteristics of the membranes are inferred from the topography of the wrinkling instability that emerges. By depositing comparable films on quartz, we also use optical (UV-Vis-NIR) absorption spectroscopy to compute the effective London dispersion spectra of the purified materials, and from these we compute the attractive part of the van der Waals potential between nanotubes of identical electronic type as a function of separation and relative orientation. We find significant differences in the strength and shape of the contact potential depending on electronic type, which in turn are evident in the modulus and yield strain measured from the deformation of the films.

[1]Supported by the NSF through CMMI-0969155 and the DOE through DE-FG36-08GO88160

3:42PM D31.00005 Electrostatic Origin of Meandering C60 Chain Formation at ZnPc Interfaces[1] , JANICE REUTT-ROBEY, QIANG LIU, LEVAN TSKIPURI, WEI JIN, JOHN WEEKS, University of Maryland, DANIEL DOUGHERTY, NC State University, STEVE ROBEY, NIST — We present STM investigations of interface-formation and nanophase separation in binary films of zinc phthalocyanine (ZnPc) and C_{60} on Ag(111) and Au(111) supports. We report ZnPc:C_{60} 1-D and 2-D interfaces with distinctive molecular orientations and unusually low C_{60} packing densities. Meandering C_{60} chains of single-molecular width arise without registration to the underlying ZnPc template, islanding into a disordered chain phase. These structures are reminiscent of dipole fluids (albeit of single molecular widths!) We present detailed measurements and analysis of C_{60} wandering chain formation on ZnPc/Ag (111) and ZnPc/Au (111) substrates. We explore the physical origin of these structures through simulations with a model potential that incorporates short-range C_{60} – C_{60} attraction and a long-range dipolar repulsion. From simulations of realized structures, we estimate the effective dipole needed for chain formation. DFT calculations on the C60/ZnPc/Ag(111) structure support these conclusions and provide more detailed insight on the electrostatic interactions that drive chain formation.

[1]This work has been supported by the UMD MRSEC (DMR 0520471) and NSF Surface and Analytical Chemistry(CHE0750203).

3:54PM D31.00006 How van der Waals interactions affect alanine-based polypeptides , M. ROSSI, V. BLUM, X. REN, A. TKATCHENKO, M. SCHEFFLER, Fritz-Haber-Institut, Berlin — van der Waals interactions play a critical role among the intramolecular interactions that stabilize secondary structure folding motifs in polypeptides. In this work, we quantify its influence *ab initio* for the series of helix-forming alanine based polypeptides Ac-Ala_n-LysH^+ (n = 4-15). We show that: (i) applying a van der Waals (vdW) correction based on the self-consistent electron density [2] to the PBE functional, a clear α-helical conformational preference emerges at n=8, in agreement with experiment [1], while a mostly 3_{10} helical structure is preferred at plain PBE; (ii) a numeric atom-centered orbital basis enhanced specifically to converge conformational energy differences from explicitly correlated methods (MP2, EX+cRPA and beyond [3]) gives us benchmark capabilities for treatments that include long-range correlations outrightly; (iii) exploring the free energy surface through *ab initio* dynamics for longer helices (n=15) we see a dramatic influence of vdW interactions for high temperature stability and surface explored by these molecules. Our results demonstrate that we are now in a position to quantify vdW contributions accurately, and thus unravel their critical qualitative role in comparison to other contributions (strain, H-bonds) in medium-sized biomolecules. [1] Kohtani and Jarrold, JACS 108, 8454 (2004); [2] Tkatchenko and Scheffler, PRL 102, 073055 (2009); [3] http://www.fhi-berlin.mpg.de/aims

4:06PM D31.00007 Dispersion Forces and Self-assembly of Styrene Nanowires on H-Si(100) 2×1 Surface[1] , GUO LI, Institute of Physics, CAS, P. R. China; U of Tennessee at Knoxville, VALENTINO COOPER, Oak Ridge National Laboratory, JUN-HYUNG CHO, Hanyang University, Korea, SHIXUAN DU, HONGJUN GAO, Institute of Physics, CAS, P. R. China, ZHENYU ZHANG, Oak Ridge National Laboratory; U of Tennessee at Knoxville — We present our first-principles investigation of the influence of dispersion forces (or van der Waals interactions) on the self-assembly of styrene nanowires on the hydrogenated Si(100) 2×1 surface. Using density functional theory (DFT) calculations and kinetic Monte Carlo (KMC) simulations we demonstrate that the dispersion forces enhance the binding between styrene molecules thus allowing us to tune the preferential growth of long wires for the fabrication of desired nanopatterns. Furthermore, this approach is a step towards accurate fully first-principles studies of the effects of dispersion forces on the dynamics at interfaces, and therefore will be invaluable to our understanding of chemical processes such as self-assembly and the catalysis of organic chemical reactions.

[1]Supported by NNSF, "863" and "973" programs of China; Research sponsored by the DOE, Office of Basic Energy Sciences, MSED, USNSF; and NRF of Korea (KRF-2009-0073123).

4:18PM D31.00008 Morphological Control in the Synthesis of Silver Nanostructures: Role of Polyvinylpyrrolidone[1] , KRISTEN FICHTHORN, HAIJUN FENG, RAJESH SATHIYANARAYANAN, Penn State University — Solution-phase syntheses are useful for assembling metallic nanostructures with desired morphologies. For example, a wide variety of silver nanostructures have been synthesized in the polyol process [1], including nanowires, nanoplates, cubes, etc. Polyvinylpyrrolidone (PVP) plays a key role in controlling nanostructure morphologies in these fabrication processes. Based on experimental observations, the interaction strength between PVP chains and Ag atoms in different crystallographic facets is expected to vary significantly and this shape selectivity is expected to play a key role in directing the formation of various nanostructures. Using first-principles calculations based on density-functional theory including van der Waals interactions, we compute the interactions of the basic elements of a repeat unit in PVP (2-pyrollidone and ethane) with various crystal faces of Ag. Our results indicate that PVP does exhibit the expected structure sensitivity and that this arises from an interesting balance between van der Waals interactions and direct chemical bonding. We discuss the ramifications of our calculations for the assembly of Ag nanostructures.

[1] B. Wiley et al., Chem. Eur. J. 11, 454 (2005).

[1]Supported by DOE Grant # DE-FG0207ER46414.

4:30PM D31.00009 Structure and Formation of Synthetic Hemozoin: Insights from First Principles Calculations , NOA MAROM, University of Texas at Austin, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut, Berlin, SERGEY KAPISHNIKOV, LEEOR KRONIK, LESLIE LEISEROWITZ, Weizmann Institute of Science, Israel — Malaria has reemerged due to parasite resistance to synthetic drugs that act by inhibiting crystallization of the malaria pigment, hemozoin (HZ). Understanding the process of HZ nucleation is therefore vital. The crystal structure of synthetic HZ, β-hematin (βH), has recently been determined via x-ray diffraction. We employ van der Waals (vdW) corrected density functional theory to study the βH crystal and its repeat unit, a heme dimer. We find that vdW interactions play a major role in the binding of the heme dimer and the βH crystal. Accounting for the βH periodicity is a must for obtaining the correct geometry of the heme dimer, due to vdW interactions with adjacent dimers. The different isomers of the heme dimer are close in energy, consistent with the observed pseudo-polymorphism. We use these findings to comment on βH crystallization mechanisms.

4:42PM D31.00010 Adsorption of methane on Zn(bdc)(ted)0.5 microporous metal-organic framework , VAIVA KRUNGLEVICIUTE, Southern Illinois University Carbondale, SANHITA PRAMANIK, Rutgers, The State University of New Jersey, ALDO MIGONE, Southern Illinois University Carbondale, JING LI, Rutgers, The State University of New Jersey — Zn(bdc)(ted)0.5 is metal-organic framework crystallized in a tetragonal space group with a 3D porous structure containing intersecting channels of two different sizes. The larger channels are parallel to the c axis and have a cross section 7.5 $\times$ 7.5Å. The smaller channels are along both the a- and b-axes and have a cross section of 4.8 $\times$ 3.2Å. We measured methane adsorption isotherms at several different temperatures between 82 and 102 K. We calculated the effective specific surface area, isosteric heat and binding energy values. Two distinct substeps were observed in the isotherms corresponding to two different adsorption sites. The origin of the substeps will be discussed.

4:54PM D31.00011 Understanding H_2-H_2 interactions in Metal Organic Frameworks (MOFs) with unsaturated metal centers[1] , NOUR NIJEM, JEAN F. VEYAN, Univeristy of Texas at Dallas, LINGZHU KONG, YONGGANG ZHAO, JING LI, DAVID LANGRETH, Rutgers University, YVES J. CHABAL, Univeristy of Texas at Dallas — Unsaturated Metal Organic Frameworks (MOFs) are particularly interesting due to their high H_2 uptakes with relatively large isosteric heats of adsorption (Q_{st} >8 kJ/mol). This work explores H_2-H_2 interactions between adsorbed H_2 at the different sites in MOF-74 (M_2(dhtp),dhtp=2,5-dihydroxyterephthalate) and combines IR spectroscopy with vdW-DFT calculations. The adsorption sites in MOF-74 are from highest to lowest binding energies the metal, oxygen, benzene and pore-center sites. The frequency of adsorbed H_2 at the metal site suffers an additional $\sim$-30 cm^{-1} red shift (for Mg and Zn) and $\sim$-84 cm^{-1} (for Co) when the neighboring oxygen site is occupied. The dipole moment of adsorbed H_2 is also affected. These interactions extend to the benzene sites for MOF-74-Co. A decrease in dipole moment of H_2 adsorbed at the metal site is observed with the partial occupation of the benzene sites. However, the complete occupation of the benzene sites induces an additional $\sim$-10 cm^{-1} red shift.

[1]DOE Grant No. DE-FG02-08ER46491

5:06PM D31.00012 First-Principles Calculations of the Role of Dispersive Interactions in CO_2 binding in metal-organic frameworks , ROBERTA POLONI, University of California, Berkeley; Molecular Foundry, LBNL; University of California, Davis, JOSHUA HOWE, University of California, Berkeley, JEFFREY B. NEATON, Molecular Foundry, LBNL, GIULIA GALLI, University of California, Davis, BEREND SMIT, University of California, Berkeley and LBNL — Metal-organic frameworks (MOFs) have attracted much attention over the past 20 years for their possible applications in gas storage. In this study, we provide computational insight into what makes a MOF structure optimum for CO_2 capture. We present a density functional theory-based study of the electronic and structural properties of recently synthesized frameworks M'$_3$[(M$_4$Cl)$_3$(BTT)$_8$]$_2$, with M'=extraframework cation and M=Ca [1]. We study the interactions between CO_2 and different binding sites, and predict an unexpected favored binding site at the organic linker. We explore how binding energies are affected by the ordering and type of the extraframework cations. Finally, we address the role of dispersion forces by employing a recent non-local van der Waals functional [2], and compare with a DFT+D approach [3].

[1] M. Dinca et al., *J. Am. Chem. Soc.* 128, 16876 (2006)
[2] M. Dion et al., *Phys. Rev. Lett.* 92, 246401 (2004)
[3] A. Tkatchenko et al., *Phys. Rev Lett.* 102, 073005 (2009)

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D32 DMP: Focus Session: Optical Properties of Nanostructures and Metamaterials III

C144

2:30PM D32.00001 Spatial gradient tuning in metamaterials , TOM DRISCOLL, Duke, UCSD, MICHAEL GOLDFLAM, UCSD, NAN JOKERST, Duke, DIMITRI BASOV, UCSD, DAVID SMITH, Duke — Gradient Index (GRIN) metamaterials have been used to create devices inspired by, but often surpassing the potential of, conventional GRIN optics. The unit-cell nature of metamaterials presents the opportunity to exert much greater control over spatial gradients than is possible in natural materials. This is true not only during the design phase but also offers the potential for real-time reconfiguration of the metamaterial gradient. This ability fits nicely into the picture of transformation-optics, in which spatial gradients can enable an impressive suite of innovative devices. We discuss methods to exert control over metamaterial response, focusing on our recent demonstrations using Vanadium Dioxide. We give special attention to role of memristance and mem-capacitance observed in Vanadium Dioxide, which simplify the demands of stimuli and addressing, as well as intersecting metamaterials with the field of memory-materials.

2:42PM D32.00002 Carrier concentration dependence of the tunability of the dipole resonance peak in optically excited metamaterials , IOANNIS CHATZAKIS, LIANG LUO, JIGANG WANG, NIAN HAI SHEN, THOMAS KOSCHNY, COSTAS SOUKOULIS, Department of Physics and Astronomy and Ames Laboratory, Iowa State University, Ames, Iowa 50011, USA — Currently, there is strong interest to explore the dynamic control of the electromagnetic properties of metamaterials, which have important implications on their optoelectronic applications. While the design, fabrication and photo-doping of metamaterial/semiconductor structures have been actively pursued, some fundamental issues related to highly photo-excited states, their dynamic tuning and temporal evolution remain open. Using optical-pump terahertz probe spectroscopy, we report on the pump fluence dependence of the electric dipole resonance tunability in metamaterials. We find a previously undiscovered large non-monotonic variation on the strength of the dipole resonance peak with the photo-injected carrier concentration.

2:54PM D32.00003 Optically-Nonactive Assorted Helices Array with Interchangeable Magnetic/Electric Resonance[1] , MU WANG, XIANG XIONG, RU-WEN PENG, XIAO-CHUN CHEN, DAJUN SHU, Department of Physics, Nanjing University, CHENG SUN, Department of Mechanical Engineering, Northwestern University — We report here the designing of optically-nonactive metamaterial by assembling metallic helices with different chirality. With linearly polarized incident light, pure electric or magnetic resonance can be selectively realized, which leads to negative permittivity or negative permeability accordingly. Further, we show that pure electric or magnetic resonance can be interchanged at the same frequency band by merely changing the polarization of incident light for 90 degrees. This design demonstrates a unique approach to construct metamaterial.

[1]Project supported by NSF of China and MOST of China under Grant Nos. 50972057, 10874068, 11034005, 61077023 and 2010CB630705

3:06PM D32.00004 Three-dimensional optical metamaterials and nanoantennas: Chirality, Coupling, and Sensing , HARALD GIESSEN, University of Stuttgart — This abstract not available.

3:42PM D32.00005 Temperature-Tunable Transparency Window in Metamaterials Utilizing Superconducting Dark Resonators , C. KURTER, University of Maryland, A.P. ZHURAVEL, National Academy of Sciences of Ukraine, P. TASSIN, T. KOSCHNY, L. ZHANG, Ames Laboratory, J. ABRAHAMS, C.L. BENNETT, University of Maryland, A.V. USTINOV, Karlsruhe Institute of Technology, C.M. SOUKOULIS, Ames Laboratory, S.M. ANLAGE, University of Maryland — We have developed a high quality-factor microwave frequency metamaterial to demonstrate a coherent optical phenomena analogous to electrically induced transparency (EIT). The two-dimensional design employs double planar Nb split rings acting as dark resonators symmetrically placed around a thick Au strip which is a bright resonator [1]. When Nb is in the superconducting state, the significant loss gradient between Nb and Au opens a transparency window along with a strongly enhanced group delay. The data show a systematic evolution with increasing temperature in the superconducting state of Nb, and the features disappear in the resistive state when the loss gradient between the two types of resonators closes. We have observed no RF power dependence of the magnetic response coming out of the EIT configuration, which indicates the process is linear. Laser scanning microscopy images of the RF current distributions in the dark resonators and the other microwave measurements are in good agreement with the simulations run on the same structure.
[1] L. Zhang, *et al.* arXiv:1010.2976

3:54PM D32.00006 Light propagation and Anderson localization in superlattices containing metamaterials: effects of correlated disorder , RAIMUNDO ROCHA DOS SANTOS, Universidade Federal do Rio de Janeiro, DMITRI MOGILEVTSEV, Institute of Physics, NASB, FELIPE PINHEIRO, Universidade Federal do Rio de Janeiro, SOLANGE CAVALCANTI, Universidade Federal de Alagoas, LUIZ OLIVEIRA, UNICAMP — We discuss the effect of correlated disorder on light propagation and Anderson localization in a one-dimensional superlattice made up of air (A) and a dispersive metamaterial (M). Disorder is incorporated by assuming the layer widths to be random variables; however, here we consider the cases of correlated (i.e., the A and M layers with the same width) and completely anti-correlated (the total width of the A and M layers is fixed). We use transfer matrix techniques to obtain the localization length, and compare with the uncorrelated case. We have found that the photonic gaps of the corresponding periodic structure are not completely destroyed in the presence of disorder, giving rise to minima in the localization length. Near a gap, the behavior the localization length depends crucially on the physical origin of the gap (Bragg or non-Bragg gaps). We have found that the asymptotic behavior for the localization length $\xi \propto \lambda^6$ for disordered metamaterials is not affected by correlations, and the Brewster anomalies, at which light is delocalized, are also present.

4:06PM D32.00007 Active Terahertz Metamaterials[1] , ANTOINETTE TAYLOR, Los Alamos National Laboratory — In recent years terahertz technology has become an optimistic candidate for numerous sensing, imaging, and diagnostic applications. Nevertheless, THz technology still suffers from a deficiency in high-power sources, efficient detectors, and other functional devices ubiquitous in neighboring microwave and infrared frequency bands, such as amplifiers, modulators, and switches. One of the greatest obstacles in this progress is the lack of materials that naturally respond well to THz radiation. The potential of metamaterials for THz applications originates from their resonant electromagnetic response, which significantly enhances their interaction with THz radiation. Thus, metamaterials offer a route towards helping to fill the so-called "THz gap". Here, we present a series of novel THz metamaterials. Importantly, the critical dependence of the resonant response on the supporting substrate and/or the fabricated structure enables the creation of active THz metamaterial devices. We show that the resonant response can be controlled using optical or electrical excitation and thermal tuning, enabling efficient THz devices which will be of importance for advancing numerous real world THz applications.

[1]We acknowledge contribution to this work from H. Chen, J. O'Hara, A. Azad, J. Zhou, R. Singh, M. Reiten, and D. Chowdhury of the Center for Integrated Nanotechnologies.

4:42PM D32.00008 Optical properties of chiral metal nanoparticle complexes: Plasmonic chirality and circular dichroism[1] , ZHIYUAN FAN, ALEXANDER GOVOROV, Department of Physics and Astronomy, Ohio University, Athens, Ohio 45701, DEPARTMENT OF PHYSICS AND ASTRONOMY, OHIO UNIVERSITY TEAM — Plasmonic nanocrystals with chiral geometries are able to create strong circular dichroism (CD) signals in the visible wavelength range. This offers an interesting possibility to design colloidal and other nanostructures with strong optical chirality for applications in biosensors and optoelectronic devices. We present a theoretical study of circular dichroism from chiral metal nanoparticle (NP) complexes. Dipolar Coulomb interactions between NPs are involved as the main mechanism of interaction between spherical NPs in a chiral complex. In our analysis, the CD signal shows strong dependence on geometry and composition of chiral pyramids, tetramers, and helices. The CD spectra have both positive and negative bands. Strongest CD signals were found in helical chains of metal NPs, which resemble helical structures of many biomolecules.

[1]This work was supported by NSF (project number CBET-0933415), Air Force Research Laboratories, Dayton, Ohio, and BNNT Initiative at Ohio University.

4:54PM D32.00009 Plasmonic Behavior of Deep Sub-Wavelength Superconducting RF Metamaterials[1] , STEVEN ANLAGE, CIHAN KURTER, LIZA SARYTCHEV, JOHN ABRAHAMS, C. BENNETT, TIAN LAN, University of Maryland, A. P. ZHURAVEL, Verkin Inst. Low Temp. Phys., NAS Ukraine, A. V. USTINOV, Karlsruhe Inst. Tech. — We have designed and built ultra-small RF metamaterials with magnetically active spiral elements made of superconducting Nb films [1]. RF transmission measurements on single, 1-D and 2-D arrays of spirals show robust magnetic response when Nb is in the superconducting state [2] at frequencies as low as 14 MHz (corresponding to wavelength $\sim$ 3000 * 'atom' size). Numerical simulations capture the main features of the experimental spectra. The resonant features are tunable via variations in temperature and RF magnetic field [3]. As temperature approaches T_c, the superconducting kinetic inductance contribution to the total inductance increases, placing this RF metamaterial in the plasmonic limit. We study this approach to the plasmonic limit and compare to the analogous situation of frequency approaching the plasma edge in normal metal metamaterials.

[1] S. M. Anlage, J. Opt. 13, 024001 (2011).
[2] C. Kurter, *et al.*, Appl. Phys. Lett. 96, 253504 (2010).
[3] C. Kurter, *et al.*, IEEE Trans. Appl. Supercond., in press. arXiv:1008.2020.

[1]Supported by ONR through Grant No. N000140811058 and CNAM.

5:06PM D32.00010 Invisibility Using Perfect Absorption CNT Carpet at Visible Frequency and Beyond , L. JAY GUO, HAOFEI SHI, JONG OK, HYOUNGWON BAAC, Center for Nanophotonics and Spintronics, University of Michigan — The concept of invisibility cloak based on transformation optics and metamaterials has tantalized the scientific community. Cloaking of wavelength-size objects were realized at microwave and NIR frequencies. However, the complexity of metamaterials based on the previous principles limits the object to several wavelengths in size. Moreover, cloaking of 3-D objects at visible band demands challenging inhomogeneous 3D nanostructured metamaterials and still unattainable. We propose a perfect absorption ground plane cloak that works at visible range and for large area arbitrarily shaped 3D objects. Such homogeneous perfect absorption carpet is demonstrated by low density carbon nanotube (CNT) forest, which can visually compress arbitrary 3D objects to appear as a 2D perfect absorption sheet. Invisibility was observed by naked eyes for unpolarized light at entire visible band with cloaking area of 10^5 larger than a wavelength. Such a cloaking approach based on perfect absorption is not restricted to CNT carpet, and can be applied to a broader frequency range from UV to THz and acts as a universal cloak for arbitrarily large objects. In this scheme the deep space is a natural and perfect "ground plane". It would only take a "cloak" consisting of low density and broadband absorbing particles to render matters and objects totally "dark" to our current instruments.

5:18PM D32.00011 Collective dynamics in optomechanical arrays , FLORIAN MARQUARDT, University of Erlangen-Nuremberg and Max-Planck Institute for the Science of Light, GEORG HEINRICH, MAX LUDWIG, University of Erlangen-Nuremberg, JIANG QIAN, University of Munich, BJÖRN KUBALA, University of Erlangen-Nuremberg — Photonic crystals can support both localized optical and vibrational modes that couple to each other, leading to a very strong optomechanical interaction. These so-called "optomechanical crystals" have been demonstrated experimentally recently. Here we explore the dynamics that results in an array of many coupled optomechanical cells, when these are driven into a regime of self-sustained oscillations. We find synchronization of these oscillations beyond a certain coupling strength. We show that the slow phase dynamics can be efficiently described by an effective Kuramoto model. Other dynamical regimes like chaos will also be accessible in these novel systems.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D33 DMP DCOMP: Focus Session: Dielectric, Ferroelectric, and Piezoelectric Oxides: Multiferroics C143/149

2:30PM D33.00001 Oxygen rotation driven ferroelectricity enables controllable magnetization-polarization coupling in $Ca_3Mn_2O_7$, CRAIG FENNIE, NICOLE BENEDEK, School of Applied and Engineering Physics, Cornell University — We show how to achieve the electric field switching of magnetism in a multiferroic with a large polarization by having the ferroelectric state arise from the same lattice instability that modulates the spin system. Oxygen octahedron rotations, ubiquitous in perovskites and related materials, are natural candidates for this lattice instability. First-principles calculations are presented for the layered perovskite $Ca_3Mn_2O_7$, in which rotations induce both ferroelectricity and weak ferromagnetism. The key point is that this rotation pattern is a combination of two non-polar structural modes with different symmetries. We introduce the term "hybrid" improper ferroelectricity to describe this phenomenon. Our results suggest a new strategy in magnetoelectronics, whereby control over magnetism is achieved through functional antiferrodistortive oxygen octahedron rotations.
N. A. Benedek and C. J. Fennie, arXiv:1007.1003 (2010).

2:42PM D33.00002 The search for multifunctional polar materials , JOSEPH BENNETT, KARIN RABE, Department of Physics and Astronomy, Rutgers University — One strategy in the search for new polar semiconducting (and possibly magnetic) materials is to check systems already synthesized and reported as polar in the literature to determine the intrinsic magnitude and switchability of the polarization, the band gap and magnetic properties. In many examples where a polar space group was found, neither polarization or band gap measurements were made because the sample as grown was too conductive. Using a combination of ICSD searching and symmetry analysis, we first identify potentially interesting polar materials and screen out those that are reported to definitely be metallic. We then use first-principles density functional theory (DFT) calculations to investigate the ground state structures of these experimentally synthesized materials for which limited data is available. These calculations will help us to develop criteria for screening candidate systems for polar, magnetic and semiconductive behavior, and broaden the search for new examples of these important functional materials.

2:54PM D33.00003 ABSTRACT WITHDRAWN –

3:06PM D33.00004 Higher-order Ginzburg-Landau Model for Multiferroic Hexagonal Manganites , KRIS DELANEY, UC Santa Barbara, SERGEY ARTYUKHIN, U Groningen, MANFRED FIEBIG, University of Bonn, NICOLA SPALDIN, UC Santa Barbara, MAXIM MOSTOVOY, U Groningen — Hexagonal manganites have been studied intensely as some of the few multiferroic materials with relatively high ordering temperatures. The recent experimental discovery of topological defects in the domain structure of YMnO3 has led to renewed interest in these materials [1, 2, 3]. Though a Landau free-energy model has already been parameterized at low order[4], we show the form of the parameterization with higher-order terms, including for the first time an angular dependence to the structural trimerization mode. Analysis of the resulting model explains clearly the origin of the topological defects in the domain structure, provides further theoretical insight into the contentious issue of the nature of the ferroelectric phase transition, and gives theoretical input into understanding the thickness of ferrelectric domain walls.

[1] Choi et al., Nature Mat. 9, 253 (2010)
[2] Mostovoy, Nature Mat. 9, 188 (2010)
[3] Jungk et al., Appl. Phys. Lett. 97, 012904 (2010)
[4] Fennie et al., Phys. Rev. B 72, 100103 (2005)

3:18PM D33.00005 Local and Long-Range High Pressure Structure of Orthorhombic $REMnO_3$[1] , H. CHEN, T. WU, T. TYSON, New Jersey Institute of Technology, R. TAPPERO, Brookhaven National Laboratory, L. HUANG, Stony Brook University, S. KIM, S.-W. CHEONG, Rutgers University — Orthorhombic perovskite $REMnO_3$ multiferroic systems were prepared by high pressure synthesis and solid state reaction. High pressure synchrotron x-ray diffraction and x-ray absorption measurements were performed to explore the structural changes. The influence of the pressure on the electrical polarization is discussed. Theoretical simulations are utilized to predict the stable magnetic phases based on the experimental parameters. This work is supported by DOE Grant DE-FG02-07ER46402.

[1]This work is supported by DOE Grant DE-FG02-07ER46402

3:30PM D33.00006 On the Nature of the Ferroelectric Transition in Multiferroic Hexagonal $REMnO_3$, TREVOR TYSON, TAO WU, HAIYAN CHEN, NJIT, JAINMING BAI, University of Tennessee, SANG-WOOK CHEONG, Rutgers University — Combined local and long range structural measurements were conducted on $REMnO_3$ for temperatures extending significantly above the ferroelectric transition temperature (T_{FE}). We find in hexagonal REMnO3 no large atomic (bond distance or thermal factors) or electronic structure changes on crossing T_{FE}. The born effective charge tensor is found to be highly anisotropic at the O sites indicating very strong hybridization of the charge. The tensor does not change significantly above T_{FE} revealing no charge redistribution and suggests an unusual transition. This work is supported by DOE Grants DE-FG02-07ER46402 (NJIT) and DE-FG02-07ER46382 (Rutgers University).

3:42PM D33.00007 Anomalous Phonon Behavior in Orthorhombic LuMnO3 at Low Temperature , PENG GAO, HAIYAN CHEN, TREVOR A. TYSON, Department of Physics, New Jersey Institute of Technology, Newark, NJ 07102, ZHENXIAN LIU, Geophysical Laboratory, Carnegie Institution of Washington DC 20015, JIANMING BAI, Oak RidgOak Ridge National Laboratory Oak Ridge, TN 37831, LIPING WANG, Mineral Physics Institute, Stony Brook University, Stony Brook, NY 11794, YOUNGJAI CHOI, SANG-WOOK CHEONG, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, Piscataway, NJ 08854 — We present the pressure dependent phonon spectra of orthorhombic-LuMnO3 which are conducted in the low temperature region (below T_N and T_L). A temperature dependent anomalous phonon coincides with the ferroelectric behavior at low pressure condition. At ∼10 GPa, this anomalous phonon exhibits an unusual softening trend which will be suppressed at higher pressure. This work is supported by DOE Grant DE-FG02-07ER46402 (NJIT), by DE-FG02-07ER46402 (Rutgers), by COMPRES (U2A beam line at NSLS), the Consortium for Materials Properties Research in Earth Sciences under NSF Cooperative Agreement EAR01-35554, U.S. Department of Energy (DOE-BES and NNSA/CDAC) and by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886 (use of NSLS at Brookhaven National Laboratory).

3:54PM D33.00008 Induction of novel macroscopic properties by local symmetry violations in spin-spiral multiferroics[1] , D. MEIER, UC Berkeley, N. LEO, University Bonn, P. BECKER, L. BOHATY, University of Cologne, R. RAMESH, UC Berkeley, M. FIEBIG, University Bonn — Incommensurate (IC) structures are omnipresent in strongly correlated electron systems as high-T_C superconductors, CMR manganites, as well as multiferroics. In each case they are origin of a pronounced symmetry reduction reflecting the complexity of the underlying microscopic interactions. Macroscopically, this can lead to new phases and possibilities to gain control of the host material. Here we report how the IC nature of a spin-spiral multiferroic induces new physical properties by renormalizing the relevant length scales of the system. Local symmetry violations directly manifest in the macroscopic response of the material and co-determine the multiferroic order giving rise to additional domain states. These usually hidden degrees of freedom become visible when non-homogenous fields are applied and condition for instance the second harmonic generation. Our study shows that incommensurabilities play a vital role in the discussion of the physical properties of multiferroics – they represent a key ingredient for further enhancing the functionality of this class of materials.

[1]This work was supported by the DFG through the SFB 608. D.M. thanks the AvH for financial support.

4:06PM D33.00009 Origin of the magnetic-field controlled polarization reversal in multiferroic $TbMn_2O_5$[1] , N. LEO, University Bonn, Germany, D. MEIER, UC Berkeley, USA, R.V. PISAREV, Ioffe Institute, St. Petersburg, Russia, S. PARK, S.-W. CHEONG, Rutgers University, USA, M. FIEBIG, University Bonn, Germany — The interplay of multi-dimensional complex magnetic order parameters leads to interesting effects like magnetically induced ferroelectricity. A particular interesting example is $TbMn_2O_5$ because of the associated magnetic-field controllable electric polarization. By optical second harmonic generation we show that the gigantic magnetoelectric effect originates in three independent ferroelectric contributions. Two of these are manganese-generated. The third contribution is related to the magnetism of the Tb^{3+} sublattice and has not been identified so far. It mediates the remarkable magnetic-field induced polarization reversal. This model is verified by experiments on the isostructural YMn_2O_5 where Y^{3+} ions are nonmagnetic and only two polarization contributions are present and no magnetoelectric coupling is observed. These results underline the importance of the $3d-4f$-interaction for the intricate magnetoelectric coupling in the class of isostructural RMn_2O_5 compounds.

[1]This work was supported by the DFG through SFB 608.

4:18PM D33.00010 Electronic mechanism for ferroelectricity and strong magneto-electric coupling in charge-ordered multiferroics , GERARDO ORTIZ, LEONID ISAEV, Indiana University Bloomington, CRISTIAN BATISTA, T-4, LANL — We study magneto-electric phenomena in multiferroic materials, which exhibit ferroelectricity due to the charge ordering. Using rare-earth iron oxides as an example, we derive an effective model, which takes into account the Coulomb interaction, magnetic superexchange and spin-orbit effects, and is consistent with the recent X-ray absorption spectroscopy measurements in multiferroic $LuFe_2O_4$. Then we demonstrate, how the interplay between quantum fluctuations and geometric frustration stabilizes the charge and ferrimagnetic spin orderings. The strong coupling, due to the double-exchange mechanism, between these orders, leads to a large magneto-electric response. Our results provide a complete physical description of the magneto-electric properties of charge-ordered multiferroics.

4:30PM D33.00011 Colossal Magnetoelectric Effect with Competing Multiferroic and Weak-Ferromagnetic Phases , YOUNG JAI CHOI, Rutgers University, CHENGLIN ZHANG, University of Tennessee, NARA LEE, SANG-WOOK CHEONG, Rutgers University — From our investigation of magnetoelectric properties of $Eu_{0.75}Y_{0.25}MnO_3$, where a multiferroic phase competes with a weak ferromagnetic phase in magnetic fields, we found intriguing hysteretic behaviors of physical properties with variation of temperature and magnetic field. These hysteretic behaviors arise from the kinetic arrest/de-arrest processes of the first order magnetic transition, resulting in freezing or melting of a magnetoelectric glass state with the coexistence of two competing phases. We note that most of large magnetoelectric coupling effects in multiferroics are associated with the large change of polarization with magnetic fields, but the control of ferromagnetic-type magnetization by applying electric fields is most relevant to technological applications, which is scarcely observed. This important issue of mutual controllability is achieved in $Eu_{0.75}Y_{0.25}MnO_3$ utilizing dynamical modulations of the coexistence of two contraindicative phases, highly susceptible to the external perturbations such as electric and magnetic fields.

4:42PM D33.00012 Pairing and Self-Organization of Vortices and Antivortices in h-$YMnO_3$, S.C. CHAE, Y. HORIBE, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA, D.Y. JEONG, Department of Mathematics, Soongsil University, Seoul 156-743, Korea, S. RODAN, N. LEE, S.-W. CHEONG, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA — Fascinating vortices and antivortices with ferroelectric domains were discovered in multiferroic hexagonal $YMnO_3$ [1]. Interlocking of ferroelectric and structural antiphase domain walls of h-$YMnO_3$ is one of the important ingredients for the topologically-nontrivial domain pattern formation. We have recently investigated the large-scale configuration of vortices and antivortices in h-$YMnO_3$ using selective chemical etching. Our results indicate the importance of pairing of vortices and antivortices, and provide valuable insights into understanding the self-organization mechanism of a zoo of vortices and antivortices. Furthermore, we have studied the response of the vortices and antivortices configuration to external stimuli such as external electric fields.

[1] T. Choi et al., Nature Mater. **9**, 253 (2010).

4:54PM D33.00013 Ferroelectricity driven by symmetric exchange striction in orthorhombic $HoMnO_3$, NARA LEE, YOUNG JAI CHOI, SANG-WOOK CHEONG, Rutgers University — Orthorhombic $HoMnO_3$ crystallizes in a distorted perovskite structure (space group *Pbnm*). It has been predicted that the spin configuration below the Néel temperature corresponds to a collinear E-type antiferromagnetic phase, which accompanies a large ferroelectric polarization originated from local oxygen distortions driven by exchange striction. In order to understand the exact nature of the E-type magnetism-driven ferroelectricity as well as the influence of Ho magnetism on ferroelectricity, we have performed comprehensive measurements of physical properties of the system, including magnetic susceptibility, dielectric constant, ferroelectric polarization and heat capacity with the variation of temperature and magnetic fields.

5:06PM D33.00014 Landau theory of composite domain walls and vortices in multiferroic hexagonal manganites , SERGEY ARTYUKHIN, U Groningen, KRIS DELANEY, NICOLA SPALDIN, UC Santa Barbara, MAXIM MOSTOVOY, U Groningen — Multiferroic materials with their coexisting magnetic and ferroelectric orders may find applications in memory devices. In hexagonal manganites, where electric polarization is induced by a periodic lattice distortion, ferroelectric and magnetic domain walls are firmly locked[1] even though electric polarization and spin ordering are decoupled in the bulk. Recent measurements showed that electric polarization changes sign at the boundaries of structural domains and revealed the existence of unusual vortices where six structural domains merge and the electric polarization changes sign six times around the defect.[2,3] We present a phenomenological theory of coupled lattice, charge and spin degrees of freedom in hexagonal manganites, which we use to calculate how electric polarization, structural distortions and magnetic ordering vary at the domain walls and vortices, and how the shape of these defects changes in an applied electric field.

[1]M. Fiebig et al., Nature 419, 818 (2002).
[2]T. Choi et al., Nature Materials 9, 253 (2010).
[3]M. Mostovoy, Nature Materials 9,188 (2010).

5:18PM D33.00015 Analysis of the magnetic structure and spin exchange interactions of multiferroic $YBaCuFeO_5$ by first principles DFT calculations , JERRY BETTIS, YUEMEI ZHANG, C. LEE, MIKE WHANGBO — In the layered perovskites $RBaCuFeO_5$ (R = Y, Lu, Tm), the $CuFeO_9$ dumbbells made up of apex-sharing CuO_5 and FeO_5 square pyramids share their basal corners to form perovskite layers, and the resulting $CuFeO_5$ slabs are stacked along the c-direction. Recently, these compounds were found to exhibit ferroelectric polarization when a modulated magnetic component is superposed on their antiferromagnetic structure. To help understand this finding, we examined the spin exchange interactions between the Fe^{3+} (d^5) ions, between the Cu^{2+} (d^9) ions, and between the Fe^{3+} and Cu^{2+} ions on the basis of DFT+U and DFT+U+SOC calculations for $YBaCuFeO_5$. The ferroelectric polarization of $YBaCuFeO_5$ was also calculated for several modulated magnetic structures that were constructed based on the cone-model.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D34 DMP: Focus Session: Interfaces in Complex Oxides - Photo and Electric Field Induced Devices C141

2:30PM D34.00001 Band profiles of Mott-insulator/band-insulator heterointerfaces revealed by photocurrent and electromodulation spectroscopies[1] , MASAO NAKAMURA, Cross-Correlated Materials Research Group (CMRG), ASI, RIKEN, Wako, 351-0198, Japan — Heterointerfaces of Mott insulators provide a good laboratory to explore unprecedented electronic states induced by the strong electron correlation. Although a number of intriguing phenomena have been reported so far, their fundamental origins have not been fully addressed yet. This is partly because the interface band profile, which is one of the most basic knowledge to understand the interface electronic states, is still left to be unveiled. In this study, we have investigated in detail the interface band profiles of Mott insulators employing photocurrent and electromodulation spectroscopies as well as the conventional current-voltage and capacitance-voltage characterizations. We chose p-type ($LaMnO_3$ and La_2CuO_4) and n-type ($SrMnO_3$ and Sm_2CuO_4) as the Mott insulators and these are epitaxially connected to Nb doped $SrTiO_3$ (electron-doped band insulator). The photocurrent action spectra for these heterojunctions showed negligibly-small band reconstruction as well as the existence of band bending and discontinuity in the Mott insulators, which are of no salient discrepancy with the rigid-band picture valid in the interface of conventional semiconductors [1]. However, the electromodulation spectra clearly indicate the band reconstruction in the Mott insulators [2]. The results mean that the rigid-band picture is valid in the low carrier-density regime even in Mott-insulator/band-insulator interfaces, but the intentional charge modulation leads the electron correlation effect in the Mott insulators. This work was done in collaboration with A. Sawa, J. Fujioka, M. Kawasaki and Y. Tokura.

[1] M. Nakamura *et al.*, Phys. Rev. B **82**, 201101(R) (2010)
[2] M. Nakamura *et al.*, Phys. Rev. B **75**, 155103 (2007).

[1]I acknowledge the support from Japan Society for the Promotion of Science (JSPS) through its "Funding Program for World-Leading Innovative R&D on Science and Technology (FIRST Program)".

3:06PM D34.00002 Mechanisms for the enhancement of the lateral photovoltage in perovskite heterostructures

, KUI-JUAN JIN, CHEN GE, HUIBIN LU, GUOZHEN YANG, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — The mechanisms for greatly enhanced lateral photovoltaic effect in the perovskite oxide heterostructures are studied by solving *time-dependent* two-dimensional drift-diffusion equations self-consistently. By our calculations, we find that the lateral photovoltage of p type material is larger than that of n type material owing to the larger drift electric field induced in the p type material than that in the n type material. Moreover, the built-in electric field at the interface between the thin film and substrate can also enhance the lateral photovoltage. The above two mechanisms can well explain one-order-of-magnitude enhancement of the LPV in the perovskite heterostructures. In addition, we find that the materials with larger mobility ratio have stronger Dember effect. Such an understanding of the mechanisms for the enhancement of lateral photovoltage in oxide heterostructures should be useful in further designing of the structures of position-sensitive detectors and new THz sources.

3:18PM D34.00003 Electronic Transport in Ion Gel-Gated Strontium Titanate[1]

, MEN YOUNG LEE, JAMES R. WILLIAMS, DAVID GOLDHABER-GORDON, Stanford University, SIPEI ZHANG, C. DANIEL FRISBIE, University of Minnesota, BHARAT JALAN, JUNWOO SON, SUSANNE STEMMER, UC Santa Barbara — In recent years much attention has been focused on the structure and properties of two-dimensional electron liquids (2DEL) in complex oxide heterostrucutres and delta- doped layers. We report on the fabrication and measurements of mesoscopic devices of metal oxides, with focus given to an electric field-induced 2DEL at the surface of undoped strontium titanate (STO). We describe the design and fabrication of field- effect structures, gated with an ionic gel, and show the measurements of induced swings of charge carrier density in STO. Other transport properties of the 2DEL are studied by magneto-transport measurements at low temperature.

[1]Studies of 2DELs in oxides were supported by MURI program of the ARO (W911-NF-09-1-0398). Development of electrolytic gating was supported by the DOE, Office of Basic Energy Sciences as part of an Energy Frontier Research Center (DE-SC0001060).

3:30PM D34.00004 Origin of Electrical Conduction in Domain Walls of $BiFeO_3$ Thin Films[1]

, JAMES LEE, ANOOP DAMODARAN, LANE MARTIN, PETER ABBAMONTE, University of Illinois at Urbana-Champaign, HELEN HE, RAMAMOORTHY RAMESH, University of California at Berkeley — $BiFeO_3$ thin films grown on $DyScO_3$ substrates unexpectedly exhibit metallic electrical conduction at ferroelectric (FE) domain walls (DWs). Resonant x-ray scattering near Fe L and O K absorption edges was used to probe the electronic structure of these films. In-plane wavevectors of resonant Fe edge magnetic scattering, and non-resonant Cu K α diffraction peaks near the (0, 0, 1) $BiFeO_3$ Bragg peak, match the domain period observed by PFM. Fe edge scattering intensifies as the beam energy is tuned to Fe 2p $\rightarrow$ ligand-3d transitions. No O K charge scattering is observed. These results suggest that metallic conduction does not arise from charge build- up at the DWs from FE polarization discontinuities, but from the bandgap closing near DWs as the crystal symmetry changes from rhombohedral-like in the domain bulk to higher-symmetries.

[1]Funding: US DOE grant DE-FG02-06ER46285.

3:42PM D34.00005 Sketched ferroelectric single-electron transistor[1]

, GUANGLEI CHENG, U. of Pittsburgh, PABLO SILES, Laboratório Nacional de Luz Síncrotron, Brazil, FENG BI, CHENG CEN, DANIELA BOGORIN, U. of Pittsburgh, CHUNG WUNG BARK, CHAD FOLKMAN, JAE-WAN PARK, CHANG-BEOM EOM, U. of Wisconsin-madison, GILBERTO MEDEIROS-RIBEIRO, HP labs, JEREMY LEVY, U. of Pittsburgh — Oxide heterostructures formed from ultrathin layers of $LaAlO_3$ grown on TiO_2-terminated $SrTiO_3$, combined with a reversible nanoscale patterning technique, provide a versatile platform for nanoscale control at the single-electron limit. Here we demonstrate the creation and characterization of "sketched" single-electron transistors made from ultrasmall (1-2 nm) quantum dots. Shell filling from N=0 up to N=2 electrons by single-electron tunneling is observed. Resonant tunneling can be controlled in a deterministic and non-volatile fashion by altering the ferroelectric polarization within the $SrTiO_3$ tunnel barrier. These single-electron devices may find use as nanoscale hybrid piezoelectric/charge sensors, and as elemental building blocks for solid-state quantum computation and quantum simulation platforms.

[1]This work was supported by NSF DMR-0704022 (JL), DARPA (W911NF-09-10258, JL), ARO (W911NF-08-1-0317, JL), The Fine Foundation (JL), AFOSR (FA9550-10-1-0524, J.L. and C.B.E), NSF DMR-0906443 (CBE), a David and Lucile Packard Fellowship (CBE).

3:54PM D34.00006 Characterizing Interfacial Bipolar Resistive Switches at Low Temperatures

, STEPHEN TSUI, Department of Physics, California State University San Marcos — Bipolar resistive switching has continued to be a topic of interest for many years because of the phenomenon's potential for memory device applications. Typically, a voltage pulse is applied to a metal-oxide sandwich structure, which drives the sample into a nonvolatile high or low resistance state depending upon the pulse polarity. A great deal of research has already been performed on a diverse array of materials with several different characteristics. However, few systematic investigations have been carried out at low temperature, which may have application to "cryo-memory." In this work, we compare the room temperature and low temperature behaviors of switches formed at the interfaces between a silver electrode and CeO_2, Al_2O_3, and $Pr_{0.7}Ca_{0.3}MnO_3$, respectively. We investigate the performance of the switching in response to temperature change and characterize the electronic transport at the interfaces in order to identify the dominant physical processes at these various temperatures.

4:06PM D34.00007 Role of the surface in writing, erasing and maintaining nanostructures at the $LaAlO_3/SrTiO_3$ interface[1]

, FENG BI, DANIELA F. BOGORIN, CHENG CEN, JEREMY LEVY, University of Pittsburgh, CHUNG WUNG BARK, JAE-WAN PARK, CHANG-BEOM EOM, University of Wisconsin-Madison — Nanoscale control of the metal-insulator transition in $LaAlO_3/SrTiO_3$ heterostructures can be achieved using local voltages applied by a conducting AFM probe. The mechanism is believed to be governed by a "water cycle" in which the surface is locally charged via hydrogen passivation, resulting in high-resolution modulation doping of the $LaAlO_3/SrTiO_3$ interface.[2] A Kelvin probe image method is applied to study how water content in the gas environment influences such charge writing. Persistence tests are performed, in which the long-term behavior is studied by keeping the AFM-written nanostructures (nanowire and sketch FET[3]) in different ambient environments. The self-erasure process is particularly obvious in moisture environments, but is slowed greatly in dry inert gas and can be even halted under modest vacuum conditions ($\sim 10^{-3}$ Torr).

[1]Supported by National Science Foundation (DMR-0704022), DARPA seedling (W911NF-09-1-0258) and the Fine Foundation.

[2]F. Bi et al., Appl. Phys. Lett.97, 173110 (2010)

[3]C.Cen et al., Science, 323, 1026 (2009)

4:18PM D34.00008 Electric field-tuning of the magneto-transport of superconducting $LaAlO_3/SrTiO_3$ interfaces , STEFANO GARIGLIO, NICOLAS REYREN, ANDREA D. CAVIGLIA, CLAUDIA CANCELLIERI, DPMC, University of Geneva, TONI SCHNEIDER, Physikinstitut, University of Zurich, JEAN-MARC TRISCONE, DPMC, University of Geneva, DPMC, UNIVERSITY OF GENEVA TEAM, PHYSIKINSTITUT, UNIVERSITY OF ZURICH TEAM — $LaAlO_3/SrTiO_3$ interfaces display a complex phase diagram that can be explored by an electric field [1,2]. Using transport measurements in magnetic fields for different doping levels, we have characterized the superconducting phase diagram in three dimensions (temperature, electric and magnetic fields). Analyses of the anisotropy for parallel and perpendicular magnetic fields [3] reveal a two-dimensional superconducting state for all doping levels. Magneto-resistances in perpendicular fields present hallmarks of superconductor-insulator and superconductor-metal transitions depending on the doping level. We will discuss scaling analyses of the magnetic field-tuned transitions and the role of fluctuations and disorder in this two-dimensional superconductor.

[1] N. Reyren et al. Science 317, 1196 (2007).
[2] A. Caviglia et al. Nature 456, 624 (2008).
[3] N. Reyren et al. Appl. Phys. Lett. 94, 112506 (2009).

4:30PM D34.00009 Cooper Pair Writing at the $LaAlO_3/SrTiO_3$ Interface[1] , CHENG CEN, DANIELA F. BOGORIN, University of Pittsburgh, CHUNG WUNG BARK, CHAD M. FOLKMAN, CHANG-BEOM EOM, University of Wisconsin-Madison, JEREMY LEVY, University of Pittsburgh — Superconducting semiconductors offer unique ways to exert electrostatic control over macroscopic quantum phases. The recently demonstrated nanoscale control over conductivity at the $LaAlO_3/SrTiO_3$ interface raises the question of whether nanoscale control over superconducting phases can be realized. Here we report low-temperature magnetotransport experiments on structures defined with nanoscale precision at the $LaAlO_3/SrTiO_3$ interface. A quantum phase transition is observed that is associated with the formation of Cooper pairs, but a finite resistance is observed at the lowest temperatures. Higher mobility interfaces exhibit larger Ginsburg-Landau coherence lengths, a stronger suppression of pairing by magnetic field as well as Shubnikov-de Haas oscillations. Cooper pair localization, spin-orbit coupling, and finite-size effects may factor into an explanation for some of the unusual properties observed.

[1]The work is supported by Department of Energy and State of Florida, NSF (DMR-0906443 and DMR-0704022), DOE (DE-FG02-06ER46327) and the Fine Foundation

4:42PM D34.00010 Electric and magnetic field control of superconducting transition at the $LaAlO_3/SrTiO_3$ heterointerface[1] , DMITRIY DIKIN, MANAN MEHTA, VENKAT CHANDRASEKHAR, Northwestern University, CHUNG WUNG BARK, CHAD FOLKMAN, CHANG-BEOM EOM, University of Wisconsin-Madison — We report on detailed measurements of the normal state-superconducting phase transition of the two-dimensional electron gas that develops at the LAO/STO interface as a function of gate voltage and magnetic field. We will discuss the specifics of the R versus T and the T-H phase diagrams for this superconductor and the potential origin of observed dissipation and hysteretic behavior. These data are analyzed in connection with magnetoresistance and Hall measurements.

[1]Funded by DOE through grant number DE-FG02-06ER46346.

4:54PM D34.00011 Metal-insulator transition at the interface of $LaAlO_3$ /$SrTiO_3$ induced by H_2O adsorption , YUN LI, School of Advanced Materials Science & Engineering, Sungkyunkwan University, Suwon, 440-746, Korea, JAEJUN YU, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea — We investigated the adsorption configurations at various H_2O coverages on the AlO_2 surface of n-type interface of 3 unit cell layers of $LaAlO_3$ (LAO) overlayer on $SrTiO_3$ (001) (STO) and the effects on the electronic properties at the interface by carrying out density-functional-theory calculations. For 0.25 monolayer (ML) and 0.5 ML coverages of H_2O the dissociation processes are barrierless. While for 1 ML coverage the mixing adsorption configuration comprising 0.5 ML molecular and 0.5 ML dissociated H_2O is most stable and the dissociation from fully molecular adsorption has to overcome 1 eV barrier. Insulator-metal transition at the n-type interface of (LAO)3/STO occurs as the coverage of dissociated H_2O reaches to 0.5ML. Insulator-metal transition at the interface can be realized by two ways: (1) changing H_2O coverage of from less than 0.5ML to equal to 0.5ML; (2) fixing H_2O coverage at 1ML and converting the adsorption configuration form fully molecular adsorption to mixing (0.5:0.5) adsorption. The second scheme can be utilized to realizing single-electron controlled nanoscale memory and switch.

5:06PM D34.00012 GHz operation of $LaAlO_3$/ $SrTiO_3$-based transistor[1] , PATRICK IRVIN, MENGCHEN HUANG, JEREMY LEVY, U. Pittsburgh, CHUNG WUNG BARK, CHAD M. FOLKMAN, CHANG-BEOM EOM, U. Wisconsin-Madison — Local modification of the metal-insulator transition of the $LaAlO_3$ /$SrTiO_3$ interface with a conducting-atomic force microscope (c-AFM) has resulted in a variety of electrical[2] and photonic[3] devices. Using a heterodyne measurement technique, we show that a sketch-based, nanoscale transistor ("SketchFET") can operate at frequencies in excess of 1 GHz. This demonstration of GHz functionality opens the door for new applications for oxide-based, rewritable nanoscale devices.

[1]This work was supported by NSF DMR-0704022 (J.L.), DARPA W911NF-09-10258 (J.L.), the Fine Foundation (J.L.), NSF DMR-0906443 (C.-B.E.), and David and Lucile Packard Fellowship (C.-B.E.)

[2]C. Cen, S. Thiel, J. Mannhart, and J. Levy, Science **323**, 1026 (2009).

[3]P. Irvin, Y. Ma, D. F. Bogorin, C. Cen, C. W. Bark, C. M. Folkman, C.-B. Eom, and J. Levy, Nature Photonics advanced online publication, 14 Nov.2010 (DOI 10.1038/nphoton.2010.238)

5:18PM D34.00013 Nanoscale control at the $LaAlO_3/SrTiO_3$ Interface grown on LSAT[1] , DANIELA BOGORIN[2], CHENG CEN, Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260, CHUNG WUNG BARK, CHANG BEOM EOM, Department of Materials Science, University of Wisconsin-Madison, Madison, WI 53706, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260 — The two-dimensional electron gas (2DEG) that forms at the interface between two semiconductors or between a semiconductor and oxide is currently the basis for some of the most useful electronic devices. We are able to control the 2DEG interface between $LaAlO_3/SrTiO_3$ with nanoscale precision and create transistors, nanodiodes and other nanostructures. Future scaling of oxide nanoelectronics requires scaling to wafer sizes larger than what can be provided from $SrTiO_3$. $(LaAlO_3)_{0.3}$–$(Sr_2AlTaO_3)_{0.7}$ (LSAT) substrates can allow for coherently strained $LaAlO_3/SrTiO_3$ heterostructures to be created. A sharp insulator to metal transition occurs at 8 uc $LaAlO_3$ thicknesses, in contrast to what is observed for unstrained $SrTiO_3$ substrates. We describe the properties of nanoscale structures created at the 2DEG interface of $LaAlO_3/SrTiO_3$ grown on LSAT wafers and compare them with structures grown on bulk $SrTiO_3$ substrates.

[1]Work supported by NSF DMR-0704022 (J.L.), DARPA W911NF-09-10258 (J.L.), the Fine Foundation (JL), NSF DMR-0906443 (C.B.E.) and David and Lucile Packard Fellowship (C.B.E.)

[2]currently at Oak Ridge National Laboratory, Oak Ridge, TN 37831

Monday, March 21, 2011 2:30PM - 5:30PM –
Session D35 DCMP: Topological Insulators: Theory II C140

2:30PM D35.00001 Antiferromagnetic topological insulators , ROGER S.K. MONG, ANDREW M. ESSIN, JOEL E. MOORE, University of California, Berkeley — We consider antiferromagnets breaking both time-reversal (Θ) and a primitive lattice translational symmetry ($T_{1/2}$) of a crystal but preserving the combination $S = \Theta T_{1/2}$. The S symmetry leads to a Z_2 topological classification of insulators, separating the ordinary insulator phase from the "antiferromagnetic topological insulator" (AFTI) phase. This state is similar to the "strong" topological insulator with time-reversal symmetry, and shares with it such properties as a quantized magnetoelectric effect. However, for certain surfaces the surface states are intrinsically gapped with a half-quantum Hall effect [$\sigma_{xy} = e^2/(2h)$], which may aid experimental confirmation of $\theta = \pi$ quantized magnetoelectric coupling. Step edges on such a surface support gapless, chiral quantum wires. In closing we discuss GdBiPt as a possible example of this topological class.

2:42PM D35.00002 Strong topological insulator phase in cold-atom systems , PETER P. ORTH, STEPHAN RACHEL, KARYN LE HUR, Yale University — With the recent technological advance of creating (electromagnetic) gauge fields for ultracold atoms, the fascinating prospect of realizing novel topological phases in these systems arises. Specifically, we consider spin-1/2 fermions on a square lattice under the influence of various experimentally feasible gauge fields. In two dimensions and if particles with different spin are exposed to magnetic fields in time-reversed directions, the system displays a quantum spin Hall ground state. We then study the influence of hopping into the third direction (2D-3D crossover), and in the three-dimensional system, we are able to identify a strong topological insulator phase. We further elaborate on the influence of the external trapping potential as well as the unambiguous detection of the topological phases.

2:54PM D35.00003 Quantum Hall Viscosity and the Torsional Response of Topological Insulators , ROBERT LEIGH, TAYLOR HUGHES, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign — In this talk I will discuss a dissipationless viscosity that has recently appeared in connection with the quantum Hall effect. I will show that this can be connected to the response of time-reversal breaking 2+1-d topological insulators under a mechanical torque. The torque is represented by a coupling of the electronic degrees of freedom to external torsion fields and gives rise to a Chern-Simons-like term commonly seen in gravitational theories in the presence of spacetime torsion. I will discuss possible thought experiments which illustrate the effects and will briefly cover the extension to 3+1-d topological insulators.

3:06PM D35.00004 Topological BF field theory description of topological insulators , JOEL E. MOORE, University of California, Berkeley and Lawrence Berkeley National Laboratory, GIL YOUNG CHO, University of California, Berkeley — Topological phases of matter are described universally by topological field theories in the same way that symmetry-breaking phases of matter are described by Landau-Ginzburg field theories. We propose that topological insulators in two and three dimensions are described by a version of abelian BF theory. For the two-dimensional topological insulator or quantum spin Hall state, this description is essentially equivalent to a pair of Chern-Simons theories, consistent with the realization of this phase as paired integer quantum Hall effect states. The BF description can be motivated from the local excitations produced when a π flux is threaded through this state. For the three-dimensional topological insulator, the BF description is less obvious but quite versatile: it contains a gapless surface Dirac fermion when time-reversal-symmetry is preserved and yields "axion electrodynamics", i.e., an electromagnetic $E \cdot B$ term, when time-reversal symmetry is broken and the surfaces are gapped. Just as changing the coefficients and charges of 2D Chern-Simons theory allows one to obtain fractional quantum Hall states starting from integer states, BF theory could also describe (at a macroscopic level) fractional 3D topological insulators with fractional statistics of point-like and line-like objects. Preprint available at http://arxiv.org/abs/1011.3485.

3:18PM D35.00005 Detecting 3d Non-Abelian Anyons via Adiabatic Cooling , SEIJI YAMAMOTO, National High Magnetic Field Lab and FSU Dept of Physics, MICHAEL FREEDMAN, Microsoft Research, Station Q, KUN YANG, National High Magnetic Field Lab and FSU Dept of Physics — Majorana fermions lie at the heart of a number of recent developments in condensed matter physics. One important application is the realization of non-abelian statistics and consequently a foundation for topological quantum computation. Theoretical propositions for Majorana systems abound, but experimental detection has proven challenging. Most attempts involve interferometry, but the degeneracy of the anyon state can be leveraged to produce a cooling effect, as previously shown in 2d. We apply this method of anyon detection to the 3d anyon model of Teo and Kane. Like the Fu-Kane model, this involves a hybrid system of topological insulator (TI) and superconductor (SC). The Majorana modes are localized to anisotropic hedgehogs in the order parameter which appear at the TI-SC interface. The effective model bears some resemblance to the non-Abelian Higgs model with scalar coupling as studied, for example, by Jackiw and Rebbi. In order to make concrete estimates relevant to experiments, we use parameters appropriate to Ca doped Bi_2Se_3 as the topological insulator and Cu doped Bi_2Se_3 as the superconductor. We find a temperature window in the milli-Kelvin regime where the presence of 3d non-abelian anyons will lead to an observable cooling effect.

3:30PM D35.00006 Topological invariants of adiabatic cycles of Bloch Hamiltonians[1] , RAHUL ROY, Oxford University — Invariants are constructed for various adiabatic cycles of Bloch Hamiltonians and discuss their physical implications. Many of these cycles lead to a pumping of fermions, but in other cases, the physical implications are more subtle. I also discuss the construction of these invariants for insulators in the various symmetry classes and periodicities in the table of these invariants.

[1]EPSRC

3:42PM D35.00007 On the stability of surface states in topological insulators , YOUNG HOON MOON, LEONID ISAEV, GERARDO ORTIZ, Indiana University Bloomington — The existence of robust surface/edge states is arguably a fingerprint of topological insulators. These states are protected against scattering by time-reversal invariant perturbations, and lead to dissipationless transport even at high temperatures. This characteristic behavior is believed to be quite insensitive to the properties of the surface of a particular sample. We investigate the above conjecture by considering the stability of edge states with respect to the *time-reversal invariant* surface perturbations in several models of topological insulators. We demonstrate that in certain regimes the surface spectrum is modified quite dramatically. In particular, the number of edge states, which cross the Fermi level inside the bulk band gap, is very sensitive to the properties of the surface. Our results can be of great importance for future transport measurements in topological insulators.

3:54PM D35.00008 Topological quantization in units of the fine structure constant , JOSEPH MACIEJKO, Stanford University, XIAO-LIANG QI, Stanford University and Microsoft Research, Station Q, H. DENNIS DREW, University of Maryland, SHOU-CHENG ZHANG, Stanford University — Fundamental topological phenomena in condensed matter physics are associated with a quantized electromagnetic response in units of fundamental constants. Recently, it has been predicted theoretically that the time-reversal invariant topological insulator in three dimensions exhibits a topological magnetoelectric effect quantized in units of the fine structure constant $\alpha = e^2/\hbar c$. In this Letter, we propose an optical experiment to directly measure this topological quantization phenomenon, independent of material details. Our proposal also provides a way to measure the half-quantized Hall conductances on the two surfaces of the topological insulator independently of each other.

4:06PM D35.00009 Refraction and interference of electrons on the topological insulator surface , RYUJI TAKAHASHI, Tokyo Institute of Technology, SHUICHI MURAKAMI, Tokyo Institute of Technology, and PRESTO, JST — We theoretically study electron transport on the topological insulator surface, in analogy with optics. The surface states are represented by spinors, unlike optics, and therefore different behaviors from those in optics are expected. First, we consider the refraction phenomena at the boundary between the surfaces of two different topological insulators, where the velocities of the surface states are different. We compare its transmission and refraction coefficients with optics. Furthermore, we discuss the case when the velocities of the surface states of the two topological insulators have opposite signs. Second, we study interference phenomena on the surface states. The result shows that if the detector is very far from the scatterer or the slit, the interference is asymptotically similar to ordinary two-dimensional scattering problems. We also study the spin directions of scattered wave due to the surface interference phenomena.

4:18PM D35.00010 Gauge field fluctuations in three-dimensional topological Mott insulators[1] , WILLIAM WITCZAK-KREMPA, TING PONG CHOY[2], University of Toronto, Canada, YONG BAEK KIM, University of Toronto, Canada & Korea Institute for Advanced Study, Korea — We discuss the low-energy properties of 3D topological Mott insulators that can be viewed as strong topological insulators of spinons interacting with a 3D gauge field. The low-energy behavior of such systems is dominated by gapless surface spinons (Dirac fermions) coupled to bulk gauge bosons. We find that a dimensional crossover from 3D to 2D in the gauge field fluctuations may occur as the system's thickness and/or temperature is varied. In the thin sample limit, the gauge field fluctuations effectively become 2D and the problem becomes analogous to the standard 2D spinon-gauge field theory. In the 3D limit, the bulk gauge field fluctuations lead to a novel low-energy theory for the coupled system that is more controlled than in the 2D regime. We discuss various experimental signatures such as the heat capacity scaling as T ln(1/T) as well as modified RKKY interactions on the surface.

[1]Research was supported by NSERC, the Canada Research Chair program, and the Canadian Institute for Advanced Research.
[2]Currently at University of Leiden, Instituut-Lorentz for theoretical Physics

4:30PM D35.00011 Symmetry aspects of localized Dirac fermions within topological defects[1] , CHI-KEN LU, Department of Physics, Simon Fraser University, IGOR HERBUT, Department of Physics, SFU — We study the conditions for the existence of zero-energy bound states within topological defects in various insulating and superconducting order parameters for Dirac fermions in graphene and topological insulators. In particular, we discuss several physically relevant realizations of the "Dirac vortex" which include the finite chemical potential and Zeeman terms, and the orbital magnetic fields, and present some explicit solutions for the zero-modes. The crucial role in our discussion is assumed by the antilinear symmetry between the positive and negative parts of the energy spectrum. The effects of the orbital symmetry of the defect's underlying order on the zero-modes are also considered.

[1]This work has been supported by NSC Taiwan (CKL) and NSERC Canada (IH).

4:42PM D35.00012 Massive Dirac Fermion on the Surface of a Magnetically Doped Topological Insulator , YULIN CHEN, SLAC National Accelerator Laboratory, JIUN-HAW CHU, JAMES ANALYTIS, ZHONGKAI LIU, KYUSHIRO IGARASHI, HSUEH-HUI KUO, XIAOLIANG QI, SUNG-KWAN MO, ROBERT MOORE, DONGHUI LU, MAKOTO HASHIMOTO, TAKAO SASAGAWA, SHOUCHENG ZHANG, IAN FISHER, ZAHID HUSSAIN, ZHI-XUN SHEN — Insulating massive Dirac fermion state is a novel state of topological insulators in which the massless surface Dirac fermion becomes massive due to the braking of time reversal symmetry. In this state a gap develops at the Dirac point, with the Fermi energy resides inside both the surface and bulk gaps. By introducing magnetic dopants into three dimensional topological insulator Bi_2Se_3 to break the time reversal symmetry, we successfully observed the formation of massive Dirac fermion on the surface, with the Dirac gap magnitude tunable by magnetic dopant concentration. Furthermore, by precise control of simultaneous magnetic and charge doping, we successfully position the Fermi level inside the Dirac gap, thus realizing the much sought after insulating massive Dirac fermion state. This discovery paves the way for realizing striking topological phenomena and testing profound theoretical predictions.

4:54PM D35.00013 Exotic Effects of Spin-Flip Scattering on Massive Dirac Fermions[1] , SHENGYUAN YANG, ZHENHUA QIAO, The University of Texas at Austin, YUGUI YAO, JUNREN SHI, Institute of Physics, Chinese Academy of Sciences, QIAN NIU, The University of Texas at Austin — We investigate the effects of spin-flip scattering on the Hall transport and spectral properties of massive Dirac fermions. We find that in the weak scattering regime, the Berry curvature distribution is dramatically compressed in the electronic energy spectrum, becoming singular at band edges. As a result the Hall conductivity suffers a sudden jump (or drop) of $e^2/2h$ when the Fermi energy sweeps across the band edges, and otherwise is a constant quantized in units of $e^2/2h$. In parallel, spectral properties such as the density of states and spin polarization are also greatly enhanced at band edges. Possible experimental methods to detect these effects are discussed.

[1]This work is supported by NSFC (10974231) (Y.Y.), DOE (DE-FG02-02ER45958) and Texas Advanced Research Program (Q.N.).

5:06PM D35.00014 Weak indices and dislocations in general topological band structures , YING RAN, Boston College — It has recently been shown that crystalline defects - dislocation lines - in three dimensional topological insulators, can host protected one dimensional modes propagating along their length. We generalize this observation to the case of topological superconductors and other insulators of the Altland Zirnbauer classification, in d=2,3 dimensions. In general, protected dislocation modes are controlled by the topological indices in (d-1) dimensions. This is shown by relating this feature to characteristic properties of surface states of these topological phases. This observation also allows us to constrain these surface states properties, which is illustrated by an addition formula for (d-1) and (d-2) indices of a topological superconductor.

5:18PM D35.00015 Topological insulator in a non-Abelian lattice model and anyonic fermions in two-body color code model[1] , MEHDI KARGARIAN, GREGORY A. FIETE, Department of Physics,The University of Texas at Austin — We investigated topological phases in several decorated lattices such as the square- octagon and spin ruby lattices. The underlying models can be potentially simulated in optical lattices or in multi-orbital transition metal oxides. In the square-octagon lattice we apply a set of non-Abelian gauge fields to modulate the hopping between sites. Inversion symmetric fields open a gap and the model realizes topological band insulating phase. If the inversion symmetry is broken, a quantum phase transition between phases with different quantum orders takes place. These phases are characterized by number of Dirac nodes and the associated winding numbers. We also probe the topological phases in the spin ruby lattice with emerging anyonic fermions coupled to nontrivial gauge fields associated with the local symmetry of the model. And we further characterize our results by topological entanglement entropy and entanglement spectrum. M. Kargarian and G. A. Fiete, Phys. Rev. B 82, 085106 (2010).

[1]We gratefully acknowledge funding from ARO grant W911NF-09-1-0527.

Monday, March 21, 2011 2:30PM - 5:30PM –
Session D36 GERA: Photovoltaics: Nanostructured Materials C142

2:30PM D36.00001 ABSTRACT WITHDRAWN –

2:42PM D36.00002 Study of photo induced optical transparency of I/I3 redox couple in Dye Sensitized Solar Cells

, JOSEF VELTEN, JULIA BYKOVA, JAVIER CARRETERO-GONZALEZ, ELIZABETH CASTILLO MARTINEZ, ANVAR ZAKHIDOV — Dye sensitized solar cells (DSCs) are an alternative to the standard silicon solar cell, consisting of a photoelectrochemical cell that has a light absorbing working electrode, a I-/I3- charge mediator and a counter electrode for reduction of I3- back to I-. Tradtionally, this counter electrode is composed of a few nanometer layer of platinum deposited onto transparent conductive oxide glass. Our work has focused on using structured carbon materials as a counter electrode. Earlier work focused on the use of carbon nanotubes, both single and multiwalled as a replacement for this platinum counter electrode material. Recent work has moved into using 2 dimensional carbon materials, such as graphene flakes and graphene ribbons. With the use of graphene ribbons we have discovered a unique effect that has not been reported for DSCs: under operating condition of AM 1.5 light, the charge mediating electrolyte undergoes a change in its absorption profile. We conclude that this phenomenon must arise from the structure of the graphene ribbons. This process has been demonstrated to be completely reversible, and shows no degradation to the DSC's operation. This presentation will also discuss the application of this phenomenon in the use of inverted DSCs and hybrid tandem cells.

2:54PM D36.00003 Dye Sensitized Solar Cells with bilayer Multi/Single Carbon Nanotubes

, ZHARKYNAY KUANYSHBEKOVA, ANVAR ZHAKHIDOV, Nano Tech Institute UTD — In this presentation, we demonstrate the fabrication of dye sensitized solar cells using bilayers of MWCNT coated by SWCNT on top. Each DSC cell uses a typical titania photoelectrode deposited onto a transparent window electrode with photosensitive dye absorbed on the surface of the TiO_2.Adding SWCNT layer to MWCNT increased short circuit current from 10 to 14 mA/cm^2. Conventional DSC uses couterelectrode with Pt coated FTO, the Pt layers play role of catalyst for better charge transfer rate from electrolyte. In our bilayer electrode MWCNT sheet play a role a good conductor (similar to FTO), while SWCNT provide better catalytic properties for charge transfer (similar to Pt). The relatively high obtained efficiency of DSS ($\sim$7-8%) cell is determined by the high generated photocurrent, which is comparable to the reference DSS made by same method using the standard PT catalyst. However, the fill-factor of the device is still low ($\sim$0.4-0.5). Therefore further improvement of electrical conductivity of these carbon based electrodes is under investrigation with CNT sheets to achieve high performance device. We acknowledge the help with transparent SWCNTs made in A.Nasibullin of Aolto University (Finland).

3:06PM D36.00004 Equivalent Circuit Description of Non-compensated n-p Codoped TiO2 as Intermediate Band Solar Cells(IBSCs)1[1]

, TIAN-LI FENG, YI XIA, GUANG-WEI DENG, FENG-CHENG WU, PING CUI, HAIPING LAN, U of Sci. and Tech. of China, ZHENYU ZHANG, Oak Ridge Nat.Lab, U of Tennessee, U of Sci. and Tech. of China — The novel concept of non-compensated n-p codoping has made it possible to create tunable intermediate bands in the intrinsic band gap of TiO2 [1] as a promising materials for developing IBSCs [2]. Here we investigate the quantum efficiency of such IBSCs with or without current extracted from the intermediate bands (IBs). Using the ideal equivalent circuit model, we find that the maximum efficiency of 57% in the first case and 53% in the second are both much higher than the Shockley-Queisser limit. We also obtain various key quantities of the circuits, allowing us to simplify the IBSCs into an ordinary cell with an intrinsic resistance, a useful step in realistic development of TiO2 based solar cells invoking device integration. These equivalent circuit results are also compared with the efficiencies obtained directly from consideration of electron transition between the energy bands, and both approaches reveal the intriguing existence of double peaks in the maximum efficiency as a function of the location of IBs.

[1] Zhu W. G., et al., Phys. Rev. Lett. 103, 226401 (2009).
[2] A. Luque, et al., J. Appl. Phys. 96, 1 (2004).

[1]Supported by NNSF of China and DMSE/BES of USDOE.

3:18PM D36.00005 Fluctuation-Induced Tunneling Conductivity in TiO_2 Nanoparticle Thin Films[1]

, STEVEN J. KONEZNY, CHRISTIAAN RICHTER, ROBERT C. SNOEBERGER III, ALEXANDER R. PARENT, GARY W. BRUDVIG, CHARLES A. SCHMUTTENMAER, VICTOR S. BATISTA, Yale University — We integrate temperature-dependent dark DC conductivity measurements and theoretical modeling to elucidate the mechanism of electron transport in nanoporous TiO_2, a common photoanode material for dye-sensitized solar cells (DSSCs) and solar photocatalysis. We show that fluctuation-induced tunneling conduction through contact junctions between sintered TiO_2 nanoparticles can account for the temperature dependence over the entire temperature range studied. We find quantitative agreement between experimental and calculated conductivities, which span over four orders of magnitude and change with decreasing temperature from thermally activated to temperature-independent. The reported results suggest that efforts to optimize charge transport in nanoporous TiO_2 thin films as a means of improving the overall efficiency of DSSCs and solar photocatalysis should focus on fabrication conditions that optimize the properties of the contact junctions between sintered TiO_2 nanoparticles.

[1]The authors acknowledge support from DOE (NERSC supercomputer time; DE-FG02-07ER15909; DE-PS02-08ER15944) and NSF (Graduate Research Fellowship to ARP; ECCS-0404191; CHE 0911520).

3:30PM D36.00006 ZnO Nanoparticles and Nanowire Arrays with Liquid Crystals for Photovoltaic Apprications[1]

, LOURDES SALAMANCA-RIBA, NICHOLAS WEADOCK, LUZ MARTINEZ-MIRANDA, University of Maryland — Liquid crystals are small monodisperse molecules with high mobilities and are easy and cheap to process. In addition, some of their phases exhibit molecular orientation that can provide a path for the electrons, or holes, to move from one electrode to the other. We have mixed a smectic A liquid crystal (8CB) with varying concentrations of ZnO nanoparticles of $\sim$5 nm in diameter and have observed a photovoltaic effect as a function of the concentration of ZnO. The liquid crystal is believed to enhance the alignment of the nanoparticles and aid in the diffusion of electrons through the particles to the collection electrode. We have also made PV cells of ZnO nanowire arrays grown on Au layers on Si substrates. The nanowire arrays are covered with 8CB liquid crystal for hole conduction. We compare the light absorption of the PV cells as a function of wavelength of the light for the ZnO nanoparticle and the ZnO nanowire cells. We present a detailed study of the structure of the two systems.

[1]Supported by the National Science Foundation under the University of Maryland MRSEC DMR 0520471.

3:42PM D36.00007 Intermediate Band Gap Solar Cells: The Effect of Resonant Tunneling on Delocalization , REID WILLIAM, DOTY MATHEW, U. Delaware, SHILPA SANWLI, U.Delaware, DAN GAMMON, ALLAN BRACKER, NRL — Quantum dots (QD's) have many unique properties, including tunable discrete energy levels, that make them suitable for a variety of next generation photovoltaic applications. One application is an intermediate band solar cell (IBSC); in which QD's are incorporated into the bulk material. The QD's are tuned to absorb low energy photons that would otherwise be wasted because their energy is less than the solar cell's bulk band gap. Current theory concludes that identical QD's should be arranged in a superlattice to form a completely delocalized intermediate band maximizing absorption of low energy photons while minimizing the decrease in the efficiency of the bulk material. We use a T-matrix model to assess the feasibility of forming a delocalized band given that real QD ensembles have an inhomogeneous distribution of energy levels. Our results suggest that formation of a band delocalized through a large QD superlattice is challenging; suggesting that the assumptions underlying present IBSC theory require reexamination. We use time-resolved photoluminescence of coupled QD's to probe the effect of delocalized states on the dynamics of absorption, energy transport, and nonradiative relaxation. These results will allow us to reexamine the theoretical assumptions and determine the degree of delocalization necessary to create an efficient quantum dot-based IBSC.

3:54PM D36.00008 Development of High Efficient Flexible Dye-Sensitized Solar Cells[1] , XIAOJUAN FAN, Marshall University — We are developing a low cost and easy process to fabricate double-layer porous metal oxide thin films on flexible substrates for high performance dye-sensitized solar cells (DSSCs**).** The research addresses on the formulation of TiO_2 precursor to create smooth and continuous porous thin films on large size plastic or metal foil substrates enabling excellent adhesion, robust mechanics, and chemical stability. A second layer built on the underline porous nanocrystalline TiO_2 thin films are primarily used as bedding to receive more organic sensitizers. A variety of blending of polymer and Ti alkoxide precursors at different concentrations has been studied. After depositing the mixture on the substrates such as Al foils, samples are annealed to remove polymer residues leading to a porous nanocrystalline structure. Photo-electricity conversion efficiency of the fabricated solar cells will be tested under one sun illumination.

[1]Acknowledge support from NASA Seed Grant and NSF MU-ADVANCE

4:06PM D36.00009 A novel nano-structured GaAs solar cell , DONG LIANG, ANJIA GU, YIJIE HUO, Stanford University, JINGZHOU YAN, OEpic Semiconductors Inc., SHUANG LI, ERIK GARNETT, EVAN PICKETT, YANGSEN KANG, MEIYUEH TAN, ANTONIO XAVIER CERRUTO, JIA ZHU, CHING-MEI HSU, YAN YAO, Stanford University, MAJID RIAZIAT, OEpic Semiconductors Inc., YI CUI, JAMES S. HARRIS, Stanford University — In this presentation, we will demonstrate a novel solar cell with nano-structured dense arrays of single crystal GaAs conformally grown on nanopillar templates with wafer-scale uniformity. The template is prepared via plasma enhanced etching with a monolayer of SiO_2 nanospheres as a mask followed by wet chemical etching. The GaAs p-n junction with an AlGaAs passivation window layer is grown via metal-organic chemical vapor deposition (MOCVD). The rectangular shape of the nano single crystal GaAs reveals anisotropic lateral growth rates of GaAs along (011) and (01$\underline{1}$) directions, which can be engineered by tuning the AsH_3 flow and temperature during growth. Optical absorption measurements show the outstanding light trapping properties of the nano-structured cell, which agree with the simulation results. I-V characteristics show an efficiency of 1.67% for the nano GaAs solar cell, which is 15% higher than its planar control cell with the same thickness of 200nm. The efficiency is the highest among all the large area GaAs nanowire core-shell solar cells reported in literature by 2010.

4:18PM D36.00010 Highly Efficient Dye Sensitized Solar Cells based on Free-Standing Titania Nanotube[1] , CHAEHYUN KIM, SUNGJIN KIM, ALEXANDER CARTWRIGHT, HAO ZENG, SUNY at Buffalo — Dye sensitized solar cells (DSSC) attract great attention due to their respectable efficiency with very low fabrication cost, good performance under diffuse light conditions and ability to be fabricated on flexible substrates. Its main efficiency limiting factor is the random hopping of electrons within the titania nanoparticle network, which causes carrier trapping and recombination. The charge transport and collection can be enhanced by employing ordered nanostructures such as nanowire or nanotube arrays. However, nanowire/nanotube based DSSCs with efficiencies higher than those of conventional DSSCs have yet to be demonstrated. In this work, we report the fabrication of DSSCs using highly crystalline free-standing titania nanotube arrays. The high crystallinity leads to high electron mobility and diffusion length, allowing thick nanotube films to be used for improving the long wavelength light absorption. This greatly enhances the photocurrent and power conversion efficiency as compared to that of nanotube DSSCs in earlier studies.

[1]Work supported by NSF DMR-0547036.

4:30PM D36.00011 Nanowire electrodeposition for advanced photovoltaics , ERIK MENKE, JUSTIN HUJDIC, SOMNATH GHOSH, University of California, Merced — According to the Department of Energy's "Basic Research Needs for Solar Energy Utilization" report, there are a number of fundamental scientific issues that need to be addressed for nanostructure based solar cells, including: a. Control of nanoarchitecture b. Light harvesting c. Control of charge separation and recombination d. Control of charge carrier transport to the contacts Here, I will describe how lithographically patterned nanowire electrodeposition (LPNE) can address these issues by discussing the synthesis of high-density semiconductor nanowire arrays, as well as their optical and electronic properties. This talk consists of three parts. Part 1 presents a brief overview of how LPNE, essentially the combination of photolithography and electrodeposition, can be used as a general method to prepare high-density nanowire arrays. Part 2 demonstrates this method specifically for CIS/CdS core-shell nanowire arrays by discussing the electrodeposition of the nanowire arrays as well as the physical and chemical properties of the resulting nanowires. Finally, part 3 presents the optoelectronic properties of the resulting nanowire arrays and their potential application as solar cells.

4:42PM D36.00012 Shedding Light on Solar Cells with Synchrotron Radiation , FRANZ HIMPSEL, PETER COOK, PHILLIP JOHNSON, UW Madison, XIAOSONG LIU, WANLI YANG, ALS, ANGEL RUBIO, JUAN-MARIA GARCÍA-LASTRA, ENRIQUE ORTEGA, CELIA ROGERO, RUBEN GONZALEZ-MORENO, Univ. San Sebastian, ENEKO AZACETA, RAMON TENA-ZAERA, CIDETEC, San Sebastian, ELENA GUILLEN, JUAN ANTA, Univ. Sevilla — X-ray absorption and photoelectron spectroscopy with synchrotron radiation are used to systematically determine the energy levels of molecules for dye-sensitized solar cells (including porphyrins and phthalocyanines [1-3]). N 1s absorption spectra combined with theoretical modeling provide the unoccupied molecular orbitals and the charge transfer between the central metal atom and the surrounding N atoms. Metal 2p-to-3d spectra provide the oxidation state of the metal. Fe and Mn, which occur frequently in biological analogs, easily change their oxidation between $+3$ and $+2$. Some dyes interact with the electronic states of nano-structured ZnO acceptor electrodes, causing a change in the electronic states of the ZnO or the dye.

[1] P. L. Cook, et al. J. Chem. Phys. 131, 194701 (2009).
[2] P. L. Cook, et al. J. Chem. Phys. 131, 214702 (2009).
[3] J.M. García-Lastra, et al., J. Chem Phys. 133, 151103 (2010).

4:54PM D36.00013 Dye Sensitized Solar Cells Using Freestanding TiO2 Nanotube Arrays , XUKAI XIN, JUN WANG, Iowa State University, LEI ZHAO, Iowa State Univeristy, ZHIQUN LIN, Iowa State University — A TiO2 photoanode was prepared by depositing TiO_2 nanoparticle on the FTO glass followed by placing TiO_2 nanotube arrays on the top of TiO_2 nanoparticle film. The resulting TiO_2 nanotube/nanoparticle photoanode was sensitized with N719 dye after $TiCl_4$ treatment and exposure to O_2 plasma. The resulting dye sensitized solar cell (DSSC) showed that the highest DSSC power conversion efficiency of 8.02% and 7.00% were yielded when a 20 μm thick TiO_2 nanoparticle and a 13/7 μm TiO_2 nanoparticle/nanotube were used as photoanode, respectively. The I$\sim$V curve analysis suggested that the nanotubes had better electron transport pathway but lower electron generation. Future work will be focused on increasing the dye loading of nanotubes to improve the power conversion efficiency.

5:06PM D36.00014 Dye-sensitized solar cells employing TiO2 nanotube arrays modified by hydrothermal process , MEIDAN YE, 5152940804, CHANGJIAN LIN, ZHIQUN LIN — Dye sensitized solar cells (DSSCs) based on TiO2 nanotube photoanode prepared by a facile combination of electrochemical anodization and hydrothermal process exhibited a remarkable performance. Well-ordered and smooth TiO2 nanotube arrays fabricated by a two-step anodic oxidation were subjected to hydrothermal process, thereby creating roughness on the surface of nanotubes and leading to increased dye loading. Subsequently, the resulting nanotubes were used to fabricate DSSC in backside illumination mode, yielding a significantly high power conversion efficiency of 7.12% that was further increased to 7.75% upon oxygen plasma treatment.

5:18PM D36.00015 Nanostructured Thin Film Solar Cells: A Heterojunction of PbS Colloidal Quantum Dots and TiO2 Nanopillars , HO-CHEOL KIM, IBM Almaden Research Center, ILLAN KRAMER, University of Toronto, JOHN BASS, TEYA TOPURIA, LESLIE KRUPP, PHILIP RICE, IBM Almaden Research Center, RATAN DEBNATH, LUKASZ BRZOZOWSKI, LARISSA LEVINA, EDWARD SARGENT, University of Toronto — Colloidal quantum dot (CQD) has been recognized as a promising solar cell material that offers tunable band gap and inexpensive solution process. Recent report demonstrated the power conversion efficiency (PCE) of above 5% (AM 1.5) using thin films of PbS CQDs and TiO_2 nanoparticles. This so-called depleted-heterojunction-CQD solar cells have overcome limitations of CQD Schottky devices and promised potential for further improvement of solar cell performance. In this paper, we report the effect of nanostructures of TiO_2 on the performance of heterojunction CQD solar cells. Well-defined nanopillars of TiO_2 were prepared on top of F:SnO_2 substrate using micro-transfer molding technique. TiO_2 nanopillars of 70 nm in diameter (half-width), 340 nm in height and 275 nm in center-to-center distance were used for subsequent layer-by-layer spin coating of PbS CQD. PCE of $>$5% was measured for the nanopillar solar cells without extensive optimization. Detailed studies on the microstructure of materials, surface properties, optical and electrical properties and optimization will be discussed along with performance of flat TiO_2-PbS CQD solar cells.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D37 DMP: Focus Session: Graphene Structure, Dopants, and Defects: Strain Engineering I C146

2:30PM D37.00001 Strain Engineering in Graphene[1] , ANTONIO CASTRO NETO[2], Department of Physics, Boston University — Graphene is a unique example of a one atom thick metallic membrane. Hence, graphene brings together properties of soft and hard condensed matter systems. The elementary electronic excitations in graphene, the Dirac quasiparticles, couple in a singular way to structural distortions in the form of scalar and vector potentials. Therefore, graphene has an effective electrodynamics where structural deformations couple to the Dirac particles at equal footing to electric and magnetic fields. This so-called strain engineering of the electronic properties of graphene opens doors for a new paradigm in terms of electronic devices, where electronic properties can be manipulated at will using its membrane-like properties.

[1]I thank partial support from from DOE Grant DE-FG02-08ER46512 and ONR Grant MURI N00014-09-1-1063.

[2]Graphene Research Centre, National University of Singapore

3:06PM D37.00002 Optical absorption and giant Faraday rotation in strained graphene , VITOR PEREIRA, National University of Singapore, NUNO M.R. PERES, RICARDO M. RIBEIRO, Universidade do Minho, Portugal, ANTONIO CASTRO NETO, Boston University — Slightly doped or undoped graphene is characterized by an universal optical absorption coefficient of $\pi\alpha$ (nearly 2%), which is constant in a frequency band spanning the near UV, down to the far IR. Strain-induced anisotropy breaks this universality, while keeping the optical response constant up to energies close to the van-Hove singularity of the spectrum. This allows for the possibility of exploring the photoelasticity of graphene towards the development of atomically thin, broadband optical elements. We show, and analytically quantify, the amount of polarization rotation and dichroism expected for uniaxially strained graphene. The effect can be used to tailor the optical response of graphene or, conversely, to use light to measure the amount and direction of uniaxial strain in graphene for sensing applications. Exposure to an external magnetic field brings about the Faraday effect, which is shown to be extremely large in comparison with conventional materials. Moreover, the sharp enhancement of Faraday rotation and absorption at the field and stain tunable cyclotron frequency opens the possibility of tunable broadband optics in atomically thin transparent membranes.

3:18PM D37.00003 Electron-electron interactions in strained graphene , ANAND SHARMA, VALERI KOTOV, University of Vermont — We present a theoretical study on the effects of electron-electron interactions under an applied weak uni-axial strain in graphene, described as anisotropic Dirac liquid. We calculate the electron self-energy using perturbation theory in both the Coulomb interactions and strain, and find that near the Dirac point the self-energy exhibits logarithmic singularity structure, similarly to an un-deformed graphene. We present results for the renormalization of the electronic anisotropy by using first the bare Coulomb interaction, as well as the random-phase approximation, which takes into account the anisotropic nature of the vacuum polarization. The mutual interplay of interactions and strain can provide a route towards understanding the role of correlations in graphene, which so far have been quite elusive in the un-deformed case.

3:30PM D37.00004 Scattering from localized strain profiles in graphene: effects on conductance , MATTHEW BARR, Harvard University, ERIC HELLER, HELLER GROUP TEAM — Graphene has attracted significant attention for, amongst other properties, its Dirac-like quasiparticles and long coherence length. In the ballistic regime, we theoretically investigate the scattering properties of localized strain profiles. Manipulating strain in graphene has been proposed as a novel method of shaping graphene devices; modulated hopping parameters effectively introduce vector potentials equivalent to pseudomagnetic fields up to 300T [1]. We determine the localized potential and scattering parameters of several such "bubbles"; with this information we calculate the effects on conductance in both valleys of introducing one or many such impurities.

[1] N. Levy, S. A. Burke, K. L. Meaker, M. Panlasigui, A. Zettl, F. Guinea, A. H. Castro Neto and M. F. Crommie, Science 30, July 2010

3:42PM D37.00005 Ab-initio study of the Kohn anomalies in strained graphene[1] , M.E. CIFUENTES-QUINTAL, R. DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico, O. DE LA PEÑA-SEAMAN, R. HEID, K.-P. BOHNEN, Institute for Solid State Physics, Karlsruhe Institute of Technology, Germany — Recent experimental studies have show that the electronic and vibrational properties of graphene can be modulated by means of strain. However, there are not studies on strain effects on the Kohn anomalies, which is a principal key to understand the electron phonon coupling in graphene. In this work we have studied the phonon band structure of graphene under biaxial and uniaxial strain using the mixed basis pseudopotential method, within the framework of the density functional perturbation theory. For tensile/compressive biaxial strain, we found an increasing/decreasing behavior on the slop of the phonon frequencies close to Kohn anomalies. Under uniaxial strain, the two highest optical branches show a discontinuity in the frequency derivative at gamma point, instead of only one branch like in the biaxial and unstrained case. The present results suggest that the electron-phonon coupling in graphene can be modulated via strain.

[1]This research was supported by Conacyt-Mexico under Grant No. 83604.

3:54PM D37.00006 Graphene rubber band: suspended graphene sheets with controlled uniaxial strain , ZENGHUI WANG, DAVID HUTCHISON, CARLOS RUIZ-VARGAS, PINSHANE HUANG, SUNIL BHAVE, DAVID MULLER, JIWOONG PARK, Cornell University — The recent advances in growth and transfer techniques of CVD graphene have made it an excellent candidate for making electrical and mechanical devices, especially at larger scale than with exfoliated graphene flakes. Nevertheless, the electrical, electromechanical and optomechanical properties of CVD graphene need to be further characterized before one can make full use of this 2D material. Here, we study the properties of CVD graphene under well controlled uniaxial strain. We fabricate devices with adjustable-width gaps actuated by comb drives, and transfer CVD graphene sheets onto these gaps. We study the slipping, straining, and breaking of CVD graphene in real time under TEM, with identification of individual single crystal domains and domain boundaries.

4:06PM D37.00007 Suspension of Graphene and Bi2Se3 Atomic Membrane , ZENG ZHAO, JAIRO VELASCO, HANG ZHANG, FENGLIN WANG, ZHIYONG WANG, PHILIP KRATZ, LEI JING, WENZHONG BAO, JING SHI, JEANIE LAU, Department of Physics and Astronomy, UCR, SHI JING'S GROUP COLLABORATION — Coupling high quality, suspended atomic membranes to specialized electrodes enables investigation of many novel phenomena, such as spin or Cooper pair transport in these two dimensional systems. However, many electrode materials are not stable in acids that are used to dissolve underlying substrates. Here we present a versatile and powerful multi-level lithographical technique to suspend atomic membranes, which can be applied to the vast majority of substrate, membrane and electrode materials. We also demonstrate, for the first time, fabrication and measurement of a free-standing thin Bi_2Se_3 membrane, which has low contact resistance to electrodes and a mobility of $\gtrsim$500 cm^2/Vs.

4:18PM D37.00008 In-situ Investigation of Electrical-Mechanical Coupling in graphene-based devices , MINGYUAN HUANG, California Institute of Technology, TOD PASCAL, HYUNGJUN KIM, WILLIAM GODDARD III, JULIA GREER, California Institute of Technology — Graphene, a truly two-dimensional gapless semiconducting material, recently deemed strongest ever measured, can sustain very high (up to 25%) in-plane tensile elastic strains. Several recent theoretical-only studies on strained graphene predict that strain can shift the Dirac cones, reduce the Fermi velocity, introduce a pseudo-magnetic field, and be used to engineer the electronic structure. However, no direct experiments on electrical measurements of highly strained graphene have yet been reported. Here, we present the results of *in-situ* investigation of electrical-mechanical coupling in graphene-based devices. In our experiment, *in-situ* nanoindentation was performed on suspended graphene transistors to introduce homogeneous tensile strain up to 3%, while electrical measurements were carried out simultaneously. We find that the electrical resistance shows only a marginal change under strain, and the electronic transport measurement confirms that there is no opening of the band gap for graphene under moderate uniform strain. We also report first-principles informed molecular dynamics simulation that lead to Young modulus consistent with our experiments and show no opening of a band gap.

4:30PM D37.00009 Radio Frequency Electrical Transduction of Graphene Mechanical Resonators , CHANGYAO CHEN, VIKRAM DESHPANDE, YUEHANG XU, FRANK DIRENNO, ALEXANDER GONDARENKO, DAVID HEINZ, SHUAIMIN LIU, PHILIP KIM, JAMES HONE, Columbia University — We report radio frequency (RF) electrical readout of graphene mechanical resonators. The mechanical motion is actuated and detected directly by using a vector network analyzer (VNA), employing a local gate to minimize parasitic capacitance. Resist-free doubly-clamped samples with resonant frequency in MHz range, Q factor ~10,000 at 77 K and signal-to-background ratio of over 20 dB, are demonstrated. In addition to being over two orders of magnitude faster than the electrical RF mixing method, this technique paves the way for use of graphene in RF devices such as filters and oscillators.

4:42PM D37.00010 Measurement of the shear modulus of single-layer graphene[1] , THOMAS METCALF, Naval Research Laboratory, XIAO LIU, JEREMY ROBINSON, KEITH PERKINS, BRIAN HOUSTON — We have measured the shear modulus of large area (2mm $\times$ 5mm), single-layer (90–95%) polycrystalline graphene sheets and found values consistent with theoretical predictions of G=200 GPa. The graphene was grown by chemical vapor deposition onto a copper foil and subsequently transferred onto a mechanical resonator known as a double-paddle oscillator (DPO). DPOs are fabricated from single-crystal, 0.3mm thick silicon wafers, and have a torsional vibratory mode at 5500 Hz which has a very large quality factor, $Q = 5 \times 10^7$, at low (< 10 K) temperatures, giving the DPO a high sensitivity to a film deposited on its torsional element. Such a film increases the (lumped-element) spring constant of the resonator, and the film's shear modulus can be deduced from the subsequent resonant frequency shift.

[1]Work supported by the Office of Naval Research

4:54PM D37.00011 Tearing of Graphene[1] , MARIA MOURA, MICHAEL MARDER, Department of Physics - University of Texas at Austin — Experiments on free standing graphene can expose the graphene sheets to out-of-plane forces. An example of that is the back-gate voltage experimental setup. Here we show that out-of-plane forces can cause free standing graphene to fracture. This fracture mode is known as tearing mode and is common in materials like paper. We present a numerical study of the propagation of cracks in clamped, free standing graphene as a function of the out-of-plane force. We report a threshold for the graphene fracture energy.

[1]We thank Fulbright and CAPES for scholarship funding and the National Science Foundation for funding through DMR 0701373.

5:06PM D37.00012 Variable strain in graphene sealed microchambers studied with Raman spectroscopy[1] , A.L. KITT, Boston University, J.W. SUK, University of Texas, Austin, S. REMI, S. AHMED, Boston University, R. PINER, K.M. LIECHTI, R.S. RUOFF, University of Texas, Austin, A.K. SWAN, B.B. GOLDBERG, Boston University — Raman measurements are a sensitive tool for evaluating strain in graphene. Graphene sealed cylindrical microchambers provide a unique way of generating strain. Suspended graphene avoids substrate interactions which make it difficult to evaluate the graphene response, e.g., combined graphene-substrate Poisson ratio, or slippage. Additionally, the system provides a wide range of strain states with different lattice symmetries. At a fixed external pressure, the strain state varies radially. The strain is biaxial in the center and changes gradually to only radial strain at the edges. The continuum model is evaluated to find the radial strain states. Combined with Raman Spectroscopy, several fundamental parameters can be measured. We will discuss the strain and polarization dependent splitting of the G and 2D bands and compare to previous works [1,2]. Furthermore, preliminary measurements of the strain dependence of thermal properties will be discussed.

[1] T. Mohiuddin et al, Phys Rev B 79, 1-8 (2009)
[2] M. Huang, et al, Nano Letters 10, 4074-9 (2010)

[1]We acknowledge support from the Advanced Energy Consortium

5:18PM D37.00013 An Effective Tensional Strain View on the Bandgap Tunability of Helical Graphene Nanoribbons with Open and Closed Edges , DONG-BO ZHANG, TRAIAN DUMITRICA, University of Minnesota — Despite the scientific importance of graphene nanoribbons, little is known about their electronic structure other than in the flat-form presupposition. To quantify the strain stored in helical graphene nanoribbons and fractional carbon nanotubes, we supplement the standard elasticity concepts with an effective tensional strain. Using π-orbital tight binding and objective molecular dynamics coupled with density functional theory, we develop a unified theory for the electromechanical response in which the consequences of the torsional deformation are taken into account via the effective tensional strain. In spite of the open and closed edges as well as the inverse Poynting effect exhibited by these nanostructures, from the effective strain perspective the twist-induced bandgap modulations appear strikingly similar with those exhibited by carbon nanotubes in tension. Our theory may be useful for designing new electromechanical devices and experiments using carbon nanocomponents, and for establishing edge-chemistry driven nanofabrication principles for helical graphene nanoribbons with tunable bandgaps.

Monday, March 21, 2011 2:30PM - 5:06PM –

Session D38 DCP: Earle K. Plyler Prize Session II: Spectroscopy A130/131

2:30PM D38.00001 Ultrafast Nonlinear Optical Spectroscopy or where would we be without Shaul Mukamel? , GRAHAM FLEMING, University of California Berkeley — The development of ultrafast nonlinear optical spectroscopy owes much to the pioneering work of Shaul Mukamel in developing a unifying framework and language with which to understand and relate the content of different types of experiment. The culmination of this work, to date, is in the development of multidimensional optical spectroscopies. In this talk, I will describe recent work in my group on two dimensional electronic spectroscopy of photosynthetic light-harvesting complexes and, if time permits, single walled carbon nanotubes and molecular systems relaxing via conical intersections.

3:06PM D38.00002 2D IR Spectroscopy of Protein Conformation, Folding, and Binding , KEVIN JONES, ANDREI TOKMAKOFF, ZIAD GANIM, JOSHUA LESSING, C. SAM PENG, MIT Department of Chemistry — 2D IR spectroscopy is an increasingly powerful tool for investigation of protein structure and dynamics. As an ultrafast spectroscopy, it provides information on protein structure and conformational variation with high time resolution, providing a tool to study the dynamics of folding and binding. Some of the unique characteristics of 2D IR result from the powerful structure based modeling that is available for amide vibrations. This talk will cover recent examples from our group in which different forms of protein 2D IR and computational spectroscopy are used to reveal conformational heterogeneity in peptides, the folding and binding of proteins, and protein-water interactions. When combined with temperature-jump experiments, the formation and interchange of these structures is probed.

3:18PM D38.00003 Three-dimensional Fourier-transform spectroscopy of potassium vapor , HEBIN LI, ALAN BRISTOW, MARK SIEMENS, GALAN MOODY, STEVEN CUNDIFF, JILA, University of Colorado and National Institute of Standards and Technology, Boulder, CO 80309 — We have implemented three-dimensional (3D) Fourier-transform spectroscopy to study potassium vapor contained in a $\sim$20 μm transmission cell with argon buffer gas. The four-wave mixing signal is measured in three time dimensions corresponding to the delays between three $\sim$100 fs, phase-stabilized excitation pulses that are arranged in the box geometry. The emission is detected using a phase-stabilized reference pulse by spectral interferometry, and other time axes are Fourier transformed to construct the 3D spectra. The 3D spectra contain the full information of third-order coherent response of the vapor, yet the contribution from each of the single-quantum excitation pathways is unambiguously isolated. Projecting a 3D spectrum onto a specific two-dimensional (2D) plane retrieves rephasing, non-rephasing, and T-scan 2D spectra, as well as the spectra that are not accessible by conventional 2D scans. The spectral features which overlap in congested 2D spectra can be isolated for studying unique processes represented by a single pathway.

3:30PM D38.00004 Reflection Geometry Electronic Two-dimensional Fourier Transform Spectroscopy[1] , THOMAS W. JARVIS, ZHENG SUN, XIAOQIN LI, Department of Physics, University of Texas at Austin, Austin, Texas 78712, MIKHAIL EREMENTCHOUK, MICHAEL N. LEUENBERGER, NanoScience Technology Center & Department of Physics, University of Central Florida, Orlando, Florida 32826 — Studying dynamics in nanostructures is vital to develop new opto-electronic devices and to understand fundamental processes in the solid state. Electronic Two-dimensional Fourier Transform Spectroscopy (2DFTS) is a powerful technique that coherently probes the nonlinear optical polarization, establishing correlations between absorption and subsequent emission or dispersion. We perform 2DFTS in reflection, a novel experimental geometry that allows us to probe structured materials. The coupling features and dimensionally extended lineshapes revealed by 2DFTS provide a description of decoherence and dephasing processes, coherent and incoherent energy transfer, and relaxation.

[1]This work is supported financially by ARO, NSF, ONR, Welch Foundation, Texas-ARP, and the Alfred P. Sloan Foundation.

3:42PM D38.00005 Ultrafast two dimensional infrared chemical exchange spectroscopy[1] , MICHAEL FAYER, Stanford University — The method of ultrafast two dimensional infrared (2D IR) vibrational echo spectroscopy is described. Three ultrashort IR pulses tuned to the frequencies of the vibrational transitions of interest are directed into the sample. The interaction of these pulses with the molecular vibrational oscillators produces a polarization that gives rise to a fourth pulse, the vibrational echo. The vibrational echo pulse is combined with another pulse, the local oscillator, for heterodyne detection of the signal. For fixed time between the second and third pulses, the waiting time, the first pulse is scanned. Two Fourier transforms of the data yield a 2D IR spectrum. The waiting time is increased, and another spectrum is obtained. The change in the 2D IR spectra with increased waiting time provides information on the time evolution of the structure of the molecular system under observation. In a 2D IR chemical exchange experiment, two species A and B, are undergoing chemical exchange. A's are turning into B's, and B's are turning into A's, but the overall concentrations of the species are not changing. The kinetics of the chemical exchange on the ground electronic state under thermal equilibrium conditions can be obtained 2D IR spectroscopy. A vibration that has a different frequency for the two species is monitored. At very short time, there will be two peaks on the diagonal of the 2D IR spectrum, one for A and one for B. As the waiting time is increased, chemical exchange causes off-diagonal peaks to grow in. The time dependence of the growth of these off-diagonal peaks gives the chemical exchange rate. The method is applied to organic solute-solvent complex formation, orientational isomerization about a carbon-carbon single bond, migration of a hydrogen bond from one position on a molecule to another, protein structural substate interconversion, and water hydrogen bond switching between ions and water molecules.

[1]This work was supported by the Air Force Office of Scientific Research (F49620-01-1-0018), the Department of Energy (DE-FG03-84ER13251), and the National Science Foundation (DMR 0652232).

4:18PM D38.00006 Can the Isomerization of Retinal in Bacteriorhodopsin be Coherently Controlled in Strong Fields? , VALENTYN PROKHORENKO[1], University of Toronto, Chemistry Department, ALEXEI HALPIN, University of Toronto, Physics Department, PHILIP JOHNSON, University of Toronto, Chemistry Department, LEONID BROWN, University of Guelph, Physics Department, DWAYNE MILLER, University of Toronto, Chemistry and Physics Departments — Conflicting results have been obtained between weak field experiments (one-photon absorption) [1] and strong field recent studies [2] (multi-photon effects). Here we present our strong field experiments performed using linearly-chirped excitation pulses. Contrary to [2], we clearly observe phase-dependent control of photoproduct yield over a wide range of excitation energies. Above the excitation limit of $\sim$200 GW/cm^2 our results do however come into agreement with [2], but only for a single observation wavelength (650 nm) whereas the transient spectra unambiguously show drastic changes in the protein due to its ionization. At these excitation levels, this deleterious side channel precludes correct determination of the amount of 13-cis isomer. As such, we argue that it is impossible to make assignments of mechanistic details of control at a high field that in effect "kills" the protein. [1] V. I. Prokhorenko, A. M. Nagy, S. A. Waschuk, L. S. Brown, R. R. Birge, and R. J. D. Miller, Science 313, 1257-1261 (2006). [2] A. C. Florean et al., PNAS 106, 10896-10900 (2009).

[1]Present: University of Hamburg, Physics Department, Germany

4:30PM D38.00007 Toward Investigating Protein Folding Using the Combination of Computer Simulation and Spectroscopy , WEI ZHUANG — Protein folding is an important problem that is attracting scientists from a wide range of disciplines. One of the major challenges comes from the gap between the experimental and the theoretical studies. We proposed a computational protocol of simulating the T-jump peptide unfolding experiments and the related transient IR and 2DIR spectra based on the Markov State Model (MSM) and Nonlinear Exciton Propagation (NEP) methods. MSMs partition the conformation space into a set of non-overlapping metastable states, and we can calculate spectra signal for each of these states using NEP method. Thus the overall spectroscopic observable for a given system is simply the sum of spectra of different metastable states weighted by their populations. Simulated spectra based on MSM have a much better agreement with the equilibrium experimental 2DIR spectra compared to MD simulations starting from the folded state. MSMs are also capable of simulating the unfolding relaxation dynamics upon the temperature jump. The agreement of the simulation using MSMs and NEP with the experiment provides a justification for our protocol as well as a physical insight underlying the spectroscopic observables.

4:42PM D38.00008 Supersymmetry and fluctuation relations for currents in closed networks , VLADIMIR CHERNYAK, Wayne State University, NIKOLAI SINITSYN, Los Alamos National Laboratory — The discovery of fluctuation theorems and nonequilibrium work relations has stimulated considerable interest in nonequilibrium statistical mechanics and theory of counting statistics. It is important to obtain exact relations that do not directly rely on the thermodynamic concepts, such as work or entropy, but rather describe unambiguous microscopic characteristics, such as statistics of particle currents in systems driven by time-dependent fields. We identify hidden supersymmetry in evolution, governed by the master equation, that survives on the level of the counting statistics of stochastic particle currents. Supersymmetry connects the evolutions in the spaces of populations (boson component) and empirical currents (fermion component). We present exact relations for statistics of currents in strongly driven mesoscopic stochastic systems. Being reminiscent of known fluctuation theorems, a part of our exact result is not directly related to the condition of microscopic reversibility but rather follows from *supersymmetry* of the counting statistics of currents.

4:54PM D38.00009 Understanding Metal-Adsorbate Binding with Surface-Enhanced Raman Spectroscopy: Theory and Experiment[1] , ALEXEY ZAYAK, Molecular Foundry, LBNL, HYUCK CHOO, EECS, UC Berkeley, YING HU, Bioengineering Dpt., Rice University, JEFFREY BOKOR, EECS, UC Berkeley, STEFANO CABRINI, JAMES SCHUCK, JEFFREY NEATON, Molecular Foundry, LBNL — Building on recent work [1], we use a combination of density functional theory (DFT) calculations and surface-enhanced Raman spectroscopy (SERS) measurements to explain experimentally observed variations in SERS data of an organic molecule, trans-1,2-two (4-pyridyl) ethylene (BPE). For the BPE on Au surfaces, our DFT calculations provide a quantitative description of chemical enhancement (CE), and elucidate that variations reported in experiments arise from a convolution of two factors: a nonuniform frequency dependent electromagnetic enhancement, and dependence of CE on the sample incubation time. The later reveals aspects of the binding kinetics of BPE to Au surfaces.

[1] A. T. Zayak,et. al., arXiv:1011.1873v1

[1]We acknowledge support from DOE and DARPA. Computational resources provided by NERSC.

Monday, March 21, 2011 2:30PM - 5:30PM –
Session D39 DBP: Physics of Physiological Systems A124/127

2:30PM D39.00001 Axonal Transport and Morphology: How Myelination gets Nerves into Shape[1] , PETER JUNG, PENG ZHAO, Ohio University, PAULA MONSMA, TONY BROWN, Ohio State University — The local caliber of mature axons is largely determined by neurofilament (NF) content. The axoskeleton, mainly consisting of NFs, however, is dynamic. NFs are assembled in the cell body and are transported by molecular motors on microtubule tracks along the axon at a slow rate of fractions of mm per day. We combine live cell fluorescent imaging techniques to access NF transport in myelinated and non-myelinated segments of axons with computational modeling of the active NF flow to show that a), myelination locally slows NF transport rates by regulating duty ratios and b), that the predicted increase in axon caliber agrees well with experiments. This study, for the first time, links NF kinetics directly to axonal morphology, providing a novel conceptual framework for the physical understanding of processes leading to the formation of axonal structures such as the "Nodes of Ranvier" as well as abnormal axonal swellings associated with neurodegenerative diseases like Amyotrophic lateral sclerosis (ALS).

[1]NSF grants # IOS-0818412(PJ) and IOS-0818653 (AB).

2:42PM D39.00002 Experimental evaluation of biophysical neurite growth models , ZACHARY WISSNER-GROSS, Harvard University, MARK SCOTT, DAVID KU, PRIYA RAMASWAMY, MEHMET YANIK, Massachusetts Institute of Technology — During nervous system development, neurons exhibit complex growth dynamics, as several neurites compete to become each neuron's axon. Numerous mathematical and biophysical models have been proposed to explain this competition, but these models remain experimentally unverified. Large-scale and repeatable measurements of neurite dynamics are difficult to perform, since neurons have varying numbers of neurites, which themselves have complex morphologies. To overcome these challenges using a minimal number of primary neurons, we generated repeatable neuronal morphologies by laser-patterning micron-wide stripes of adhesive proteins on an otherwise highly non-adherent substrate. Upon analyzing thousands of time-lapse measurements, we observed three key neuronal behaviors: total neurite growth accelerated until neurons polarized, immature neurites competed even at very short lengths, and neuronal polarity underwent an apparent phase transition as the neurites grew beyond a critical length. Proposed biophysical neurite growth models agreed only partially with our experimental observations, and simple yet specific modifications significantly improved these models. The protein patterning and high-content analyses presented here could also be employed for studying other structural or biomechanical cellular phenomena.

2:54PM D39.00003 Deep Brain Stimulation using Magnetic Fields , DAVID JILES, Iowa State University, Ames, Iowa 50011, PAUL WILLIAMS, LAWRENCE CROWTHER, Wolfson Centre for Magnetics, Cardiff University, United Kingdom, IOWA STATE UNIVERSITY TEAM, WOLFSON CENTRE FOR MAGNETICS TEAM — New applications for transcranial magnetic stimulation are developing rapidly for both diagnostic and therapeutic purposes. Therefore so is the demand for improved performance, particularly in terms of their ability to stimulate deeper regions of the brain and to do so selectively. The coil designs that are used presently are limited in their ability to stimulate the brain at depth and with high spatial focality. Consequently, any improvement in coil performance would have a significant impact in extending the usefulness of TMS in both clinical applications and academic research studies. New and improved coil designs have then been developed, modeled and tested as a result of this work. A large magnetizing coil, 300mm in diameter and compatible with a commercial TMS system has been constructed to determine its feasibility for use as a deep brain stimulator. The results of this work have suggested directions that could be pursued in order to further improve the coil designs.

3:06PM D39.00004 Growth of Necrotic Cores in Vulnerable Plaque , PAK-WING FOK, Mathematical Sciences — Plaques are fatty deposits that grow mainly in arteries and develop as a result of a chronic inflammatory response. Plaques are called *vulnerable* when they are prone to mechanical rupture. Vulnerable Plaques (VPs) are characterized by lipid-rich, necrotic cores that are heavily infiltrated with macrophages. The rupture of VPs releases thrombogenic agents into the bloodstream, usually resulting in myocardial infarctions. We propose a quantitative model to predict the development of a plaque's necrotic core. By solving coupled reaction-diffusion equations for macrophages and dead cells, we explore the joint effects of hypoxic cell death and chemo-attraction to Ox-LDL, a molecule that is strongly linked to atherosclerosis. Our model predicts cores that have approximately the right size and shape. Normal mode analysis and subsequent calculation of the smallest eigenvalues allow us to compute the times required for the system to reach its steady state. This study allows us to make quantitative predictions for how quickly vulnerable plaques develop and how their growth depends on system parameters such as chemotactic coefficients and cell death rates.

3:18PM D39.00005 Understanding cellular architecture in cancer cells , SIMONE BIANCO, CHAO TANG, Department of Bioengineering and Therapeutic Science, University of California San Francisco — Understanding the development of cancer is an important goal for today's science. The morphology of cellular organelles, such as the nucleus, the nucleoli and the mitochondria, which is referred to as cellular architecture or cytoarchitecture, is an important indicator of the state of the cell. In particular, there are striking difference between the cellular architecture of a healthy cell versus a cancer cell. In this work we present a dynamical model for the evolution of organelles morphology in cancer cells. Using a dynamical systems approach, we describe the evolution of a cell on its way to cancer as a trajectory in a multidimensional morphology state. The results provided by this work may increase our insight on the mechanism of tumorigenesis and help build new therapeutic strategies.

3:30PM D39.00006 A two-scale model for correlation between B cell VDJ usage in zebrafish , KEYAO PAN, MICHAEL DEEM, Rice University — The zebrafish (Danio rerio) is one of the model animals for study of immunology. The dynamics of the adaptive immune system in zebrafish is similar to that in higher animals. In this work, we built a two-scale model to simulate the dynamics of B cells in primary and secondary immune reactions in zebrafish and to explain the reported correlation between VDJ usage of B cell repertoires in distinct zebrafish. The first scale of the model consists of a generalized NK model to simulate the B cell maturation process in the 10-day primary immune response. The second scale uses a delay ordinary differential equation system to model the immune responses in the 6-month lifespan of zebrafish. The generalized NK model shows that mature B cells specific to one antigen mostly possess a single VDJ recombination. The probability that mature B cells in two zebrafish have the same VDJ recombination increases with the B cell population size or the B cell selection intensity and decreases with the B cell hypermutation rate. The ODE model shows a distribution of correlation in the VDJ usage of the B cell repertoires in two six-month-old zebrafish that is highly similar to that from experiment. This work presents a simple theory to explain the experimentally observed correlation in VDJ usage of distinct zebrafish B cell repertoires after an immune response.

3:42PM D39.00007 Modelling Nanoparticle Diffusion into Cancer Tumors , VISHWA PRIYA PODDUTURI, Louisiana Tech University, Institute for Micromanufacturing, PEDRO DEROSA, Louisiana Tech University,Institure for Micromanufacturing. Grambling State University, Physics Department — Cancer is one of the major, potentially deadly diseases and has been for years. Non-specific delivery of the drug can damage healthy tissue seriously affecting in many cases the patient's living condition. Nanoparticles are being used for a targeted drug delivery thereby reducing the dose. In addition, metallic nanoparticles are being used in thermal treatment of cancer cells where nanoparticles help concentrate heat in the tumor and away from living tissue. We proposed a model that combines random walk with diffusion principles. The particle drift velocity is taken from the Hagen-Poiseuille equation and the velocity profile of the particle at the pores in the capillary wall is obtained using the Coventorware software. Pressure gradient and concentration gradient through the capillary wall are considered. Simulations are performed in Matlab using the Monte Carlo technique. Number of particles leaving the blood vessel through a pore is obtained as a function of blood pressure, the osmotic pressure, temperature, particle concentration, blood vessel radius, and pore size, and the relative effect of each of the parameters is discussed.

3:54PM D39.00008 ABSTRACT WITHDRAWN –

4:06PM D39.00009 Hearing and Infinite-Period Bifurcations , SEUNG JI, UCLA, DOLORES BOZOVIC, ROBIJN BRUINSMA, UCLA — Auditory and vestibular systems present us with biological sensors that can achieve sub-nanometer sensitivity orders of magnitude in the dynamic range, while operating in a fluid-immersed, room-temperature environment. While the mechanisms behind this extreme sensitivity and robustness of the inner ear have not been fully explained, nonlinear response has been shown to be crucial to its proper function. Recent experiments have recorded innate motility of hair cells of the bullfrog sacculus, under varying degrees of steady-state offset. The bundle deflection was shown to suppress or enhance spontaneous oscillations, and affect the sensitivity of the mechanical response. We will present a theoretical model based on cubic nonlinearity and show that in different parameter regimes, the system can be induced to cross a supercritical Hopf bifurcation, an infinite-period bifurcation, or a multi-critical point. Comparing the numerical simulation to the experiment, we will present evidence that the multi-critical point corresponds most closely to the dynamic state of saccular hair cells. Further, we will discuss the crossing of the bifurcation, and the sensitivity of the phase-locked response in various frequency regimes.

4:18PM D39.00010 Axonal Transport and Morphogenesis near Retinal Excavation of the eye[1] , YINYUN LI, Department of Physics and Astronomy, Ohio University, ANTHONY BROWN, Center for Molecular Neurobiology and Department of Neuroscience, Ohio State University, PETER JUNG, Department of Physics and Astronomy, Ohio University — Neurofilaments(NFs) represent the main space-filling elements of mature axons. NFs are transported on microtubule (MT) tracks along the axon at a slow rate of mm/day and thus form a dynamic cytoskeleton. During development, the optic nerve forms a sharp increase of caliber at about $150\mu m$ from the retinal excavation of the eye. Our key hypothesis is a relation between NF kinetics and nerve morphology based on the continuity of the active flow of NFs. We use computational modeling of axonal transport to infer modulation of NF kinetics consistent with the observed increase of nerve caliber. We show that the inferred kinetics is also consistent with reported spatial distribution of NFs and MTs near the retinal excavation. We further show that the predicted time course of development of the observed nerve swelling is consistent with the time course of animal development.

[1]This work has been sponsored by NSF under grants IOS-0818412(PJ) and IOS-0818653(AB)

4:30PM D39.00011 Hydroxyapatite in Physiological Environment , ALEXANDER SLEPKO, ALEXANDER A. DEMKOV, The University of Texas at Austin — A carbonated form of hydroxyapatite (HA) [$Ca_{10}(PO_4)_6(OH)_2$] is one of the most abundant materials in mammal bone. It crystallizes within the spaces between tropocollagen protein chains in an aqueous solution and strengthens the bone tissue. An emerging application of synthetic HA is bone repair and replacement. Bulk electronic and chemical properties of HA were studied theoretically recently. However, the absorption of H_2O molecules and amino acids of the tropocollagen chains at HA surfaces remains an area of active research. Using density functional theory we analyze the electronic properties and surface energetics of HA for different orientations and terminations and generate a theoretical surface phase diagram of HA. The reactivity of these surface models is analyzed using the frontier orbital approach. We find two dominant surfaces which are most stable over the widest chemical range. However, we expect them to show little surface reactivity. Using a HA slab with a highly reactive surface we build atomistic models of HA covered with up to one monolayer of water and analyze interactions between this surface and the water molecules.

4:42PM D39.00012 Excitable signal relay in Dictyostelium discoideum , TROY MESTLER, DAVID SCHWAB, PANKAJ MEHTA, THOMAS GREGOR, Department of Physics, Princeton University — The social amoeba D. discoideum transitions when starved from a collection of individual cells into a multicellular spore-complex. During this process, amoebae display several interesting phenomena including intercellular signaling, pattern formation, and cell differentiation. At the heart of these phenomena is the exchange of the signaling molecule cyclic-AMP, which has previously been extensively studied using a variety of indirect methods. Here we employ a sensor that uses a compound fluorescent protein whose emission spectrum changes in the presence of bound cyclic AMP to directly monitor, in real time and in vivo, intracellular cAMP concentrations. We use cells expressing this sensor in microchemostats to study intracellular cAMP concentrations at the single-cell level in response to precise, dynamically-controlled external cAMP stimulation. Specifically, we show that these cells display excitability much like that found in neurons and agree experimentally quite well with a modified FitzHugh-Nagumo dynamical systems model. This single-cell model sets groundwork for a comprehensive multicellular model that promises to explain emergent behavior in D. discoideum.

4:54PM D39.00013 Modeling Intracellular Oscillations and Polarity Transition in Fission Yeast , TYLER DRAKE, Lehigh University, MAITREYI DAS, FULVIA VERDE, Miami University, DIMITRIOS VAVYLONIS, Lehigh University — Fission yeast, a pill-shaped model organism, restricts growth to its tips. These cells maintain an asymmetric growth state, growing at only one tip, until they meet length and cell-cycle requirements. With these met, they grow at both. The mechanism of this transition, new-end take-off (NETO), remains unclear. We find that NETO occurs due to long-range competition for fast-diffusing signaling protein Cdc42 between the old and new tips. From experimental results, we suppose that symmetric tips compete for Cdc42, which triggers growth. We describe a symmetric growth model based on competition between tips. This model restricts short cells to monopolar states while allowing longer cells to be bipolar. Autocatalytic Cdc42 recruiting at both cells tips leads to broken symmetry, and the recruiting cuts off as tip Cdc42 levels saturate. Non-linear differential equations describe the model, with stable attractors indicating valid distributions. Linear stability analysis and numerical methods identify stable fixed points over a twofold increase in cell length. The model reproduces qualitative behavior of the organism. We show that observed pole-to-pole Cdc42 oscillations may facilitate the polarity transition and discuss their relationship to the Min system in E. Coli.

5:06PM D39.00014 Biomineral Structure and Strength of Barnacle Exoskeletons , NATHAN SWIFT, Colgate University — Studying the construction of organic-inorganic compound structures through biomineralization is potentially very useful. During biomineral formation, organisms restructure naturally occurring minerals in conjunction with their own organically produced minerals to create new structures. While there is extensive knowledge about material properties and structure of the raw minerals themselves, insight into how specific biomineral structures and compounds contribute to an object's mechanical properties is lacking. In this study, the exoskeletons of barnacles from the genus *Balanus* were examined, both for their physical structure (how they're put together) and for their mechanical properties (strength, hardness, and elasticity). Scanning electron microscopy produced close-up, detailed images of the inner shell structure to determine what type of structure barnacles build during exoskeleton formation. Energy dispersive x-ray spectroscopy was used to map the elemental components of the shells. Nanoindentation tested the mechanical properties of these mapped structures to determine how certain characteristics of the exoskeleton contribute to its mechanical properties.

5:18PM D39.00015 Enhancing mechanical properties of calcite by Mg substitutions: An ab initio study , PAVLINA ELSTNEROVA, MARTIN FRIAK, TILMANN HICKEL, HELGE OTTO FABRITIUS, LIVERIOS LYMPERAKIS, MICHAL PETROV, DIERK RAABE, JOERG NEUGEBAUER, Max Planck Institute for Iron Research, Duesseldorf, Germany, SVETOSLAV NIKOLOV, Institute of Mechanics, Bulgarian Academy of Sciences, Sofia, Bulgaria, ANDREAS ZIGLER, Central Facility for Electron Microscopy, University of Ulm, Ulm, Germany, SABINE HILD, Department of Polymer Science, Johannes Kepler University Linz, Linz, Austria — Arthropoda representing a majority of all known animal species are protected by an exoskeleton formed by their cuticle. The cuticle represents a hierarchically structured multifunctional bio-composite based on chitin and proteins. Some groups like Crustacea reinforce the load-bearing parts of their cuticle with calcite. As the calcite sometimes contains Mg it was speculated that Mg may have a stiffening impact on the mechanical properties of the cuticle. We present a theoretical parameter-free quantum-mechanical study of thermodynamic, structural and elastic properties of Mg-substituted calcite. Our results show that substituting Ca by Mg causes an almost linear decrease in the crystal volume with Mg concentration and of substituted crystals. As a consequence the calcite crystals become stiffer giving rise e.g. to substantially increased bulk moduli.

Monday, March 21, 2011 2:30PM - 4:42PM –

Session D40 DBP: Lipid Bilayers and Biological Membranes: Peptide Interactions A122/123

2:30PM D40.00001 Molecular Simulations of Sequence-Specific Association of Transmembrane Proteins in Lipid Bilayers , MANOLIS DOXASTAKIS, ANUPAM PRAKASH, LORANT JANOSI, University of Houston — Association of membrane proteins is central in material and information flow across the cellular membranes. Amino-acid sequence and the membrane environment are two critical factors controlling association, however, quantitative knowledge on such contributions is limited. In this work, we study the dimerization of helices in lipid bilayers using extensive parallel Monte Carlo simulations with recently developed algorithms. The dimerization of Glycophorin A is examined employing a coarse-grain model that retains a level of amino-acid specificity, in three different phospholipid bilayers. Association is driven by a balance of protein-protein and lipid-induced interactions with the latter playing a major role at short separations. Following a different approach, the effect of amino-acid sequence is studied using the four transmembrane domains of the epidermal growth factor receptor family in identical lipid environments. Detailed characterization of dimer formation and estimates of the free energy of association reveal that these helices present significant affinity to self-associate with certain dimers forming non-specific interfaces.

2:42PM D40.00002 An amino acid composition criterion for membrane active antimicrobials , NATHAN SCHMIDT, GHEE HWEE LAI, Physics, UIUC, ABHIJIT MISHRA, Bioengineering, UCLA, DENNIS BONG, Chemistry, Ohio State U, PAUL MCCRAY, JR., Pediatrics, U. Iowa, MICHAEL SELSTED, ANDRE OUELLETTE, Pathology, USC, GERARD WONG, Bioengineering, UCLA — Membrane active antimicrobials (AMPs) are short amphipathic peptides with broad spectrum anti microbial activity. While it is believed that their hydrophobic and cationic moieties are responsible for membrane-based mechanisms of action, membrane disruption by AMPs is manifested in a diversity of outcomes, such as pore formation, blebbing, and budding. This complication, along with others, have made a detailed, molecular understanding of AMPs difficult. We use synchrotron small angle xray scattering to investigate the interaction of model bacterial and eukaryotic cell membranes with archetypes from beta-sheet AMPs (e.g. defensins) and alpha-helical AMPs (e.g. magainins). The relationship between membrane composition and peptide induced changes in membrane curvature and topology is examined. By comparing the membrane rearrangement and phase behavior induced by these different peptides we will discuss the importance of amino acid composition on AMP design.

2:54PM D40.00003 Interaction between Cell Penetrating pVEC and cell membranes , ABHIJIT MISHRA, Bioengineering Dept., University of California Los Angeles, GHEE HWEE LAI, NATHAN SCHMIDT, GERARD WONG, Bioengineering Dept., University of California Los Angeles, Dept. of Physics University of Illinois Urbana Champaign — Vascular Endothelial Cadherin (VEC) is a transmembrane-spanning glycoprotein that belongs to the family of cell adhesion molecules and plays an active role in control of vascular permeability and angiogenesis. PVEC, an 18 amino acid domain, has been shown to be able to traverse cell membranes with attached macromolecules. pVEC is an amphiphilic molecule with a high content of basic amino acids resulting in a net positive charge. Electrostatic and hydrophobic interactions can perturb membrane self-assembly and stability and are likely to be responsible for peptide uptake. We use synchrotron x-ray scattering and confocal microscopy to examine the phase behavior of the pVEC lipid system, and its relation to membrane permeation mechanisms.

3:06PM D40.00004 Interactions between cyclic cell penetrating peptides and lipid membranes , KUN ZHAO, Bioengineering Department, University of California, Los Angeles, TAO LIU, Chemistry Department, the Ohio State University, MIKE CHOE, DANIEL KAMEI, Bioengineering Department, University of California, Los Angeles, DEHUA PEI, Chemistry Department, the Ohio State University, GERARD WONG, Bioengineering Department, University of California, Los Angeles — Cyclic peptides exhibit strong enhancement in receptor-binding affinity, specificity, and stability relative to their linear counterparts, partially due to their reduced conformational freedom. In this work, we examine cyclic versions of cell penetrating peptides. Using small-angle x-ray scattering (SAXS) measurements, we show that cyclic polyarginine peptides generate saddle-splay curvature more efficiently than their linear counterparts, We show how this increase in induced saddle splay curvature impinges on the efficiency of cell penetration in a series of giant vesicle and intracellular trafficking experiments.

3:18PM D40.00005 Interaction of a P. aeruginosa Quorum Sensing Signal with Lipid Membranes , REBECCA MORRISON, AMELIA HALL, ELLEN HUTCHISON, THUC NGUYEN, BENJAMIN COOLEY, VERNITA GORDON, University of Texas at Austin — Bacteria use a signaling and regulatory system called "quorum sensing" to alter their gene expressions in response to the concentration of neighboring bacteria and to environmental conditions that make collective activity favorable for bacteria. P. aeruginosa is an opportunistic human pathogen that uses quorum sensing to govern processes such as virulence and biofilm formation. This organism's two main quorum sensing circuits use two different signaling molecules that are amphiphilic and differ primarily in the length of their hydrocarbon side chain and thus in their hydrophobic physical chemistry. How these physical chemistries govern the propagation and spatial localization of signals and thus of quorum sensing is not known. We present preliminary results showing that signals preferentially sequester to amphiphilic lipid membranes, which can act as reservoirs for signal. This is promising for future characterization of how the quorum sensing signals of many bacteria and yeast partition to spatially-differentiated amphiphilic environments, in a host or biofilm.

3:30PM D40.00006 Criticality in Plasma Membranes , BENJAMIN MACHTA, STEFANOS PAPANIKOLAOU, JAMES SETHNA, Cornell University, SARAH VEATCH, University of Michigan — We are motivated by recent observations of micron-sized critical fluctuations in the 2d Ising Universality class in plasma membrane vesicles that are isolated from cortical cytoskeleton. We construct a minimal model of the plasma membrane's interaction with intact cytoskeleton which explains why large scale phase separation has not been observed in Vivo. In addition, we use analytical techniques from conformal field theory and numerical simulations to investigate the form of effective forces mediated by the membrane's proximity to criticality. We show that the range of this force is maximized near a critical point and we quantify its usefulness in mediating communication using techniques from information theory. Finally we use theoretical techniques from statistical physics in conjunction with Monte-Carlo simulations to understand how criticality can be used to increase the efficiency of membrane bound receptor mediated signaling. We expect that this sort of analysis will be broadly useful in understanding and quantifying the role of lipid "rafts" in a wide variety of membrane bound processes. Generally, we demonstrate that critical fluctuations provide a physical mechanism to organize and spatially segregate membrane components by providing channels for interaction over relatively large distances.

3:42PM D40.00007 Fluctuation-induced forces between inclusions in a fluid membrane under tension , HSIANG-KU LIN, ROYA ZANDI, LEONID P. PRYADKO, Department of Physics and Astronomy, University of California at Riverside — We discuss the fluctuation-induced force, a finite-temperature analog of the Casimir force, between two inclusions embedded in a fluid membrane under tension. We suggest a method to calculate this Casimir interaction in the most general case, where membrane fluctuations are governed by the combined action of surface tension, bending modulus, and Gaussian rigidity. We find that the surface tension strongly modifies the power law in the separation dependence of the Casimir interaction. Furthermore, the method allows us to calculate the Casimir force both at short and large separations.

3:54PM D40.00008 Nanoparticles Induced Microscaled Pore Formation on Supported Lipid Bilayer , BENXIN JING, Y. ELAINE ZHU — Most of recent researches on the cytotoxicity of nanomaterials focused on hydrophilic nanomaterials because of their good dispersion in water, but much less on hydrophobic ones. In this work, we have investigated the effect of semi-hydrophobic nanoparticles (NPs) on the dynamics and morphology of model cell membrane. We have found carboxyl functionalized polystyrene nanoparticles can induce the formation of microscaled pores on neutral supported Egg PC lipid bilayer at the ionic strength range similar to that in the human body with a strong dependence on nanoparticle size and concentration. The hydrophobic interaction between the NP surface and lipid bilayer is accounted for the induced line tension in lipid bilayer; when the tension exceeds a critical value, pores are formed and grow rapidly with dependence on nanoparticle size and ionic strength.

4:06PM D40.00009 Modeling the Elastic Properties of Lipid Bilayer Membranes , EDWARD BARRY[1], MRSEC at Brandeis University, THOMAS GIBAUD, MRSEC at Brandeis Universiy, MARK ZAKHARY, ZVONIMIR DOGIC, MRSEC at Brandeis University — Model membranes such as lipid bilayers have been indispensable tools for our understanding of the elastic properties of biological membranes. In this talk, I will introduce a colloidal model for membranes and demonstrate that the physical properties of these colloidal membranes are identical to lipid bilayers. The model system is unique in that the constituent molecules are homogenous and non-amphiphilic, yet their self-assembly into membranes and other hierarchical assemblages, such as a lamellar type phases and chiral ribbons, proceeds spontaneously in solution. Owing to the large size of the constituent molecules, individual molecules can be directly visualized and simultaneous observations at the continuum and molecular lengthscales are used to characterize the behavior of model membranes with unprecedented detail. Moreover, once assembled in solution, molecular interactions can be controlled in situ. In particular, the strength of chiral interactions can be varied, leading to fascinating transitions in behavior that resembles the formation of starfish vesicles. These observations point towards the important role of line tension, and have potential implications for phase separated lipid mixtures or lipid rafts.

[1]Author gratefully acknowledges support from the co-sponsored HHMI and NIBIB Quantitative Biology Program

4:18PM D40.00010 Dielectric sensors for measuring membrane potential[1] , KIMAL RAJAPAKSHE, ASANGA WIJESINGHE, JIE FANG, WILLIAM WIDGER, JOHN MILLER — Membrane potential in a biological cell depends on the ionic concentration difference between the extracellular and the intracellular medium. Ions close to the membrane show high polarizations under an electric field. Recent theoretical studies have related these polarizations to the alpha (α) dispersions in the impedance spectroscopy of a cell suspension. Therefore these dispersions can be used to measure the membrane potential of a single cell. Here we report the dielectric properties of phosphatidylcholine liposomes and its changes with the membrane potential. Liposomes have been prepared to have a higher concentration of potassium ions (K^+) inside the membrane compared to external medium. Under valinomycin (K^+ ionophores) these liposomes generate a negative membrane potential, as verified by fluorescent voltage sensitive dye measurements. Both dielectric and conductivity spectra display low frequency dispersions that are dependent on membrane potential. Possible future applications include noninvasive sensors for in vitro testing of new drugs and other applications.

[1]The authors acknowledge support by R21CA122153 from NHLBI & NCI, NIH, & from NSF, by the Welch Foundation (E-1221), and by TcSUH.

4:30PM D40.00011 Laser Transmission Spectroscopy and applications to liposome studies , FRANK LI, JAMES MARR, CHING-TING HWANG, ROBERT SCHAFER, ZACHARY SCHULTZ, STEVEN RUGGIERO, CAROL TANNER, University of Notre Dame — We describe the implementation of precision laser transmission spectroscopy (LTS) for sizing nanoparticles in suspension. Our apparatus incorporates a tunable laser and balanced optical system which measures light transmission over a wide (210 – 2300 nm) wavelength range with high precision and sensitivity. Spectral inversion was employed to determine both the particle size distribution and absolute density of particles with diameters over a total range of 5 to 3000 nm. LTS has a dynamic range of $\sim 10^3$ particles/mL to $\sim 10^{10}$ particles/mL ($5x10^{-8}$ vol.% to 0.5 vol.%). Currently, LTS is being applied as a tool to investigate the behavior of liposomes, dipalmitoylphosphatidycholine (DPPC) and dipalmitoylphosphatidylserine (DPPS), under the presence of fusing and de-aggregating agents. Our measurements indicate a maximum diameter of 400 nm for liposomes suspended in solution after fusion.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D41 DCP: LeRoy Apker Prize Session: Clusters and Nanoscale Systems A115/117

2:30PM D41.00001 LeRoy Apker Award Talk: Self-Assembly of DNA-Functionalized Nanoparticles , CHIA WEI HSU, Wesleyan University / Harvard University — Nanoparticles tethered with DNA strands can self-assemble into highly organized structures through the bonding of complementary nucleobases. These are promising building blocks for the bottom-up nanotechnology, and computational tools are useful to probe the behaviors of such complex materials. In this talk I will summarize my work on the phase behavior of nanoparticles tethered with a small number of DNA strands, and on the development of theories for the clustering and self-assembly kinetics of a specific case. Due to a separation of repulsion and attraction length scales, these nanoparticles exhibit an interesting hierarchy of phases made up of multiple interpenetrating structures.

3:06PM D41.00002 DNA-driven assembly of phospholipid bilayer nanodiscs , NIENKE GEERTS, Department of Chemical Engineering, Yale University, New Haven, CT 06511, PAUL A. BEALES, Centre for Molecular Nanoscience, School of Chemistry, University of Leeds, Leeds LS2 9JT, UK, T. KYLE VANDERLICK, Department of Chemical Engineering, Yale University, New Haven, CT 06511 — Phospholipid nanodiscs are a rare form of stable lipid self-assembly. The discs are formed by allowing lipids to self-assemble in the presence of membrane scaffold proteins (MSP). Each disc contains two MSP, wrapping around the edge of a leaflet of the bilayer. Although nanodiscs have become an important and versatile tool among model membrane systems to functionally reconstitute membrane proteins, they are yet to be utilized as building blocks in material science. However their highly monodisperse nanoscale structure make them ideal for this purpose. Here we report the first superstructures of nanodiscs self-assembled via membrane anchored single stranded DNA. The discs assemble into columnar stacks with high aspect ratio. The MSPs provide another powerful feature, as the His-tags of the protein can be used to attach the discs to colloids or other molecules of interest. This has strong potential for assembly of nanomaterials with greater degrees of complexity.

3:18PM D41.00003 Orthogonal DNA-colloid Clusters[1] , JESSE W. COLLINS, Harvard SEAS, VINOTHAN N. MANOHARAN, Harvard Physics and SEAS — We experimentally investigate the self-assembly of colloids labelled with different DNA strands into small clusters. We coat 1 micron diameter spheres with 65 base DNA strands having highly specific "sticky ends." Particles with different surface-bound DNA sequences represent different particle "types." We tune the short-ranged, pairwise interactions between some types to be attractive and interactions between other types to be purely repulsive; in this sense, the interactions are orthogonal. The magnitude of attraction (and repulsion) is constant across various types. We control the number and types of colloids at the single particle level, and distinguish the type of each particle from the types of their binding partners within each cluster. In an example experiment, 2 particles of each of 3 different types explore a volume less than 100 picoliters and assemble into equilibrium configurations. We characterize the structures with a microscope and compare observed averages with statistical mechanical predictions.

[1]We acknowledge support from NSF through MRSEC (DMR-0820484), NIRT (ECCS-0709323), and IGERT programs.

3:30PM D41.00004 Size Characterization of Surfactant and Polymer Coated Gold Nanorods[1] , CHRISTOPHER GRABOWSKI, PAUL LUCHETTE, PETER PALFFY-MUHORAY, Liquid Crystal Institute - KSU — Polarization-dependent dynamic light scattering was conducted on gold nanorods (Au NRs) coated with CTAB (hexadecyltrimethylammonium bromide) in water and coated with 50k MW PS (polystyrene) in toluene. The autocorrelation function of the scattered light intensity was determined for a series of scattering angles under VH and VV scattering geometries. The data were fit to a model of rotational and translational diffusivities. From this fit, we estimate the effective length (L) and diameter of the coated nanorods in solution. Au NRs coated with 50k PS show greatly reduced rotational diffusion compared to CTAB-coated NRs. Since the rotational diffusion coefficient scales as $1/L^3$, this implies significant extension of the grafted PS chains in toluene. We investigate this phenomenon for PS grafted onto Au nanoparticles and nanorods of varying aspect ratio to determine the impact of surface curvature on polymer layer thickness.

[1]This work was supported by the AFOSR under MURI grant FA9550-06-1-0337.

3:42PM D41.00005 A ligand phase transition on nanorods and its effect on their surface forces[1] , ASAPH WIDMER-COOPER, University of Sydney, PHILLIP GEISSLER, U.C. Berkeley — Synthesizing nanometer-scale objects with controlled optical and electronic properties is now a relatively straightforward task, however organizing such objects into extended structures that could revolutionize technology remains a challenge, especially for anisotropic particles. Nanorods behave like liquid crystals in solution and can assemble into structures with the rods oriented perpendicular with respect to a substrate upon drying, assemblies that could potentially be used to print nanostructured solar cells and photoelectrochemical devices. Achieving complete control of this process, however, requires detailed understanding of the rod-rod and rod-surface interactions. Like most nanoparticles, CdS nanorods are passivated with ligands to stabilize them from random aggregation in solution. Using molecular dynamics simulations with explicit ligands and solvent we investigate the structure of phosphonic acid ligands on CdS nanorods as a function of temperature and show that they can undergo an ordering transition close to room temperature. We calculate the potential of mean force between the rods and show that this changes the rod-rod interaction from purely repulsive to attractive. This should have a significant effect on their self-assembly behavior.

[1]This work was supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

3:54PM D41.00006 Chemical Preparation and Characterization of Elemental Cu, Ni, and Cu/Ni Core/Shell Nanoparticles , LAURA HIGGINS, MICHAEL LATTANZI, BRIAN KELLY, University of Delaware, GERALD POIRIER, Princeton University, KARL UNRUH, University of Delaware — Elemental Ni, Cu, and Cu core/Ni shell nanoparticles have been prepared in a polyol-type process. The elemental nanoparticles were prepared by dissolving $NiCl_2{\cdot}6H_2O$ and/or $CuCl_2{\cdot}2H_2O$ in ethylene glycol (EG) and heating the solution to reflux prior to the addition of NaOH. The resulting precipitate was then extracted, dried, and characterized by scanning electron microscopy (SEM) with elemental analysis, x-ray diffraction (XRD), and in the case of the elemental Ni nanoparticles, vibrating sample magnetometry (VSM) measurements. The best fit lattice parameters obtained from the elemental Ni and Cu nanoparticles were 0.35289(28) and 0.36171(23) nm, respectively, in good agreement with the corresponding bulk values. On the other hand, the measured saturation magnetization of about 49 emu/g was somewhat smaller than the bulk Ni value. In the case of the Cu/Ni nanoparticles, the best fit lattice parameters for the Ni and Cu components of the core/shell structure were 0.35299(26) and 0.36101(10) nm, indicating the formation of an essentially pure Ni shell and a slight amount of Ni incorporation in the Cu core.

4:06PM D41.00007 Solid-State Homogenization Reactions in Cu Core/Ni shell Nanoparticles , MICHAEL LATTANZI, LAURA HIGGINS, BRIAN KELLY, University of Delaware, GERALD POIRIER, Princeton University, KARL UNRUH, University of Delaware — Air stable Cu core/Ni shell nanoparticles have been prepared in a polyol-type process by heating an ethylene glycol (EG) solution containing $CuCl_2{\cdot}2H_2O$ and $NiCl_2{\cdot}6H_2O$ to its boiling temperature, adding an appropriate amount of NaOH, and allowing the reaction to proceed at reflux for 30 minutes prior to cooling. The as-prepared nanoparticles were characterized by scanning electron microscopy (SEM) with elemental mapping, x-ray diffraction (XRD), and vibrating sample magnetometry (VSM) measurements. Chemical composition maps of the particles revealed a well-defined core/shell structure consisting of a Cu core about 100-150 nm in diameter surrounded by a Ni shell about 30-40 nm in thickness. XRD measurements indicated that while the Cu core contained a small amount of incorporated Ni, the shell was essentially pure Ni. The solid-state transformation from the as-prepared core/shell structure to an essentially homogeneous Cu-Ni alloy was studied by high temperature VSM and XRD measurements as a function of annealing temperature and time. These measurements reveal that the core/shell structure remains largely intact to temperatures above 400 $^\circ$C and that complete homogenization occurs at temperatures above about 600 $^\circ$C.

4:18PM D41.00008 The Discovery of a New Class of Magnetic Superhalogens , P. JENA, M.M. WU, H. WANG, Y. KO, Q. WANG, Q. SUN, B. KIRAN, A. KANDALAM, K. BOWEN, VIRGINIA COMMONWEALTH UNIVERSITY TEAM, PEKING UNIVERSITY COLLABORATION, JOHNS HOPKINS UNIVERSITY COLLABORATION, MCNEESE STATE UNIVERSITY COLLABORATION — We report the discovery of a new class of magnetic superhalogens and their unusually stable molecular anions. These are formed when a hot plume of manganese atoms is cooled through collisions with an inert gas in the presence of chlorine atoms. The anions, with a composition of $(Mn_xCl_{2x+1})^-$ (x = 1, 2, 3. . .), appear as prominent (magic) peaks in mass spectra. Using calculations based on density functional theory and experiments utilizing anion photoelectron spectroscopy, we traced the origin of their unusual stability to the half-filled d-shell of the Mn atoms in anionic clusters and the large electron affinities of their neutral counterparts. The calculated and measured electron affinities are almost twice as high as that of the chlorine atom. However, unlike conventional superhalogens which are non-magnetic and consist of a single metal atom at the core surrounded by halogen atoms, the superhalogens discovered here are magnetic and have $(MnCl_2)_x$ moiety as a core to which a chlorine atom is attached. In addition, our calculations show that Mn atoms carry large magnetic moments and Mn_xCl_{2x+1} superhalogen moieties can serve as building blocks of a new category of salts with magnetic properties.

4:30PM D41.00009 Dielectron Attachment and Hydrogen Evolution Reaction in Water Clusters[1] , ROBERT BARNETT, Georgia Institute of Technology, RINA GINIGER, ORI CHESHNOVSKY, Tel-Aviv University, UZI LANDMAN, Georgia Institute of Technology — Binding of excess electrons to nano-size water droplets, with a focus on the hitherto largely unexplored properties of doubly-charged clusters, were investigated experimentally using mass spectrometry and theoretically with large-scale first-principles quantum simulations. Doubly-charged clusters were measured in the range of $83 \leq n \leq 123$, with $(H_2O)_n^{-2}$ clusters found for $83 \leq n < 105$, and mass-shifted peaks corresponding to $(H_2O)_{n-2}(OH^-)_2$ detected for $n \geq 105$. Simulations revealed surface and internal dielectron, e_2^-, localization modes and elucidated the mechanism of the reaction $(H_2O)_n^{-2} \rightarrow (H_2O)_{n-2}(OH^-)_2 + H_2$ (for $n \geq 105$), which was found to occur via concerted approach of a pair of protons belonging to two water molecules located in the first shell of the dielectron internal hydration cavity, culminating in hydrogen formation $2H^+ + e_2^- \rightarrow H_2$. Instability of the dielectron internal localization impedes the reaction for smaller ($n < 105$) clusters.

[1]Support: US Office of Basic Energy Sciences (RB, UL), Israel Science Foundation (RG,OC).

4:42PM D41.00010 Investigations into aggregate growth dynamics *via in situ* structural quantification of flame synthesized silica nanoparticle aggregates , DURGESH RAI, GREGORY BEAUCAGE, University of Cincinnati, JAN ILAVSKY, Argonne National Laboratory, HENDRIK KAMMLER, Clariant Corporation, SOTIRIS PRATSINIS, ETH Zurich — Ramified aggregates are formed in many dynamic processes such as in flames. The structures are disordered and present a challenge to quantification. The topological quantification of such nanostructured materials is important to understand their growth processes. Small-angle X-ray scattering (SAXS) is widely used to characterize such nanoparticle aggregates. Recently, we have developed a method for the quantification of topology in aggregated material using SAXS. This methodology will be used to describe topologies from *in-situ* SAXS studies on flame synthesized silica aggregates on millisecond time scales. This is an important step to facilitate understanding of the growth dynamics and the structural rearrangements that occur during flame synthesis.

4:54PM D41.00011 Influence of Nanoparticles on Fragility and Collective Particle Motion in Polymer Glass-Formation , JACK DOUGLAS, Polymers Division, NIST, FRANCIS STARR, Department of Physics, Wesleyan University — We investigate the impact of nanoparticles (NP) on glass-formation in polymer melts by molecular dynamics simulation. The NP cause significant changes in both fragility and the average length of string-like cooperative motion, where the extent of the effect depends on the NP-polymer interaction and NP concentration. These dynamical changes can be interpreted via the Adam-Gibbs (AG) theory if we assume the strings represent the abstract cooperatively rearranging regions (CRR) of the AG model, whose basic assumptions are reviewed. Molecular additives are also effective at altering the fragility of glass-formation and extent of string-like collective motion so the modulation of fragility and cooperative motion with additives seems to be a general effect. We find that the fragility of glass formation is mainly controlled mainly by the differential change of L with respect to T near the glass transition rather than the actual size L of the collective motion. We also find a near proportionality between m and the glass transition temperature in our nanocomposite system, which greatly simplifies the T dependence of structural. The classical entropy theory of glass-formation is considered as a complementary tool to gain analytic insights into these additive effects on polymer glass formation.

5:06PM D41.00012 Anion Photoelectron Spectroscopy and First-Principles Study of PbxIny Clusters[1] , S. VINCENT ONG, Virginia Commonwealth University, JOSHUA MELKO, UJJWAL GUPTA, The Pennsylvania State University, J. ULISES REVELES, Virginia Commonwealth University, JONATHAN D'EMIDIO, The Pennsylvania State University, SHIV KHANNA, Virginia Commonwealth University, A.W. CASTLEMAN, The Pennsylvania State University, DEPARTMENT OF PHYSICS, VIRGINIA COMMONWEALTH UNIVERSITY COLLABORATION, DEPARTMENTS OF CHEMISTRY AND PHYSICS, THE PENNSYLVANIA STATE UNIVERSITY COLLABORATION — Anionic and neutral Pb_xIn_y clusters containing up to 5 Pb and up to 7 In atoms have been investigated using negative ion photodetachment spectroscopy along with first-principles electronic structure studies within a gradient corrected density functional approach. The stability and electronic properties of these clusters have been characterized through studies of the detachment energies, gaps in the electronic spectrum, variations in binding energy, and nature of the electronic states. Particularly stable clusters have been grouped into two families of stable species. $PbIn_3^-$, Pb_2In_2, and Pb_3In_2 exhibit enhanced stability compared to their neighbors and the stability is linked to the aromatic character identified in their molecular orbitals. On the other hand, $PbIn_5^-$ and Pb_2In_4 exhibit enhanced stability associated with filled electronic shells within a confined nearly free electron gas.

[1]We acknowledge support from the U.S. Department of the Army through a MURI Grant W911NF-06-1-0280.

5:18PM D41.00013 Structural Analysis of Bonding in Au-Ge Clusters , DANIELLE MCDERMOTT, KATHIE NEWMAN, University of Notre Dame — The study of Gold-Germanium clusters is important in understanding systems such as gold catalyzed nanowire growth. Of particular concern is the bonding behavior between the two chemical elements, one tending to form metallic bonds, the other covalent. DFT calculations and Conjugate Gradient relaxations were performed on clusters ranging in size from 50 to 150 atoms using the SIESTA code to find the geometries of metastable states. Emphasis has been placed on developing accurate and dependable bases to be used to study nano-sized systems. The binding energy, coordination number, bond lengths and bond angles are studied as a function of the size and composition of Ge-Au clusters. We will discuss a nanoscale "phase diagram" for gold and germanium and will also discuss the topology of the bonding network.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D42 DFD: Colloids Theory & Computation, Emulsions, and Foams A302/303

2:30PM D42.00001 Liquid loss from foams with low water content , MICHAEL CONROY, JUSTIN TAYLOR, JOHN FARLEY, JAMES FLEMING, RAMAGOPAL ANANTH, Naval Research Laboratory — The liquid content of a foam can be significantly affected by liquid loss (drainage), a process that occurs both during and after the foam fills a space. We develop a theoretical model to describe liquid loss and evolution of average liquid volume fraction over time for advancing and static foams. We also perform bench-scale drainage experiments on foams with low water content. The theoretical model shows a constant drainage rate during the filling process which decays exponentially after a static column is formed. The measured loss of liquid is found to be in good agreement with the theoretical predictions. We find that drainage is greatly affected by the time scale for filling a space with foam. Significant effects on drainage are also found by varying bubble size, foam column height, and initial liquid content. The study indicates that drainage behavior can substantially deviate from that described by free-drainage theories, which assume that drainage initiates from a foam of static height.

2:42PM D42.00002 Molecular Dynamics Study of the Foam Stability of a Mixed Surfactant System with and without Calcium Ions , XIAOZHEN YANG, WENHONG YANG, Institute of Chemistry, CAS, INSTITUTE OF CHEMISTRY, CAS TEAM — Foam stability performance of a mixture surfactant system with and without calcium ions, including linear alkylbenzene sulfonate (LAS) and sodium dodecyl sulfate (SDS), has been studied by molecular dynamics. Microscopic interaction analysis reveals that the fraction of free calcium ions, X_f, in film system indicates the extent of the foam stabilities when X_f is in different calcium ion zones. In the system without ions, we found the variable of the surfactant tail mass out of water film, W, is indicator of foam stability. Performance of the mixture system predicted here was supported by experiments.

2:54PM D42.00003 Structural Properties of a Sheared Dense Emulsion[1] , S.K. DUTTA, E.D. KNOWLTON, D.L. BLAIR, Department of Physics, Georgetown University — The flow of a compressed emulsion above its yield point can be described by a velocity profile in addition to a rearrangement of individual droplets on top of this time averaged motion. Using a confocal microscope, we have tracked the droplets of an oil-in-water emulsion as they are sheared in a rheometer. When the applied stress is large, the velocity profile shows a nearly affine deformation, while there is strong strain localization close to yield. The crossover between these two behaviors occurs at higher shear rates as the volume fraction of the droplets is increased. At shorter length scales, rearrangement events are heterogeneously distributed, reflecting the disordered packing of the emulsion droplets. This characterization is a step towards linking bulk viscoelastic properties to local structural relaxation as the system leaves the jammed state.

[1]This work is funded by the NSF through Grant DMR 0847490.

3:06PM D42.00004 Janus and Gemini Nanoplates , ZHENGDONG CHENG, ANDRES MEJIA, YA-WEN CHANG, PENG HE, Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX 77840, AGUSTIN DIAZ, ABRAHAM CLEARFIELD, Department of Chemistry, Texas A&M University, College Station, TX 77842 — Janus particles were used to make stable Pickering emulsions (emulsions stabilized by particles). Here we demonstrated a novel method to produce high aspect ratio Janus plates with atomic thickness. Gemini plates with only the edges functionalized are also fabricated. These novel nanoplates are observed to have super surface activity. Most importantly, these particles overcome the two *opposite* effects in the stabilization of Pickering emulsions using spherical particles: stabilization requires particles as small as possible; but smaller particles are easy to escape the interface due to Brownian motion since the adsorption energy to the oil-water interface is proportional to the diameter of the spheres. Our nanoplates have a *large* aspect ratio due to the extremely thin thickness, which offers extraordinary stability to the liquid film between two emulsions to prevent coalescence. In the meantime, their large lateral surface area offers strong adsorption energy at the oil-water interface.

3:18PM D42.00005 Control over the number, size, and type of inner drops inside a double emulsion , LAURA ADAMS, YUANJIN ZHAO, ANDERSON SHUM, DAVID WEITZ, Harvard University — The formation of monodisperse double emulsions, drops inside of drops, has revealed a rich range of configurations not possible without the precise control of microfluidics. Yet-to-date, development of double emulsions with a controlled number of two different inner drops has not emerged. Here we demonstrate exquisite control over the number, size and type of inner drops encapsulated inside a double emulsion. These are fabricated using glass capillary devices implemented with a dual bore injection tube. We will show our latest results and discuss the scientific and technological opportunities made possible by these stable binary configurations.

3:30PM D42.00006 Yielding and Shear Induced Structure Formation in Emulsions with Attractive Interactions , ZHEN SHAO, AJAY NEGI, CHINEDUM OSUJI, Yale University, OSUJI LAB TEAM — The yielding behavior of colloidal suspensions is a strong function of inter-particle interactions. Recent results [Pham et al. 2006, 2008] indicate that attractive colloidal glasses display a two-step yielding due to inter-particle bond rupture followed by particle cage escape. From this perspective, we examine the yielding behavior of an oil-in-water emulsion system with attractive interactions using dynamic bulk rheology. In strain sweep experiments, after a limited linear regime, the system yields with a pronounced bump in the viscous modulus, a sharp decrease in the elastic modulus and a crossover between the two. The yielding response is marked by bond-breaking at low volume fractions and bond-breaking accompanied by cage escape above a critical concentration. An increase in the complex modulus is observed at yet higher strains (>100%), with both the elastic and viscous components showing small frequency dependent peaks. The onset, peak strains and peak stress display different dependences on volume fraction. We speculate that this display is due to the formation of shear induced structures at high strains and advance a simple model for this behavior.

3:42PM D42.00007 Force Network in a 2D Frictionless Emulsion Model System , KENNETH W. DESMOND, PEARL YOUNG, DANDAN CHEN, ERIC R. WEEKS, Emory University — We confine oil-in-water emulsion droplets between two parallel plates to create a quasi-two-dimensional model system to study the jamming transition. This model system is analogous to granular photoelastic disks with the exception that there is no static friction between our droplets. To study the jamming transition we compress the droplets in small increments and investigate how the force network evolves with increasing area fraction, where the forces are measured using a calibration technique we have developed. The forces in our system are spatial heterogeneous with a probability distribution that is similar to that found for photoelastic disks. We also find that the probability distribution of the forces narrows with area fraction, and that the correlation length of the largest forces is only few particle diameters.

3:54PM D42.00008 New activated dynamical regimes in dense suspensions of attractive uniaxial colloids , RUI ZHANG, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — Our microscopic theory of cooperative translational-rotational activated glassy dynamics of hard uniaxial particles [PRE,80,011502(2009); JCP,133,104902(2010)] is extended to treat short range attractions. For small aspect ratio dicolloids, a plastic glass (PG) state exists for weak attractions, but is destroyed beyond a critical attraction strength resulting in a new dynamic triple point (fluid, PG, gel), and two novel re-entrant behaviors: PG-fluid-gel, and repulsive glass(RG)-PG-gel. A new mixed "glass-gel" state also emerges characterized by center-of-mass and rotational angle localization parameters of intermediate magnitude. At high volume fractions, increasing attraction transforms the RG to an attractive glass (AG) characterized by a dynamic free energy surface with a gel-like localization state but a glass-like saddle point, and a non-monotonic variation of relaxation time and diffusion constant. AG dynamics is of a 2-step nature where physical bonds first break followed by hopping over a glass-like barrier. At high attractions a sharp crossover from a gel to AG with increasing volume fraction is predicted. As the particle aspect ratio grows, the PG state is destroyed, and translational motion becomes increasingly more important for escaping dynamical traps.

4:06PM D42.00009 A new analysis methodology for the motion of self-propelled particles and its application , YOUNG-MOO BYUN, PAUL LAMMERT, VINCENT CRESPI, Penn State University — The self-propelled particle (SPP) on the microscale in the solution is a growing field of study, which has a potential to be used for nanomedicine and nanorobots. However, little detailed quantitative analysis on the motion of the SPP has been performed so far because its self-propelled motion is strongly coupled to Brownian motion, which makes the extraction of intrinsic propulsion mechanisms problematic, leading to inconsistent conclusions. Here, we present a novel way to decompose the motion of the SPP into self-propelled and Brownian components; accurate values for self-propulsion speed and diffusion coefficients of the SPP are obtained for the first time. Then, we apply our analysis methodology to ostensible chemotaxis of SPP, and reveal the actual (non-chemotactic) mechanism of the phenomenon, demonstrating that our analysis methodology is a powerful and reliable tool.

4:18PM D42.00010 Diffraction effects on optical trapping of small particles , RACHAEL HARPER, ALEX LEVINE, University of California, Los Angeles — Geometric ray optics is an elegant and computationally efficient means of numerically calculating the forces on particles of arbitrary shape due to their interaction with a beam of light. This method is limited to the regime in which the particle is much larger than the wavelength of light. Ashkin's pioneering work [1] on force exerted by a laser trap on a spherical dielectric particle relies on this geometric optics limit. In current experiments, however, the size of the trapped particles can be comparable to the wavelength of the trapping radiation field. In this talk, we discuss the corrections to ray-tracing-based calculations of the laser trapping forces due to diffraction effects. Specifically, we compare the momentum transfer from a uniform beam of light to hollow dielectric cylindrical shells obtained from two different calculations using: (i) ray-tracing and (ii) the full physical optics formulation. By changing the radii of the inner and outer edges of the hollow cylinder with respect to the wavelength of light we determine the limits of validity of the ray-tracing solution. In the limit in which the radius of the inner cylinder is comparable to the wavelength radiation we show that the corrected momentum transfer is smaller than that predicted by geometric optics. We attribute this result to the reduction in the scattering force on the cylinder due to diffraction effects not accounted for in the geometric optics formalism. [1] A Ashkin, Biophys. J., 61, 569 (1992).

4:30PM D42.00011 Capillary Interactions among Spherical Particles at a Curved Liquid Interface , CHUAN ZENG, University of Massachusetts Amherst, FABIAN BRAU, Physique Theorique, Universite de Mons, BENNY DAVIDOVITCH, ANTHONY D. DINSMORE, University of Massachusetts Amherst — Colloidal particles tend to adsorb on liquid interfaces, where in- plane interactions can arise from a variety of mechanisms. We focus on capillary interactions induced by the curvature of the liquid interface, where particles were assumed to have a constant Young-Laplace contact angle at the three-phase contact line. Whereas spherical particles can adsorb on flat or spherical interfaces without deforming the interface, adsorption on a cylindrical interface deforms the interface because of the lack of azimuthal symmetry around the contact line. We present an analytical model of the interfacial shape and energy upon adsorption of a single particle as well as the interaction between two particles. Based on our result on a cylindrical interface, we propose a general formula for the force on a particle on a curved interface. This study provides an important step toward understanding the interactions among interfacial particles when the interface is distorted by an external field. We acknowledge support from the NSF-supported MRSEC on Polymers at UMass (DMR- 0820506) and NSF CBET-0967620.

4:42PM D42.00012 Slow relaxations of individual colloidal spheres following the breach of a fluid interface , MADHAV MANI, KITP & UCSB Physics, DAVID M. KAZ, RYAN MCGORTY, VINOTHAN N. MANOHARAN, Harvard University — Although the equilibrium state of a micron sized spherical particle at an interface is well understood, the dynamics associated with the approach to equilibrium is not. Recent high-resolution experiments from the Manoharan Lab (Ref: David M. Kaz's Talk) have shown that the dynamics are richer than expected. Subsequent to the initiation of a contact-line at a fluid interface the dynamics towards equilibrium are much slower than predicted by a hydrodynamic theory and the center of mass of the particle appears to follow a logarithmic law in time. We propose the importance of thermally agitated interactions between the contact-line and physical/chemical defects that pin the contact-line locally, thereby leading to an enhancement of the overall dissipation. We deduce that the interface must remain flat during this dynamic process and derive a force-velocity relation, which agrees with both the slow velocities and the logarithmic law. This surprisingly slow approach to equilibrium has significant consequences for processes where interactions between colloids and interfaces are present.

4:54PM D42.00013 Using Micron-Sized Ellipsoids as a New Tool for Microrheology , DAVID KILGORE, KENNETH W. DESMOND, ERIC R. WEEKS, Emory University — It is a well-established principle that the viscosity of a fluid can be calculated by observing the diffusion of microspheres, provided the diameter of the microspheres is known. We are developing a microrheology technique using ellipsoids, where the rheology can be measured without prior knowledge of the length and width of the ellipsoid. The advantage of using ellipsoids is that their asymmetry allows for the diffusion to be decomposed into two translational motions and one rotational motion. For each of these diffusive motions, we can measure a diffusion constant and relate the constant to the three unknowns: the length and width of the ellipsoid, and the viscosity. By measuring the three diffusion constants, we can determine the three unknowns. To verify this technique, we produce ellipsoids in the lab and suspend them in a viscous solution for three-dimensional imaging of the diffusion with a confocal microscope. We are able to get good agreement between the microrheological measurements and macroscopic viscosity measurements.

5:06PM D42.00014 Inferring elastic properties in colloidal solids: artifacts of a restricted observation window , ASAD HASAN, CRAIG MALONEY, Carnegie Mellon University — Recently, it has been shown how to extract information about the effective elasticity in colloidal solids, granular packings, *etc.*, using two point displacement correlations as obtained in, *e.g.*, optical microscopy experiments or computer simulations. At its core, this technique relies on the observation that, within the harmonic approximation, the Hamiltonian, H, is the inverse of the elastic response function, G, *defined over the whole domain of the elastic body*. However, most experiments (and even most simulations) have access to G only over some restricted sub-domain of the experimental system. Here, we study restricted observation domains of various size and dimensionality in face centered cubic (fcc) crystals of various size using a pseudo-analytic approach in which G is obtained analytically and is inverted numerically *on a compact sub-domain* to obtain the projected Hamiltonian, $\tilde{H}$. We show that the effective plane-wave energy, $E_k = \langle\psi_k|\tilde{H}|\psi_k\rangle$, for either a [111] or [100] planar subdomain has an unusual dispersion, $E \sim k$, rather than the familiar $E \sim k^2$ and motivate this observation from continuum considerations. We also show how this leads to an anomaly in the density of states of $\tilde{H}$.

5:18PM D42.00015 Enhancing tracer diffusivity by tuning interparticle interactions and solvation shell structure , JAMES CARMER, GAURAV GOEL, TOM TRUSKETT, University of Texas at Austin Chemical Engineering — Using computer simulations, we explore how tuning the tracer-solvent interactions affects the dynamics of a tracer particle. Optimizing the tracer particle contribution to excess entropy results in significant increases in tracer particle diffusivity. We also observe increases in dynamics while increasing the effective particle size. These changes are investigated at various densities and particle size ratios.

Monday, March 21, 2011 2:30PM - 5:30PM –
Session D45 DAMOP: Many Body Physics of Quantum Gases in Reduced Dimension A310

2:30PM D45.00001 Moving Impurities and Spin-Boson Systems in One-Dimensional BECs , THOMAS SCHMIDT, PETER ORTH, KARYN LE HUR, Yale University — We theoretically investigate the dynamics of two moving impurities immersed in a one-dimensional interacting Bose liquid. Interactions between the two impurities are mediated via excitations in the quantum liquid, and lead to correlations between them. For certain parameter regimes, the system can be mapped onto a spin-boson model, in which the relative momentum of the impurities plays the role of a spin-1/2 or spin-1. We will discuss the implications of the spin-impurity model onto observables of the liquid and impurities.

2:42PM D45.00002 Exact result for the three-body local correlator in the 1D Bose gas at finite temperature , MARTON KORMOS, ADILET IMAMBEKOV, Rice University — The 1D Bose gas with Dirac-delta interaction (Lieb–Liniger model) gives a very good description of cold atomic gases confined in quasi one-dimensional waveguides. While the model is integrable by means of the Bethe Ansatz it can also be regarded as a particular non-relativistic limit of an integrable relativistic quantum field theory, the sinh-Gordon model. This fact can be exploited to calculate form factors and correlation functions for the Bose gas. We derive an exact expression for the finite temperature expectation value of the third power of the density operator $:\rho^3:$, a quantity which is closely related to the three-body losses in cold atom experiments. We achieve this by summing up an infinite integral series obtained using the connection with the sinh-Gordon model. Our method can be generalized to other local correlators.

2:54PM D45.00003 The density profile of interacting Fermions in a one-dimensional optical trap[1] , SEBASTIAN EGGERT, Univ. of Kaiserslautern, Germany, STEFAN SOEFFING, Univ of Kaiserslautern, Germany — The density distribution of the Hubbard model in a one-dimensional external harmonic potential is investigated in order to study the effect of the confining trap. The broadening of the Fermion cloud with increasing interaction is analyzed in detailed, which can be described by a surprisingly simple scaling form. Strong superimposed "Friedel" oscillations are always present despite the absence of any hard wall boundaries. The wavelength of the dominant oscillation changes with interaction, which indicates the crossover to a spin-incoherent regime. We present an analytical formula, which describes the behavior of the oscillations very well for all interactions strengths and in return gives some insight for the use of bosonization in a trapping potential.

[1]Financial support has been received from the DFG funded TRANSREGIO 49, the research center OPTMAS, and the graduate school of excellence MAINZ/MATCOR

3:06PM D45.00004 Pairing correlations in one-dimensional Bose-Fermi mixtures with molecular boundstates , SHIMUL AKHANJEE, RIKEN - Condensed Matter Theory Laboratory, MASAHISA TSUCHIIZU, Nagoya University, AKIRA FURUSAKI, RIKEN - Condensed Matter Theory Laboratory — We study the ground-state properties of one-dimensional (1D) 3-component mixtures of Tonks bosons having infinite repulsion and nearly free fermionic atoms that can combine to form molecular fermions. Using a bosonization scheme, the form of the interaction is equivalent to the hopping term between weakly coupled spinless Tomonaga Luttinger liquids (TLL). Upon reduction of the energy scale, the 3-component TLL system scales down into a phase with coupled massive modes accompanied by pairing correlations.

3:18PM D45.00005 Scaling of noise correlations in one-dimensional lattice hard-core boson systems , KAI HE, MARCOS RIGOL, Department of Physics, Georgetown University — Noise correlations are studied for systems of hard-core bosons in one-dimensional lattices. We use an exact numerical approach based on the Bose-Fermi mapping and properties of Slater determinants. We focus on the scaling of the noise correlations with system size in superfluid and insulating phases, which are generated in the homogeneous lattice, with period-two superlattices, and with uniformly distributed random diagonal disorder. For the superfluid phases, the leading contribution is shown to exhibit a density independent scaling proportional to the system size, while the first subleading term exhibits a density dependent power-law exponent.

3:30PM D45.00006 Double occupancy as a probe of the Mott transition for fermions in one-dimensional optical lattices[1] , JORGE QUINTANILLA, SEPnet, University of Kent and Rutherford Appleton Laboratory, VIVALDO L. CAMPO, JR, UFScar, Brazil, VITO SCAROLA, Virginia Tech, USA, CHRIS HOOLEY, SUPA and University of St Andrews, UK, KLAUS CAPELLE, UFABC, Brazil — We study theoretically double occupancy D as a probe of the Mott transition for trapped fermions in one-dimensional optical lattices and compare our results to the three-dimensional case. The ground state is described using the Bethe Ansatz in a local density approximation and the behavior at finite temperatures is modelled using a high-temperature series expansion. In addition, we solve analytically the model in the limit in which the interaction energy is the dominant energy scale. We find that enhanced quantum fluctuations in one dimension lead to increased double occupancy in the ground state, even deep in the Mott insulator region of the phase diagram. Similarly, thermal fluctuations lead to high double occupancies at high temperatures. Nevertheless, D is found to be a good indicator of the Mott transition just as in three dimensions. We discuss possible experiments to verify these results and argue that the one-dimensional Hubbard model could be used as a benchmark for quantitative quantum analogue simulations.

[1]JQ acknowledges support from STFC and HEFCE

3:42PM D45.00007 ABSTRACT WITHDRAWN –

3:54PM D45.00008 Analysis of the single-particle excitation spectrum of ultracold fermions in 1D optical lattices , ATSUSHI YAMAMOTO, SUSUMU YAMADA, MASAHIKO MACHIDA, CCSE, Japan Atomic Energy Agency — We present single-particle excitation spectra of ultracold fermions in one-dimensional(1D) optical lattices by using dynamical density-matrix renormalization group (DDMRG) method. Our model is described by a Hubbard model with the harmonic trap potential. We find that the spectra show many kinds of intriguing structures owing to the harmonic trap potential and on-site interaction. In an analysis of weakly-interaction regimes, we find that the spectrum structure changes from a typical Hubbard band as obtained from periodical 1D lattice to band branching as increasing the trap potential, and finally, we observe clear discrete bound-state levels. On the other hand, in case of strongly-interacting regimes, we confirm the multiple flat bound-state levels lying above 1D Tomonaga-Luttinger (TL) liquid spectrum on a central Mott-plateau phase surrounded by metallic regions. Furthermore, we also investigate spectral changes as a metallic state partially emerges at the center region and find one-dimensional TL spectrum breakdown with an emergence of a new dispersive band due to the central metal portion. The observed features are closely related with the spectral changes when doping into Mott insulator. We will show the more details of spectra in 1D fermionic optical lattices by comparing non-trapped uniform 1D spectra.

4:06PM D45.00009 A quantum Monte Carlo study of the two-component mixture of hard-core bosons in one dimension , MIN-CHUL CHA, JONG-GEUN SHIN, INHO JEON, Hanyang University — The two-component mixture of hard-core bosons in one dimension is studied by quantum Monte Carlo simulations. A rich variety of phases exists in the parameter space of the inter-species interaction strengths, the ratio of the hopping amplitudes between two species, and the filling fractions. Physical properties of different phases are investigated by measuring the superfluid stiffness, the counter-flow stiffness, the compressibility, and the structure factor. We examine the nature of some phase transitions between a superfluid and an insulator and the 1st-order transition in the occurrence of phase separations.

4:18PM D45.00010 Fermionic Cold Atom Systems in Mixed Dimensions , KYLE IRWIN, SHAN-WEN TSAI, Dept. of Physics and Astronomy University of California, Riverside — Cold atom experiments can now realize mixtures of components that move in different dimensions [1]. We investigate such a system with two species of fermions. One species, f-fermions, moves on a two-dimensional square lattice. Another species, c-fermions, is constrained to move on a one-dimensional lattice embedded in the square lattice of f-fermions. We investigate the effective one-dimensional system who's interactions are mediated by the two-dimensional system, and explore effective theories, quantum phases, correlations, and relevant energy scales for various fillings of the mixed dimensional system using a functional renormalization group approach.

[1] G. Lamporesi, J. Catani, G. Barontini, Y. Nishida, M. Inguscio, and F. Minardi, Phys. Rev. Lett. 104, 153202 (2010)

4:30PM D45.00011 Long range bosonic correlations in 2D optical lattice traps , K.W. MAHMUD, University of California, Davis, E.N. DUCHON, Ohio State University, Y. KATO, Los Alamos National Laboratory, N. KAWASHIMA, University of Tokyo, R.T. SCALETTAR, University of California, Davis, N. TRIVEDI, Ohio State University — We use quantum Monte Carlo (QMC) simulations to study the combined effects of harmonic confinement and temperature for bosons in a two dimensional optical lattice. We present the scale invariant, finite temperature, state diagram for the Bose- Hubbard model in terms of experimental parameters - the particle number, confining potential and interaction strength. We examine the correlation decay of the superfluid trapped in annular rings, and find that the width of the superfluid ring determines a distance after which the correlation decays faster than in an equivalent 2D superfluid. At zero temperature, the correlation decay is intermediate between 1D and 2D decay, while at finite temperature, the decay is similar to a 1D decay at a much lower temperature. These provide the strongest evidence for the breakdown of the local density approximation (LDA) in trapped superfluid bosons.

4:42PM D45.00012 Interference signatures of thermal and quantum phase fluctuations in the two dimensional Bose-Hubbard Model[1] , MASON SWANSON, YEN LEE LOH, NANDINI TRIVEDI, The Ohio State University — Superfluidity in the Bose-Hubbard model is destroyed by the interplay of thermal and quantum phase fluctuations. In two dimensions, Berezinskii-Kosterlitz-Thouless theory predicts that deep in the superfluid phase quasi-long-range order is destroyed by the proliferation of thermally induced free vortices. As the Mott insulator regime is approached, the effect of quantum phase fluctuations must also be taken into account. By using a $(2+1)$-dimensional XY phase model, we investigate the signatures of thermal and quantum vortices in interference patterns. The possibility of extracting spatial and temporal correlation lengths from such interference images provides a new experimental probe for characterizing the state of ultracold atomic gases in 2D optical lattices.

[1]We acknowledge support from the NSF Graduate Research Fellowship Program and ARO/DARPA Grant No. W911NF-08-1-0338

4:54PM D45.00013 The Fluctuation-Dissipation Theorem at Low Temperatures in a 2D Optical Lattice[1] , ERIC DUCHON, Department of Physics, The Ohio State University, YASUYUKI KATO, Theoretical Division, Los Alamos National Laboratory, NAOKI KAWASHIMA, Institute for Solid State Physics, University of Tokyo, NANDINI TRIVEDI, Department of Physics, The Ohio State University — We calculate local density fluctuations and the local compressibility[2] of bosons in a two dimensional optical lattice as a function of temperature T and the tuning parameter U/t, the on-site boson repulsion strength in units of hopping, using worldline Quantum Monte Carlo. Our numerical results, coupled with the quantum fluctuation-dissipation theorem applied locally, make significantly different predictions for direct simulations of lattice bosons in a harmonic trap versus simulations that treat the trap within a local density approximation, especially at low temperatures. We discuss implications of our results for local thermometry, equilibration and characterization of the quantum critical regime.

[1]Work supported by NSF grant 06840 590000 60019607
[2]Q. Zhou, et al., *Phys. Rev. Lett.* **103**, 085701 (2009).

5:06PM D45.00014 The Effects of Disorder on a Quasi-2D System of Ultracold Atoms , MATTHEW BEELER, MATTHEW REED, TAO HONG, STEVEN ROLSTON, UMD/JQI — An ultra-cold gas of atoms can be used to create many different model Hamiltonians. When tightly confined in one spatial dimension, the gas can become effectively two-dimensional. At low temperature, a quasi-2D Bose gas undergoes a Berezinskii-Kosterlitz-Thouless phase transition to a superfluid, mediated by the binding and unbinding of vortex pairs. As disorder affects vortex transport properties, a slight amount of fine-grain disorder in the potential energy may alter the properties of this phase transition. We will present experimental observations of a 2D Bose gas of rubidium atoms in the presence of disorder created by a laser speckle field.

5:18PM D45.00015 Atomic Fermi superfluids in a honeycomb optical lattice: Supercurrents and dynamical instabilities , SHUNJI TSUCHIYA, Department of Physics, Tokyo University of Science, RAMACHANDRAN GANESH, ARUN PARAMEKANTI, Department of Physics, University of Toronto — Cold Fermi and Bose atoms on a honeycomb lattice have been of great recent interest given the possibility to simulate graphene physics and to realize interesting topological phases of matter.[1,2,3] We study the attractive Hubbard model of fermions on the honeycomb lattice in order to explore the strongly correlated superfluid state in this lattice geometry. We calculate the superfluid order parameter and collective modes in the presence of a superfluid flow in order to investigate the superflow stability. We find that the superfluid order parameter and density fluctuations exhibit nontrivial dependence on the flow, and these collective modes lead to novel dynamical instabilities.

[1]A. H. Castro Neto et al., Rev. Mod. Phys. 81, 109 (2009).
[2]C. L. Kane and E. J. Mele, Phys. Rev. Lett, 95, 226801 (2005).
[3]A. Kitaev, Ann. Phys. (N.Y.) 321, 2 (2006).

Monday, March 21, 2011 5:45PM - 6:45PM –

Session E1 APS: APS Prizes and Awards Ceremonial Session Ballroom C1

5:45PM E1.00001 Presentation of Prizes and Awards –

Monday, March 21, 2011 6:45PM - 7:45PM –

Session F1 Welcome Reception Hall A

6:45PM F1.00001 Welcome Reception –

Monday, March 21, 2011 7:45PM - 8:45PM –

Session G1 DCMP: Physics Community Outreach: Small Wonders: Bringing Nano to the Public Through Museum Partnership Ballroom C1

7:45PM G1.00001 Small Wonders: Public Adventures with Nanoscience[1] , VINCENT CRESPI, Penn State University — Hands-on activities in nanoscience can convey complex topics in rapid, accessible forms to audiences of all ages. We will show these entertaining demos in action, and discuss how their development has been facilitated by a partnership between the Penn State MRSEC and Philadelphia's science museum, The Franklin Institute.

[1]We aknowledge contributions from the Penn State MRSEC and The Franklin Institute

Tuesday, March 22, 2011 8:00AM - 11:00AM –

Session H1 DCMP: Spin-Triplet Supercurrents in Superconductor/Ferromagnet/Superconductor Josephson Junctions Ballroom A1

8:00AM H1.00001 Odd Triplet superconductivity in Superconductor-Ferromagnet hybrid structures

, SEBASTIAN BERGERET, Centro de Fisica de Materiales CSIC/UPV and DIPC, San Sebastian — Since the prediction of a long-range triplet component of the superconducting condensate in ferromagnetic-superconductor (S/F) proximity structures in 2001 [1], the activity in the field has increased considerably, both theoretically and experimentally The coexistence of conventional singlet superconductivity and ferromagnetism in S/F structures is closely related with the appearence of a triplet component of the condensate, which is odd in frequency and even in momentum and therefore insensitive to nonmagnetic impurities. The presence of the triplet component leads to new effects as for example, long-range Josephson coupling in SFS junctions [1], flow of a supercurrent through a half-metallic link [2] and screening of the magnetic moment of ferromagnetic particles embbeded in a superconductor [3]. In this talk I will review the main issues of the odd-triplet superconductivity, its manifestation in physical properties, and briefly discuss the relevant experiments in the field [4].

[1] F.S. Bergeret, A. F. Volkov and K. B. Efetov, Phys. Rev. Lett. 86, 4096 (2001); see also by the same authors Rev. Mod. Phys. 77, 1321 (2005).
[2] M. Eschrig and T. Löfwander, Nature Phys. 4, 138 (2008).
[3] F. S. Bergeret, A. F. Volkov and K. B. Efetov, Phys. Rev. B 69, 174504 (2004).
[4] R. S. Keizer et al, Nature 439, 825 (2006); T. S. Khaire et al., Phys. Rev. Lett. 104, 137002 (2010); J. W. A. Robinson, J. D. S. Witt and M. G. Blamire, Science 329, 59 (2010), Jian Wang et al, Nature Phys. 6, 389 (2010).

8:36AM H1.00002 Proximity effect-induced superconductivity in crystalline metallic and ferromagnetic nanowires[1]

, JIAN WANG, The Pennsylvania State University — In a single crystal gold nanowire of 1.2 microns contacted by superconducting contacts, the proximity effect induced superconductivity was found to appear in two distinct steps. The superconducting and normal regions are separated by a mini-gap state of low critical field. We suggest that a superposition of two distinct magnetic-flux states, which correspond to quantum flux 0 and 1 trapped in the nanowire, can explain the mini-gap state. Furthermore, we observed clear periodic differential magnetoresistance oscillations in the superconducting to normal transition region, which corresponds to the generation or annihilation of one vortex. In crystalline ferromagnetic Co and Ni nanowires, unexpected long-range proximity effect was observed. Josephson current associated with weakly damped singlet superconducting correlations or triplet correlations produced by the contact regions may lead to the observed long ranged proximity effect. In addition, a large and sharp resistance peak around the transition temperature was observed in the wires exhibiting incomplete superconductivity. Further theoretical model needs to be developed to reveal the physics behind the "peak effect."

[1]This work was supported by the Penn State MRSEC under NSF grant DMR-0820404.

9:12AM H1.00003 Observation of spin-triplet supercurrent in Co-based Josephson junctions[1]

, NORMAN BIRGE, Michigan State University — When a superconductor (S) and a ferromagnet (F) are put into contact with each other, the combined S/F system may exhibit altogether new properties. There is a proximity effect where pair correlations from S penetrate into F, but these correlations decay over a very short distance due to the large exchange splitting between the spin-up and spin-down electron bands in F. Theory predicts that, under certain conditions, electron pair correlations can be generated with spin-triplet rather than spin-singlet symmetry [1]. The two electrons in such a spin-triplet pair have parallel spins and are not subject to the exchange splitting in F; hence they propagate long distances. We have measured a long-range supercurrent in Josephson junctions of the form S/X/N/SAF/N/X/S, where S is a superconductor (Nb), N is a normal metal (Cu), SAF is a synthetic antiferromagnet of the form Co/Ru/Co, and X is a thin ferromagnetic layer necessary to induce spin-triplet correlations in the structure [2]. Spin-triplet correlations are generated due to non-collinearity of the magnetizations in each X layer and the nearest Co layer. Using X = PdNi, CuNi, and Ni, we observe enhancements of the critical current of up to 300 times relative to similar samples lacking the X layers. We also observe a large additional enhancement of the spin-triplet supercurrent after the samples are magnetized in a large field. This result is counter-intuitive, since one would expect magnetizing the samples to suppress the occurrence of non-collinear magnetization. We will present a model of the SAF magnetization structure that explains these intriguing results.

[1] F.S. Bergeret, A.F. Volkov, and K.B. Efetov, Phys. Rev. Lett., 86, 4096 (2001).
[2] T.S. Khaire, M.A. Khasawneh, W.P. Pratt, Jr., N.O. Birge, Phys. Rev. Lett. 104, 137002 (2010).

[1]Work supported by the U.S. Dept. of Energy under grant DE-FG02-06ER46341.

9:48AM H1.00004 Triplet supercurrents in ferromagnets[1]

, MARK BLAMIRE, University of Cambridge — In almost all superconductors the pairs of electrons which carry the charge are in the so-called singlet state in which the quantum spin of the two electrons is antiparallel. During the past five years there has been increasing evidence that proximity coupling between singlet superconductors and ferromagnets can sometimes generate triplet pairs within the ferromagnet in which the spins of the electrons are parallel rather than antiparallel – the evidence being that supercurrents can be passed through thicknesses of ferromagnetic material which are simply too large for singlet pairs to survive. The superconductor-ferromagnet proximity effect describes the fast decay of a spin-singlet supercurrent originating from the superconductor upon entering the neighboring ferromagnet. For strong ferromagnets such as Co, a thickness of only a few nanometres is sufficient to almost completely suppress the critical current of a Nb/Co/Nb Josephson junction. Here we report experiments in which a conical magnet (holmium) is placed at the interface between the superconductor and ferromagnet. The results showed that a long-ranged supercurrent can occur through the ferromagnetic Co layer but only for certain critical thicknesses of the Ho [1]. These thicknesses correspond to maximum magnetic inhomogeneity on the Ho and are therefore consistent with models which predict that a spin-mixing interface between the superconductor and ferromagnet can generate triplet pairs which are long-ranged in the ferromagnet. This paper reports recent experiments which aim to understand further the behaviour of triplet pairs in superconductor / ferromagnet heterostructures.

[1] J. W. A. Robinson, J. D. S. Witt, and M. G. Blamire, "Controlled Injection of Spin-Triplet Supercurrents into a Strong Ferromagnet" Science **329**, 59-61 (2010).

[1]Work supported by EPSRC: grant EP/F016611/1

10:24AM H1.00005 Long-ranged supercurrents through half-metallic ferromagnetic CrO_2[1]

, JAN AARTS, Leiden University — In the last few years, the scenery in the physics of superconductor/ ferromagnet hybrids has changed considerably with the realization that spin triplets may be induced in the ferromagnet through the mechanism of odd-frequency pairing. Since the equal-spin component of the triplet is not susceptible to pair breaking by the exchange field, such correlations can sustain supercurrents over long lengths, in particular in fully spin polarized materials where only one spin band is available. In halfmetallic ferromagnetic CrO_2 for instance, where superconducting contacts were deposited on top of the ferromagnetic films, we observed the current to flow over 700 nm at 4.2 K [1]. Still, we also have fabricated devices where the supercurrent is absent, which indicates that the mechanism of triplet generation is not yet well in hand. The presence of non-homogeneous magnetization is important, and here the grain structure of the film appears to play a key role, as can be illustrated with data for films grown on different substrates (TiO_2 and Al_2O_3). Moreover, recent data will be presented which suggest that triplet generation can be improved by using an additional ferromagnetic layer in the contact area.
[1] M. S. Anwar, F. Czeschka, M. Hesselberth, M. Porcu, and J. Aarts, Phys. Rev. B **82**, 100501(R) (2010).

[1]Work is supported by the Dutch Foundation F.O.M.

Tuesday, March 22, 2011 8:00AM - 11:00AM –

Session H2 DCMP: New Materials for Spin Quantum Hall Effect and Topological Insulators

Ballroom A2

8:00AM H2.00001 Bulk Topological Insulators and Superconductors: Discovery and the new Frontiers , M. ZAHID HASAN, Princeton University, Department of Physics — While most known phases of matter are characterized by broken symmetries, the discovery of quantum Hall effects (1980s) revealed that there exists an organizational principle based on topology rather than broken symmetry. In the past few years, theory and experiments have suggested that new types of topological states of matter exist in certain bulk insulators without any applied magnetic field. These topological insulators are characterized by a full band gap in their bulk and gap-less conducting edge or surface states protected by time-reversal symmetry. Unlike the quantum Hall systems, the bulk 3D topological insulators can be doped into superconductors and magnets revealing the interplay between topological-order and broken-symmetry-order [Rev. Mod. Phys 82, 3045 (2010)]. In this talk, I will highlight the experimental observations and focus on recent experimental developments on bulk topological insulators. I will then draw connections between the topological physics and their potential applications in electronics and the emergent new frontiers in fundamental physics. Work in collaboration with D. Hsieh, Y. Xia, L. Wray, D. Qian, C.L. Kane, H. Lin, A. Bansil, D. Grauer, R.J. Cava, Y.S. Hor, J. H. Dil, F. Meier, L. Patthey, J. Osterwalder, A.V. Fedorov.

8:36AM H2.00002 Tunable multifunctional topological insulators in ternary Heusler and related compounds , CLAUDIA FELSER, University of Mainz — Recently the quantum spin Hall effect was theoretically predicted and experimentally realized in quantum wells based on the binary semiconductor HgTe. The quantum spin Hall state and topological insulators are new states of quantum matter interesting for both fundamental condensed-matter physics and material science. Many Heusler compounds with C1b structure are ternary semiconductors that are structurally and electronically related to the binary semiconductors. The diversity of Heusler materials opens wide possibilities for tuning the bandgap and setting the desired band inversion by choosing compounds with appropriate hybridization strength (by the lattice parameter) and magnitude of spin–orbit coupling (by the atomic charge). Based on first-principle calculations we demonstrate that around 50 Heusler compounds show band inversion similar to that of HgTe. The topological state in these zero-gap semiconductors can be created by applying strain or by designing an appropriate quantumwell structure, similar to the case of HgTe. Many of these ternary zero-gap semiconductors (LnAuPb, LnPdBi, LnPtSb and LnPtBi) contain the rare-earth element Ln, which can realize additional properties ranging from superconductivity (for example LaPtBi) to magnetism (for example GdPtBi) and heavy fermion behaviour (for example YbPtBi). These properties can open new research directions in realizing the quantized anomalous Hall effect and topological superconductors. Heusler compounds are similar to a stuffed diamond, correspondingly, it should be possible to find the "high Z" equivalent of graphene in a graphite-like structure with 18 valence electrons and with inverted bands. Indeed the ternary compounds, such as LiAuSe and KHgSb with a honeycomb structure of their Au-Se and Hg-Sb layers feature band inversion very similar to HgTe which is a strong precondition for existence of the topological surface states. These materials have a gap at the Fermi energy and are therefore candidates for 3D-topological insulators. Additionally they are centro-symmetric, therefore, it is possible to determine the parity of their wave functions, and hence, their topological character. Surprisingly, the compound KHgSb with the strong SOC is topologically trivial, whereas LiAuSe is found to be a topological non-trivial insulator.

9:12AM H2.00003 Quantized Anomalous Hall Effect in Magnetic Topological Insulators , ZHONG FANG, Institute of Physics, Chinese Academy of Sciences — The anomalous Hall effect is a fundamental transport process in solids arising from the spin-orbit coupling. In a quantum anomalous Hall insulator, spontaneous magnetic moments and spin-orbit coupling combine to give rise to a topologically nontrivial electronic structure, leading to the quantized Hall effect without an external magnetic field. Based on first-principles calculations, we predict that the tetradymite semiconductors Bi_2Te_3, Bi_2Se_3, and Sb_2Te_3 form magnetically ordered insulators when doped with transition metal elements (Cr or Fe), in contrast to conventional dilute magnetic semiconductors where free carriers are necessary to mediate the magnetic coupling. In two-dimensional thin films, this magnetic order gives rise to a topological electronic structure characterized by a finite Chern number, with the Hall conductance quantized in units of e^2/h. References:

[1] R. Yu, W. Zhang, H.J. Zhang, S. C. Zhang, X. Dai, Z. Fang, "Anomalous Hall Effect in Magnetic Topological Insulators," Science 329, 61 (2010).
[2] Y. Zhang, K. He, C. Z. Chang, et.al., "Crossover of the 3D topological insulator Bi_2Se_3 to the 2D limit," Nature Physics 6, 584 (2010)

9:48AM H2.00004 Search for Topological Insulators in Ternary Chalcogenides[1] , CHAOXING LIU, Physikalisches Institut(EP3), Institut fuer Theoretische Physik und Astrophysik, Universitaet Wuerzburg — A topological insulator (TI) is a novel quantum state, which is a bulk insulator but has gapless surface states. Recently, binary chalcogenides, Bi2Te3, Bi2Se3 and Sb2Te3 have been theoretically predicted and experimentally observed to be a family of TIs [1]. In this talk, we extend our search of TIs to ternary chalcogenides by replacing some of Bi or Sb atoms by other atoms, such as thallium and rare earth atoms. It is found that for thallium-based materials [2], only TlSbS2 is trivial and all the others are TIs, while for rare earth-based materials[3], LaBiTe3 is a TI and the others are trivial. The search in ternary chalcogenides not only bring new members of TIs in the family of chalcogenides but also may provide candidates for other new topological states such as topological superconductor, quantum anomalous Hall insulator, axionic insulator and topological Kondo insulator.

Reference:
[1] Topological insulators in Bi2Se3, Bi2Te3 and Sb2Te3 with a single Dirac cone on the surface, Haijun Zhang, Chao-Xing Liu, Xiao-Liang Qi, Xi Dai, Zhong Fang and Shou-ChengZhang, Nature Physics 5, 438 - 442 (2009).
[2] Theoretical prediction of topological insulators in thallium-based III-V-VI2 ternary chalcogenides, Binghai Yan, Chao-Xing Liu, Hai-Jun Zhang, ChiYung Yam, Xiao-Liang Qi, Thomas Frauenheim and Shou-Cheng Zhang, Europhysics Letters, 90, 37002 (2010).
[3] Theoretical prediction of topological insulator in ternary rare earth chalcogenides, Binghai Yan, Hai-Jun Zhang, Chao-Xing Liu, Xiao-Liang Qi, Thomas Frauenheim, Shou-Cheng Zhang, Phys. Rev. B 82, 161108(R) (2010).

[1]Here I acknowledge the financial support by the Alexander von Humboldt Foundation of Germany.

10:24AM H2.00005 Magnetotransport studies of new topological insulators: Bi_2Te_2Se and others[1]

, ALEXEY TASKIN, Institute of Scientific and Industrial Research, Osaka University — A topological insulator (TI) is a material that has a gapped insulating bulk and a gapless metallic surface. However, presently available TI materials are not truly insulating, making surface transport measurements to be a challenge. The second generation of TIs, Bi_2Se_3 and related compounds, turned out to be more suitable for the experimental studies of the topological 2D states than the first discovered Bi-Sb alloys, due to a much larger bulk gap and a simpler surface state consisting of a single Dirac cone. Unfortunately, near-stoichiometric Bi_2Se_3 is always a metallic n-type material owing to a finite amount of Se vacancies. We searched for new TI materials that are better suited for achieving a bulk insulating state and found that Bi_2Te_2Se, which has an ordered tetradymite structure with the Te-Bi-Se-Bi-Te layer sequence, is a very promising material. It was found that high-quality single crystals of Bi_2Te_2Se show a high resistivity exceeding 1 Ωcm, together with a variable-range hopping behavior which is a hallmark of an insulator; yet, they present Shubnikov-de Haas oscillations which signify the 2D surface state consistent with the topological one observed by photoemission spectroscopy. Moreover, we are able to clarify both the bulk and surface transport channels, establishing a comprehensive understanding of the transport in this material. Our results demonstrate that Bi_2Te_2Se is the best material to date for studying the surface quantum transport in a topological insulator. Transport properties of other new TI materials are also presented.

[1]Work in collaboration with Yoichi Ando, Zhi Ren, Kouji Segawa, Satoshi Sasaki. Supported by JSPS (KAKENHI 19674002), MEXT (KAKENHI 22103004), and AFOSR (AOARD 10-4103).

Tuesday, March 22, 2011 8:00AM - 11:00AM –
Session H3 GMAG: Collective Effects in Molecular Magnets Ballroom A3

8:00AM H3.00001 Experimental realization of random-field Ising ferromagnetism in a molecular magnet[1]

, MYRIAM P. SARACHIK, Physics Department, City College of New York, CUNY, New York, New York 10031 — The longitudinal magnetic susceptibility of single crystals of the molecular magnet Mn_{12}-acetate obeys a Curie-Weiss law, indicating a transition to a ferromagnetic phase at $\sim$ 0.9 K [1,2]. With increasing magnetic field applied transverse to the easy axis, a marked change is observed in the temperature dependence of the susceptibility, with a considerably more rapid suppression of the Curie-Weiss temperature than predicted by mean-field theory for an ordered single crystal. Our results can instead be fit by a Hamiltonian for a random-field Ising ferromagnet in a transverse magnetic field, where the randomness derives from the intrinsic distribution of locally tilted magnetic easy axes known to exist in Mn_{12}-acetate crystals. Mn_{12}-ac and other single molecule magnets may thus serve as clean model systems for the study of random field ferromagnetism where the random fields are controllable and considerably larger than typical hyperfine fields. This discovery promises to enable widespread and convenient experimental study of magnetism in a random field in a broad class of new materials.

Work performed by and in collaboration with: Bo Wen, and Lin Bo, Physics Dept. City College of New York, CUNY (funded by NSF-DMR-0451605), P. Subedi and A. D. Kent, Physics Dept., NYU, (funded by NSF-DMR-0506946 and ARO-W911NF-08-1-0364) Y. Yeshurun, Physics Dept., Bar Ilan U, (funded by Deutsche Forschungsgemeinschaft), A. J. Millis, Physics Dept. Columbia U. (funded by DMR DMR-0705847), C. Lampropoulos and G. Christou, Chemistry Dept., U. of Florida (funded by NSF -CHE-0910472).

[1] B. Wen et al., Phys. Rev. B 82, 014406 (2010).
[2] Luis, et al., Phys. Rev. Lett. 95, 227202 (2005).

[1]Funding provided by NSF award DMR-0451605.

8:36AM H3.00002 Pure and Random–field quantum criticality in dipolar Ising magnets[1]

, ANDREW MILLIS, Columbia University — A theoretical model for Mn_{12} acetates and related materials is derived. Isomer effects present in some families of host acetate materials are argued to lead to a random field of a strength which may be tuned by a magnetic field applied in a direction perpendicular to the easy axis of the Mn_{12} unit. A mean field phase diagram is presented and consequences of beyond-mean-field physics are outlined. Measureable consequences in the experimentally accessible high temperature regime are presented and in this regime the importance of a complete treatment of the molecular level structure is emphasized. Open theoretical problems are described. Work reported in Phys. Rev. B 82, 014406 (2010) and Phys. Rev. B 82, 174405 (2010)). and performed in collaboration with: M. Sarachik, Bo Wen, and Lin Bo, Physics Dept. City College of New York, CUNY (funded by NSF-DMR-0451605), P. Subedi and A. D. Kent, Physics Dept., NYU, (funded by NSF-DMR-0506946 and ARO-W911NF-08-1-0364) Y. Yeshurun, Physics Dept., Bar Ilan U, (funded by Deutsche Forschungsgemeinschaft), C. Lampropoulos and G. Christou, Chemistry Dept., U. of Florida (funded by NSF -CHE-0910472).

[1] Phys. Rev. B 82, 014406 (2010).
[2] Phys. Rev. B 82, 174405 (2010)).

[1]Funding provided by NSF award DMR–0705847.

9:12AM H3.00003 Deflagration, fronts of tunneling, and dipolar ordering in molecular magnets

, DMITRY GARANIN, CUNY — Although there is no exchange interaction in crystals of molecular magnets characterized by a giant effective spin S (S =10 for Mn_{12}, and Fe_8), magnetic field $B^{(D)}$ generated by magnetic moments $g\mu_B S$ of magnetic molecules creates energy bias $W^{(D)}$=2$Sg\mu_B B^{(D)}$ on a molecule that largely exceeds the tunnelling splitting Δ of matching quantum states on different sides of the anisotropy barrier. Thus the dipolar field has a profound influence on the processes of tunnelling and relaxation in molecular magnets. Both theoretical and experimental works showed a slow non-exponential relaxation of the magnetization in both initially ordered and completely disordered states since most of the spins are off tunneling resonance at any time. Recently a new mode of relaxation via tunneling has been found, the so-called fronts of tunneling, in which (within a 1d theoretical model) dipolar field adjusts so that spins are on resonance within the broad front core. In this "laminar" regime fronts of tunnelling are moving fast at speeds that can exceed that of the temperature-driven magnetic deflagration, if a sufficiently strong transverse field is applied. However, a "non-laminar" regime has also been found in which instability causes spins to go off resonance and the front speed drops. In a combination with magnetic deflagration, the laminar regime becomes more stable and exists in the whole dipolar window 0$\leq W \leq W^{(D)}$ on the external bias W, where the deflagration speed strongly increases. Another dipolar effect in molecular magnets is dipolar ordering below 1 K that has recently been shown to be non-uniform because of formation of magnetic domains. An object of current research is possible non-uniformity of magnetic deflagration and tunneling fronts via domain instability that could influence their speed.

9:48AM H3.00004 Experiments on Magnetic Deflagration , JAVIER TEJADA, University Barcelona — Magnetic deflagration was first observed in molecular magnets [1,2] and then in glassy magnetic materials like manganites [3,4] and intermetallic systems like Gd_5Ge_4 [5]. The role of the chemical energy is played by the magnetic energy of the material. In the case of a molecular magnet, this is Zeeman energy, while in manganites and Gd_5Ge_4 the free energy is a combination of the Zeeman energy and the energy of the metastable magnetic phase. In molecular magnets both the ignition process and the speed of the flame are assisted by quantum spin reversal [2]. There also exists some evidence of the transition from deflagration to detonation [6]. Various experimental techniques have been used to detect the speed of the magnetic flame. They include SQUID magnetometry, Hall bars and coils. Magnetic deflagration has been ignited by local heating, application of external fields, by surface acoustic waves and microwaves. High frequency EPR measurements of the population of spin levels permitted observation of magnetic deflagration in real time. The talk will review these experiments and their interpretation.

[1] Y. Suzuki et al. Phys. Rev. Lett. 95, 147201 (2005).
[2] A. Hernandez-Minguez et al. Phys. Rev. Lett. 95, 217205 (2005).
[3] F. Macia et al. Phys. Rev. B79, 092403 (2009).
[4] F. Macia et al. Phys. Rev. B76, 174424 (2007).
[5] S. Velez et al. Phys. Revc. B81, o64437 (2010).
[6] W. Decelle et al. Phys. Rev. let. 102, 027203 (2009)

10:24AM H3.00005 Electronic Structure and Transport Through Single Molecule Magnets[1] , KYUNGWHA PARK, Dept. of Physics, Virginia Tech — Over the past decade, single-molecule magnets have drawn considerable attention due to observed magnetic quantum tunneling and interference and a possibility of using them for information storage or devices. There have been so far significant experimental efforts to build and characterize monolayers of single-molecule magnets on various surfaces or single-molecule magnets connected to electrodes. There is need to understand changes of electronic and magnetic properties of single-molecule magnets in those environments using quantum mechanical simulations. We simulate, within density-functional theory, a nanostructure in which prototype single-molecule magnets Mn12 are adsorbed onto a gold surface. We investigate coupling between the Mn12 and the surface and discuss electronic structure and magnetic anisotropy of the Mn12 on a gold surface in comparison to an isolated Mn12. In addition, we present electron transport properties through a Mn12 bridged between gold electrodes, using the nonequilibrium Green's function method in conjunction with density-functional theory. We discuss a possibility of using a Mn12 molecule as a spin filter and an effect of interface geometry and bonding type on transport across a Mn12.

[1]Supported by NSF DMR.

Tuesday, March 22, 2011 8:00AM - 11:00AM –
Session H4 DPOLY: Polymer Physics Prize Ballroom A4

8:00AM H4.00001 Polymer Physics Prize Talk: Polymer Brushes: Why do we still care?[1] , GARY S. GREST, Sandia National Laboratories — Polymer molecules have been widely used to modify the properties of surfaces including its adhesion. Among the most studied have been polymer brushes, in which polymer chains are grafted at one end to a surface and immersed in a small molecule solvents. Experiments and simulations have shown that the conformation of the chains grafted onto a flat surface depends on the grafting density and the interaction of the polymer with the solvent. As the molecular weight of the solvent increases, the structure of the brush changes. Consequently the brush chains are expelled from the solvent due to entropic loss that originate from the fact that the melt chains penetrating the brush cannot overcome the translational, or mixing, entropy. This crossover from wetted to non-wetted brushes, has important implications for polymer adhesion, where the phase separation of melt and brush chains reduces entanglements at the interface. As polymers are grafted to nanoparticles, the curvature of the surface offers the polymer brush chains a significantly larger space to explore compared to a flat surface, reducing the tendency for autophobic dewetting. Using large scale molecular dynamics simulations we have studied the interface between brush coated nanoparticles and a polymer melt. Effects of chain length of the brush, and that of the polymer melt, the coverage of the nanoparticle and its curvature on the brush/melt interface will be discussed. The role of individual entanglements, between the brush chains and the melt, as identified by primitive path analysis will be introduced. These simulations provide insight into the structure of the brush/polymer interface which is not accessible through other theoretical or experimental means.

[1]Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract No. DE-AC04-94AL85000.

8:36AM H4.00002 Polymer Physics Prize Talk: Topological Constraints Matter – or Back to the Origin[1] , KURT KREMER, Max Planck Institute for Polymer Research, Mainz, Germany — Topological constraints, being permanent or temporal, influence many properties of soft matter, especially polymers. While at a first glance the simple Rouse models describes the motion of short chains surprisingly well, the fact that chains cannot cut through each other dominates the dynamics of long chain melts, ring polymers and the relaxation in networks and gels. Furthermore new phenomena in special melts and mixtures even make this more obvious. The talk will review some developments and will also address new problems linked to material science as well as biology. To illustrate the importance of topological constraints, numerical simulations for a melt on non concatenated ring polymers with and without linear contaminants will be presented. While the static properties of long rings can be rationalized by the concept of a crumpled globule, dynamic properties are much less understood. Our simulations clearly show that diffusion and stress relaxation in such a system of globules decouple. In addition the first results for non concatenated rings added to a melt of linear polymers and for a few linear polymers added to a melt of rings will be discussed.

[1]The work over the years benefited from intense and fruitful collaborations with many colleagues. For the topics discussed above I especially want to thank K. Binder, G. S. Grest. B. Duenweg, R. Everaers, M. Pütz, A. Yu Grosberg and J. Halverson.

9:12AM H4.00003 Bottle-brush polymers versus worm-like chains: Do we understand the stiffness of macromolecules? , KURT BINDER, Johannes Gutenberg Universitaet Mainz — Bottle-brush polymers contain a long flexible macromolecule as a backbone to which flexible side-chains are grafted. Through the choice of the grafting density of the length of the side chains to the local stiffness of this cylindrical molecular brush can be controlled. However, understanding mesoscopic length scales (cross-sectional radius, persistence length, contour length) of these semiflexible cylindrical brushes poses a challenging problem. While self-avoiding walks of variable stiffness show a crossover to the Kratky-Porod worm-like chain model, and hence a (pre-asymptotic) regime of Gaussian behavior, bottle-brushes under good solvent conditions are not compatible with this model. Consequences for the description of chain stiffness in terms of the concept of the persistence length are discussed, as welll as pertinent experiments.

9:48AM H4.00004 Entanglements and the Mechanical Properties of Glassy Polymers[1] , MARK ROBBINS, Johns Hopkins University — The response of glassy polymers to shear or tensile strain is strongly influenced by the entanglement network that is inherited from the melt. Molecular dynamics simulations are used to probe the microscopic origins of stress-strain curves and their connection to entanglements. The latter are identified in real space by examining topological constraints along the primitive path. The first part of the talk will consider the process of craze formation, where the entanglement density is correlated to the volume increase during crazing. Simulations show that entanglements are preserved during crazing, but the craze density does not correspond to pulling chains taut between entanglements. The second part of the talk will examine the effect of entanglements on strain hardening under uniaxial strain. The stress is directly associated with the degree of orientational order along the strain axis, and nearly independent of order along perpendicular directions [1]. Studies with mixtures of short and long chains show that the degree of order is independent of the surrounding chains [2]. The final part of the talk will examine the strength of welds formed by diffusion across polymer interfaces. The shear stress follows the bulk response until chains are pulled taut on the scale of the length of segments that have diffused across the interface. When this length is several times the entanglement length, the maximum shear stress saturates at the bulk value and chains fail through scission. Similar trends are found for the fracture energy in tensile loading.

[1] T. Ge and M. O. Robbins, J. Polymer Sci. B: Polymer Physics **48**, 1473-1482 (2010).
[2] R. S. Hoy and M. O. Robbins, J. Chem. Phys. **131**, 244901 (2009)

[1]This material is based upon work supported by NSF Grant DMR 108474.

10:24AM H4.00005 Conjugated Polymer Nanoparticle Hybrids: Structure, Dynamics and Forces[1] , DVORA PERAHIA, Clemson University — While nanoparticles (NPs) have unique tunable elctro-optical properties and exceptional mechanical strength, it remains a challenge to integrate them into devices while retaining the advantages of the nanoscale. Tethering polymeric materials to the NPs surfaces has the potential to stabilize single NPs and direct their assembly. The polymers may serve in several capacities from a simple tether to a matrix to directed assembly tool taking advantage of the inherent structure of the polymers and as an active component in a complex material. However confining a large molecule to a highly curved surface affects the inherent configuration of the polymer. These effects are of particular interests in conjugated polymer-nanoparticle hybrids, where the conformation of the polymers affects not only the assembly of the nanoparticles but also the optical and electronic communication between the NPs. Using molecular dynamic simulations we have studied the structure of a single hybrid of *para* dialkyl phenylene ethynelyne (PPE) grafted nanoparticles. PPEs are polymers whose conformation determines their degree of conjugation and therefore their electro-optical response. Using simulations coupled with neutron scattering studies we have shown that PPE is a rigid polymer that is fully extended in dilute solutions in good and theta solvents but can be forced into a collapsed configuration in a poor a solvent. When confined to a nanoparticle surface, the PPE chains are fully extended but cluster as the solvent quality is reduced. Results for the conformation of grafted PPE molecules on a single nanoparticle and the forces between two nanoparticles as a function of chain length and solvent quality will be presented. These simulations provide insight to the interactions that result in formation of tunable hybrids.

[1]This work has been done in collaboration with Gary S. Grest.

Tuesday, March 22, 2011 8:00AM - 11:00AM –

Session H5 FIAP GERA DNP: Drowning in Carbon: The Imperative of Nuclear Power Ballroom C1

8:00AM H5.00001 A Strategy for Expanded Nuclear Power: The Role of the U.S. Department of Energy , VICTOR REIS, U.S. Department of Energy — This abstract not available.

8:36AM H5.00002 What happened to the US nuclear renaissance? , ROBERT ROSNER , The University of Chicago — While nuclear power generation is seeing a distinct revival internationally, especially in Asia, a corresponding revival within the United States has not yet occurred. I will discuss the various reasons for this difference, as well as the consequences - some distinctly unintended - for the future U.S. role in the spread of nuclear power generation as well as in non-proliferation internationally.

9:12AM H5.00003 Used Nuclear Fuel: From Liability to Benefit , RAYMOND L. ORBACH, The University of Texas at Austin — Nuclear power has proven safe and reliable, with operating efficiencies in the U.S. exceeding 90%. It provides a carbon-free source of electricity (with about a 10% penalty arising from CO_2 released from construction and the fuel cycle). However, used fuel from nuclear reactors is highly toxic and presents a challenge for permanent disposal – both from technical and policy perspectives. The half-life of the "bad actors" is relatively short (of the order of decades) while the very long lived isotopes are relatively benign. At present, spent fuel is stored on-site in cooling ponds. Once the used fuel pools are full, the fuel is moved to dry cask storage on-site. Though the local storage is capable of handling used fuel safely and securely for many decades, the law requires DOE to assume responsibility for the used fuel and remove it from reactor sites. The nuclear industry pays a tithe to support sequestration of used fuel (but not research). However, there is currently no national policy in place to deal with the permanent disposal of nuclear fuel. This administration is opposed to underground storage at Yucca Mountain. There is no national policy for interim storage—removal of spent fuel from reactor sites and storage at a central location. And there is no national policy for liberating the energy contained in used fuel through recycling (separating out the fissionable components for subsequent use as nuclear fuel). A "Blue Ribbon Commission" has been formed to consider alternatives, but will not report until 2012. This paper will examine alternatives for used fuel disposition, their drawbacks (e.g. proliferation issues arising from recycling), and their benefits. For recycle options to emerge as a viable technology, research is required to develop cost effective methods for treating used nuclear fuel, with attention to policy as well as technical issues.

9:48AM H5.00004 Fuel Cycle R&D Requirements for Future Nuclear Power , LEE SCHROEDER, Lawrence Berkeley National Lab and TechSource — Recently, DOE Nuclear Energy completed its Road Map for a science-based approach to future nuclear energy development. Fuel cycle R&D is a central element of the Road Map, which covers nuclear energy through the period 2040-2050 and perhaps beyond. Examples of fuel cycle R&D activities will be presented, along with an outline of the types of research facilities needed to support this effort. Experimental facilities within several areas of the DOE, including DOE's Office of Nuclear Energy and its Office of Science, will be required for this task. In addition, advanced modeling and simulation will play a growing major role in these activities.

10:24AM H5.00005 Roundtable Discussion and Q&A –

Tuesday, March 22, 2011 8:00AM - 11:00AM –

Session H6 DAMOP: Ultracold Molecules and Quantum Many Body Physics Ballroom C2

8:00AM H6.00001 Control of dipolar collisions of polar molecules in the quantum regime[1] , AMODSEN CHOTIA, JILA, University of Colorado, Boulder and National Institute of Standards and Technology — Ultracold polar molecular quantum gases promise to open new research directions ranging from the study of ultra-cold chemistry, precision measurements to novel quantum phase transitions. Based on the preparation of high-phase space density gases of polar KRb molecules, I will discuss the control of dipolar collisions and chemical reactions of polar molecules in a regime where quantum statistics, single scattering partial waves, and quantum threshold laws play a dominant role. In particular, I will discuss the crucial role of electric dipole-dipole interactions and external confinement in determining the chemical reaction rate. Finally, I will discuss prospects of reaching quantum degeneracy in bi-alkali samples of polar molecules and prospects for these systems as novel dipolar quantum many-body systems.

[1] Experimental work done in collaboration with Silke Opselkaus, M. H. G. de Miranda, B. Neyenhuis, K.-K. Ni, D. Wang, D. S. Jin, and J. Ye

8:36AM H6.00002 Ultracold high-density samples of rovibronic ground-state molecules in an optical lattice , JOHANN GEORG DANZL, Institute of Experimental Physics, University of Innsbruck — Ultracold molecules controlled at the level of single quantum states with respect to all internal and external degrees of freedom will enable a series of fundamental studies in physics and chemistry, ranging from novel quantum gas experiments and cold controlled chemistry to quantum information and quantum simulation. Ultracold molecules trapped in an optical lattice at high density and prepared in their lowest internal quantum state are an ideal starting point for these studies. We create ultracold and dense samples of molecules in a single hyperfine sublevel of the rovibronic ground state while each molecule is individually trapped in the motional ground state of an optical lattice well [1,2]. Starting from an atomic Mott-insulator state with optimized double-site occupancy, weakly bound Cs dimer molecules are efficiently formed on a Feshbach resonance and subsequently transferred to the rovibronic ground state by a stimulated 4-photon process with the Stimulated Raman Adiabatic Passage (STIRAP) technique. The molecules are trapped in the lattice with a lifetime of 8 s. We aim at producing Bose-Einstein condensates of ground-state molecules by adiabatically removing the lattice. Our results, when suitably generalized to heteronuclear molecules, present an important step towards the realization of dipolar quantum-gas phases in optical lattices. I will report on recent progress in Innsbruck on the formation of RbCs ground state molecules.

[1] Science **321**, 1062 (2008)
[2] Nature Physics **6**, 265 (2010)

9:12AM H6.00003 Theory of ultracold heteronuclear polar molecules , JOHN BOHN, Univ of Colorado - Boulder — This abstract not available.

9:48AM H6.00004 Laser Cooling of a Diatomic Molecule , EDWARD SHUMAN, Yale University — Laser cooling techniques to produce ultracold (T<1μK) atoms have lead to rapid advances in a wide array of fields. However, extending laser cooling to molecules has remained elusive. The primary problem is that laser cooling requires a large number (>104) of photon absorption/emission cycles. Molecules, however, have vibrational and rotational degrees of freedom, which typically lead to high branching probabilities into a large number of unwanted sublevels. Here we report on experiments demonstrating the laser cooling of a diatomic molecule which have overcome this problem. We use the molecule strontium monofluoride (SrF) where only three lasers and a magnetic field are necessary to scatter >105 photons. We have demonstrated 1-D transverse cooling of a beam of SrF, dominated by Doppler or Sisyphus-type cooling forces depending on experimental parameters. We observe a reduction in the velocity distribution by a factor of 3 or more, corresponding to final 1-D temperature T $<$ 1 mK. This transverse cooling may be useful for a variety of experiments; in addition, our results open a path to trapping and 3D cooling of SrF to the ultracold regime.

10:24AM H6.00005 Meta-stable 1-D gases of polar molecules with attractive dipole forces[1] , ROBIN CÔTÉ, University of Connecticut — The recent achievements in the formation and manipulation of ultracold polar molecules have opened the gate to exciting new studies in several fields of physical sciences. Polar molecules could find uses in quantum information science and in precision measurements, while dense samples could provide a fertile ground for novel quantum gases because of their long-range and anisotropic interactions. Until now, stable dipolar gases were thought to require a repulsive dipole-dipole interaction, such as provided by parallel dipoles aligned perpendicularly to a two-dimensional (2-D) trap. However, to observe interesting new correlations and condensed matter phases, attractive interactions are needed. Here, we explore how meta-stable one-dimensional (1-D) samples of ultracold polar molecules could be created with attractive long-range dipole-dipole interaction. We show that a repulsive barrier due to a strong quadrupole interaction can stabilize a gas of ultracold KRb molecules and even lead to long-range wells supporting bound states. The properties of these wells can be controlled by external electric fields, allowing the formation of long chains of KRb polymers, and the further study of Luttinger liquid transition. We also discuss the general molecular properties necessary for the existence of a repulsive barrier.

[1]Partially supported by AFOSR

Tuesday, March 22, 2011 8:00AM - 11:00AM –
Session H7 DBP DPOLY: Physics of Proteins II: Dynamics and Functions Ballroom C3

8:00AM H7.00001 Energy Landscapes Encoding Function in Enzymes Investigated Over Broad Time Scales[1] , ROBERT CALLENDER, Albert Einstein College of Medicine — The operating hypothesis of much of our current work is that atomic motion, over broad time scales (femtoseconds to milliseconds, the latter being the time scale of most enzyme catalyzed reactions), contributes to enzymic catalysis in proteins. It is clear from our work that specific types of motions are important in binding of ligands to proteins and transition state formation in enzymatic catalysis. Since new experimental and theoretical approaches are needed to understand the dynamical nature of proteins broadly and enzymatic catalysis specifically, we have employed time-resolved "pump-probe" spectroscopic techniques because of the sensitivity of these type of approaches to all relevant time scales. And we have also developed and applied new theoretical methods. The talk will focus on how lactate dehydrogenase brings about catalysis based on current experimental and theoretical studies.

[1]Work supported by NIH Grant P01GM068036.

8:36AM H7.00002 NMR investigations of molecular dynamics , ARTHUR PALMER, Columbia University — NMR spectroscopy is a powerful experimental approach for characterizing protein conformational dynamics on multiple time scales. The insights obtained from NMR studies are complemented and by molecular dynamics (MD) simulations, which provide full atomistic details of protein dynamics. Homologous mesophilic (*E. coli*) and thermophilic (*T. thermophilus*) ribonuclease H (RNase H) enzymes serve to illustrate how changes in protein sequence and structure that affect conformational dynamic processes can be monitored and characterized by joint analysis of NMR spectroscopy and MD simulations. A Gly residue inserted within a putative hinge between helices B and C is conserved among thermophilic RNases H, but absent in mesophilic RNases H. Experimental spin relaxation measurements show that the dynamic properties of *T. thermophilus* RNase H are recapitulated in *E. coli* RNase H by insertion of a Gly residue between helices B and C. Additional specific intramolecular interactions that modulate backbone and sidechain dynamical properties of the Gly-rich loop and of the conserved Trp residue flanking the Gly insertion site have been identified using MD simulations and subsequently confirmed by NMR spin relaxation measurements. These results emphasize the importance of hydrogen bonds and local steric interactions in restricting conformational fluctuations, and the absence of such interactions in allowing conformational adaptation to substrate binding.

9:12AM H7.00003 Kinetic vs. Thermodynamic Control of Bacteriorhodopsin Pumping[1] , MARILYN GUNNER, City College of New York — Bacteriorhodopsin is a transmembrane proton pump that converts light energy to a transmembrane electrochemical gradient. Retinal, bound in the center of the protein, absorbs light and isomerizes from the all-trans to 13-cis configuration. A series of conformational changes and proton transfers then restores the structure to the all-trans ground state while pumping one proton from the high pH cell interior to the low pH exterior, saving energy in an electrochemical gradient. Poorly understood gating elements control key steps where incorrect proton transfer would return the protein to the ground state without pumping. The gate's barrier height determines how much the pump leaks. Analysis of high-resolution structures trapped in different intermediates has produced ideas for how bacteriorhodopsin ensures pumping. There are two contrasting strategies, one primarily thermodynamic and the other relying on kinetic control to ensure that protons are moved uphill. With thermodynamic control, residue protonation states always remain in quasi-equilibrium. Relatively slow conformational changes shift the energy landscape modifying site pKas. Residues then change ionization remaining in equilibrium in each metastable intermediate. The sequence of intermediates imparts the directionality to the transfers. Alternatively, the direction of transfer is determined by the accessibility of low energy pathways so is thus is under kinetic control. We will discuss which steps in the bacteriorhodopsin photocycle are under thermodynamic or under kinetic control. The role of three specific conformational changes (retinal isomerization, Arg82 reorientation and Glu194 and 204 separations) on the degree of proton transfer will be described. Supported by NFS MCB 1022208.

[1]Carried out with Yifan Song now at the University of Washington Department of Biochemistry

9:48AM H7.00004 Beller Lectureship Talk: Ultrafast Excitation Energy Transfer and the Mechanism of Non-Photochemical Quenching in Plant Photosynthesis , RIENK VAN GRONDELLE, VU University Amsterdam — The success of photosynthesis relies on two ultrafast processes: excitation energy transfer in the light-harvesting antenna followed by charge separation in the reaction center. LHCII, the peripheral light-harvesting complex of Photosystem II, plays a major role. At the same time, the same light-harvesting system can be 'switched' into a quenching state, which effectively protects the reaction center of Photosystem II from over-excitation and photodamage. In this talk I will demonstrate how LHCII collects and transfers excitation energy. Using single molecule spectroscopy we have discovered how LHCII can switch between this light-harvesting state, a quenched state and a red-shifted state. We show that the switching properties between the light-harvesting state and the quenched state depend strongly on the environmental conditions, where the quenched state is favoured under 'NPQ-like' conditions. It is argued that this is the mechanism of non-photochemical quenching in plants.

10:24AM H7.00005 Protein Dynamics, Ligand Binding, and Biological Function , HUAN-XIANG ZHOU, Florida State University — Dynamics is essential for protein function. To demonstrate this point, this talk presents three studies. (1) For a ligand-gated ion channel, ligand binding leads to channel activation by modulating the dynamics of the channel protein. A common theme that emerges from different families of ligand-gated ion channels is that agonist binding closes the ligand-bidning domain (LBD), leading to pore opening in the transmembrane domain (TMD); in contrast, antagonist binding opens the LBD, leading to pore closing in the TMD [1]. (2) When the structure [2] and gating dynamics [3] of the influenza M2 proton channel are accounted for, the calculated rate of ion transport is in quantitative agreement with experimental data [4]. (3) In enzymes, gating dynamics afford substrate selectivity [5].

[1] M. Yi, H. Tjong, and H.-X. Zhou (2008). Spontaneous conformational change and toxin binding in α7 nicotinic acetylcholine receptor: insight into channel activation and inhibition. Proc. Natl. Acad. Sci. 105, 8280-8285.
[2] M. Sharma, M. Yi, H. Dong, H. Qin, E. Peterson, D. D. Busath, H.-X. Zhou, and T. A. Cross (2010). Insight into the mechanism of the influenza A proton channel from a structure in a lipid bilayer. Science 330, 509-512.
[3] M. Yi, T. A. Cross, and H.-X. Zhou (2009). Conformational heterogeneity of the M2 proton channel and a structural model for channel activation. Proc. Natl. Acad. Sci. USA 106, 13311-13316.
[4] H.-X. Zhou (2010). Diffusion-influenced transport of ions across a transmembrane channel with an internal binding site. J. Phys. Chem. Lett. 1, 1973-1976.
[5] H.-X. Zhou, S. T. Wlodek, and J. A. McCammon (1998). Conformation gating as a mechanism for enzyme specificity. Proc. Natl. Acad. Sci. USA 95, 9280-9283.

Tuesday, March 22, 2011 8:00AM - 10:24AM –
Session H8 FPS: Science, Art and Culture Ballroom C4

8:00AM H8.00001 Robotics in the World of Entertainment , DAVID HANSON, Hanson Robotics — This abstract not available.

8:36AM H8.00002 XPower plus the Physics of Rodeo , STEPHEN WHARTON, Skycam Inc. — This abstract not available.

9:12AM H8.00003 Singing Tesla Coils , JOE DIPRIMA, Arc Attack — This abstract not available.

9:48AM H8.00004 The Science of Barbecue (Texas Style) , DAVEY GRIFFIN, Texas A & M University — This abstract not available.

Tuesday, March 22, 2011 8:00AM - 11:00AM –
Session H9 DFD: Colloids: Experimental D220

8:00AM H9.00001 Universality in the delayed failure of colloidal gels , JORIS SPRAKEL, DAVID WEITZ, Harvard University — The mechanical failure of heterogeneous solids is not always instantaneous with the application of a load, but can be significantly delayed. We use colloidal gels, a prototypic heterogeneous material, to unravel the microscopic mechanisms behind this delayed failure. A universal behavior is revealed; the delay time depends only on the magnitude of the applied stress not on its origin. Whether the gel succumbs to internal tension, gravitational compression or shear stresses, the behavior can be quantitatively explained using a generalized bond-rupture model that describes the microscopic events triggering macroscopic failure.

8:12AM H9.00002 Glassy dynamics of 2D colloid crystals in a random pinning potential[1] , SUNGCHEOL KIM, ALEXANDROS PERTSINIDIS[2], XINSHENG LING, Brown University — Recently, we have demonstrated that a monolayer charged colloidal crystal confined to a rough charged surface provides a realization of the Larkin-Ovchinnikov random-pinning model in two dimensions [1]. The statics of the system is found to agree with Larkin's prediction of balkanization into small ordered domains. However, the dynamics are in disagreement with the collective creep model. Detailed analysis of the particle trajectories suggest that collective creep is preempted by channel flow. We also find that the velocity response to a step-like driving force shows a stretched exponential behavior similar to that found in structural glasses. Here, we provide a detailed analysis of this process.

[1] A. Pertsinidis and X.S. Ling PRL **100** 028303 (2008)

[1]This research was supported by the NFS-DMR.

[2]Current Address: Memorial Sloan-Kettering Cancer Center New York, NY 10065

8:24AM H9.00003 Field-driven pattern formation of charged particles in nonpolar solvent , TINA LIN, SHMUEL RUBINSTEIN, DAVID WEITZ, Harvard University — We combine microfluidics and high-speed imaging to investigate transport dynamics of charged colloidal particles in a nonpolar solvent as the polarity of an external electric field is switched periodically. Immediately following a switch, particles which were initially all packed against one electrode move towards the opposite electrode in an unstable manner; instead of remaining uniform, the particle front develops undulations. This results in a heterogeneous deposition of particles on the electrode wall. For a range of wait times between switches, we find that the particles localize at exceptionally well-defined periodic modes and we offer a simple physical model to account for this pattern formation.

8:36AM H9.00004 Colloids with magnetic patches: synthesis and self-assembly , STEFANO SACANNA, NYU, LAURA ROSSI, Utrecht University, WILLIAM IRVINE, DAVID PINE, NYU — We developed a new class of colloidal particles that programmably and reversibly self-assemble into well-defined clusters by virtue of "magnetic patches" carrying a permanent magnetic dipole moment. The resulting clusters form spontaneously in a zero external field, and their geometry is entirely determined by the interplay between magnetic, steric, and electrostatic interactions. Imposing an external magnetic field enables the clusters to unbind or change their geometry allowing, in principle, to create materials with tunable structural arrangements.

8:48AM H9.00005 Melting Dynamics of Colloidal Thin Films on Patterned Substrates , JOHN MERGO, School of Applied and Engineering Physics, Cornell University, JOHN SAVAGE, Department of Physics, Cornell University, ITAI COHEN, Deparment of Physics, Cornell University — We present results of experiments on the melting dynamics of colloidal crystals formed on patterned substrates. Our system consists of micron-sized colloidal particles and a tunable short- range attractive depletion interaction that can be controlled by small temperature changes. We investigate the melting rates of crystalline islands that form on substrates with square and hexagonal symmetry. We find that crystals with square symmetry melt significantly slower than those with hexagonal symmetry despite the fact that particles at the edge of the hexagonal crystal are on average bound more strongly than those at the edge of a square crystal. We find that the symmetry of the substrate affects the ability of particles to diffuse away from a melting crystal, and these differences in single-particle diffusion rates account for the difference in melting rates.

9:00AM H9.00006 Dynamics of Transient Vorticity Aligned Structures in Attractive Colloidal Suspensions , AJAY NEGI, Yale University, MICHELLE BEBRIN, McGill University, CHINEDUM OSUJI, Yale University — Shear rate jumps from high to low flow rates in an attractive colloidal suspension of carbon black particles in a non-polar solvent result in the formation of transient log-like structures aligned in the vorticity direction. Optical microscopy in situ with bulk rheology shows that the appearance of these aggregates is attended by an increase in the suspension viscosity. The viscosity shows a peak and then gradually recedes with passage of time under flow in concordance with the disappearance of the log-like structures. The time at which the viscosity reaches its maximum scales inversely with the shear rate applied to the system. This emergence of the peak in viscosity appears to be controlled by a critical strain and rescaling in these terms produces a common response across several different shear rates. Alteration of the attraction strength between particles by the addition of surfactant severely inhibits the structure formation. We present a simple model to account for these observations.

9:12AM H9.00007 Two-dimensional Fibonacci spiral optical thermal ratchets , KE XIAO, DAVID GRIER, Center for Soft Matter Research at New York University — A novel two-dimensional optical thermal ratchet has been implemented with holographic optical trapping arrays structured as the "Fibonacci spiral" for diffusing colloidal particles. Periodically rotating the optical trapping array by an angle in a three-step cycle yields a two-dimensional time-varying optical landscape that acts either as (1) a deterministic pump when traps are closely dispersed in space, whose induced radial and azimuthal fluxes can be quantitatively mapped out according to the geometry of Fibonacci spiral, or else as (2) an optical thermal ratchet when traps are widely dispersed, whose transport property depends on the competition between the temporal evolution in optical landscapes and Brownian particles' diffusivity. The Fibonacci ratchet displays independent flux reversals in both the radial and azimuthal directions as a function of the cycle frequency and the inter-trap separation.

9:24AM H9.00008 Using shear to assemble colloidal strings , ITAI COHEN, XIANG CHENG, Dept. of Physics, Cornell University — Sheared colloidal suspensions exhibit various fascinating phases under the influence of hydrodynamic, interparticle and thermal interactions. These shear-induced phases have been intensively studied for suspensions well above the crystalline threshold, but remain relatively unexplored for amorphous suspensions. Here, we report a novel string phase in less concentrated colloidal suspensions under shear, where particles assemble into long strings normal to the plane of shear. This finding contradicts previous numerical results that predict the formation of particle strings along the shear velocity direction. We systematically investigate how the phase depends on the shear rates, the confinement of shear plates, and the volume fractions of samples. We demonstrate the relation between the string phase of low volume fraction samples and the shear-induced crystallization of high volume fraction samples. A simple mechanism for the formation of this novel phase is suggested.

9:36AM H9.00009 Biomembrane-mediated control of like-charge colloidal attraction , MAUNTA MANANDHAR, YUPENG KONG, RAGHUVEER PARTHASARATHY, Department of Physics and Material Science Institute, The University of Oregon — The nature of attractions observed between like-charged colloidal particles near a confining wall is still mysterious, due in part to the lack of experimental systems with tunable inter-particle interactions. Biomembranes are appealing candidates for colloidal functionalization, enabling access to electrostatic and chemical properties that influence inter-particle relations. Previous optical-trap based examinations of lipid membrane functionalized particles revealed a surprising linear relationship between the magnitude of the attractive pair potential and the particle charge in presence of a wall of constant charge density. Here, using lipid membranes to also functionalize the confining wall, thereby controlling its charge density, we find a non-linear relationship between inter-particle attraction and charge. Our results highlight the role of substrate-induced fields in controlling pair interactions between colloidal microparticles.

9:48AM H9.00010 Colloidal Gas-Liquid Condensation induced by the Critical Casimir Effect , DUC NGUYEN, SUZANNE FABER, GERARD H. WEGDAM, PETER SCHALL, University of Amsterdam — We explore a new temperature control over colloidal phase formation by using the Critical Casimir effect. This effect allows direct control over particle interactions via temperature-dependent solvent fluctuations: In analogy to the confinement of fluctuations of the electromagnetic field between two dielectrics (quantum mechanical Casimir effect), the confinement of fluctuations of a critical solvent leads to an attraction between surfaces that are immersed in this solvent. This allows exquisite temperature control over the interactions of colloidal particles that are suspended in this critical solvent. We show that this temperature control allows us to "freeze" a dilute colloidal gas into a dense colloidal liquid, and a crystalline solid. By using confocal microscopy, we follow these phase transitions directly in real space, and we measure the particle pair potential. We show that we can quantitatively account for the gas-liquid condensation by using Van der Waals theory. We study the growth of colloidal liquid droplets by following the mean droplet radius <R> with dynamic light scattering. We find <R> $\sim$ t1/2 and <R> $\sim$ t1/3 indicating that the droplets form by nucleation, followed by diffusion limited growth.

10:00AM H9.00011 Comparison of different analysis techniques in inline holographic video microscopy , FOOK CHIONG CHEONG, New York University — Holographic video microscope can be analyzed on a frame-by-frame basis to track individual colloidal particles' three-dimensional motions with nanometer resolution. In this work, we compare the performance of two complementary analysis techniques, one based on fitting to the exact Lorenz-Mie theory and the other based on phenomenological interpretation of the scattered light field reconstructed with Rayleigh-Sommerfeld back-propagation. Although Lorenz-Mie tracking provides more information and is inherently more precise, Rayleigh-Sommerfeld reconstruction is faster and more general.

10:12AM H9.00012 Dynamics of colloidal particles in ice , MELISSA SPANNUTH, S.G.J. MOCHRIE, Yale University, S.S.L. PEPPIN, Oxford University, J.S. WETTLAUFER, Yale University — Solidification of the solvent phase of a colloidal suspension occurs in many natural and technological settings and is becoming a popular technique for creating microporous structures and composite materials. During freezing, regions of high particle density can form as particles are rejected from the growing solid and guided into a variety of macroscopic morphologies. The particles in the high density regions form an amorphous colloidal solid that deforms in response to internal and external stresses. Using X-ray Photon Correlation Spectroscopy, we studied this deformation for silica particles in polycrystalline ice. We found that the particles in the high density regions underwent ballistic motion coupled with a non-exponential decay of the intensity autocorrelation function (ACF) that transitions from a stretched to a compressed exponential with increasing scattering vector q. While ballistic motion and a compressed exponential decay of the ACF is common, the coupling with a stretched exponential decay is very rare and a transition with increasing q has not previously been reported. We explain this behavior in terms of ice grain boundary migration.

10:24AM H9.00013 Imaging the microscopic structure of shear thinning and thickening colloidal suspensions , XIANG CHENG, Dept of Physics, Cornell University, JONATHAN MCCOY, Department of Physics and Astronomy, Colby College, JACOB ISRAELACHVILI, Dept. of Chemical Engineering, University of California, Santa Barbara, ITAI COHEN, Dept. of Physics, Cornell University — The viscosity of colloidal suspensions varies by orders of magnitude depending on how quickly they are sheared. Such non- Newtonian behavior arises from the arrangement of suspended particles and their mutual interactions. Although numerical simulations and various scattering experiments have revealed much about the local and average suspension structures, particle dynamics at mesoscopic length scales, where non- Newtonian behaviors are believed to originate, are still poorly understood. Here, by combining fast confocal microscopy with simultaneous rheological measurements, we systematically investigate changes in suspension structure over a range of length scales, as the suspension transitions through regimes with different rheological signatures. Our measurements bridge previous simulation and scattering results, and unambiguously show that shear thinning is coupled to particle layering, that shear thickening is decoupled from suspension order-to-disorder transitions, and that there exists a novel phase where particles self-assemble into strings oriented normal to the plane of shear.

10:36AM H9.00014 Cubic crystals from cubic colloids , LAURA ROSSI, Van't Hoff Laboratory, Utrecht University, STEFANO SACANNA, WILLIAM IRVINE, PAUL CHAIKIN, DAVID PINE, Center for Soft Matter Research, New York University, ALBERT PHILIPSE, Van't Hoff Laboratory, Utrecht University — We have studied the crystallization behavior of colloidal cubes by means of tunable depletion interactions. The colloidal system consists of novel micron-sized cubic particles prepared by silica deposition on hematite templates and various non-adsorbing water-soluble polymers as depletion agents. We show that under certain conditions the cubes can self-organize into crystals with a simple cubic symmetry, which is set by the size of the depletant. The dynamic of crystal nucleation and growth is investigated monitoring the samples in time by optical microscopy. Furthermore, by using temperature sensitive microgel particles as depletant it is possible to fine tune depletion interactions as to induce crystal melting. Assisting crystallization with an alternating electric field improves the uniformity of the cubic pattern allowing the preparation of macroscopic (almost defect-free) crystals that show visible Bragg colors.

10:48AM H9.00015 Spin-coating of rapidly dried colloidal suspensions: model and experiments[1] , MAXIMILIANO GIULIANI, University of Guelph, WENCESLAO GONZÁLEZ-VIÑAS, University of Navarra, ANAND YETHIRAJ, Memorial University of Newfoundland — The study of the formation of colloidal crystals has been a very active field in recent years. The spin-coating technique has proven to be a highly reproducible process to form large area colloidal crystals. Here, we present recent results on spin- coating of rapidly dried colloidal suspension. We show that the dynamics observed can be represented by an extension of classical Emslie model to highly volatile fluids. We obtained this extension while maintaining the explicit solution for the temporal evolution of the fluid thickness. We observed that the dynamics can be separated in two regimes: one dominated by non-evaporative effects and a second dominated by evaporative effects. The transition between these two dynamical regimes corresponds well with the transition between two symmetries observed during the fluid phase (six and four-fold). Similarly, the quality of the deposited structure is also well correlated to the relative strength of the capillary forces with respect to the viscous ones.

[1]Support from NSERC, and MEC (FIS2008-01126).

Tuesday, March 22, 2011 8:00AM - 11:00AM –
Session H10 DCMP: Semiconductor Surfaces and Interfaces D221

8:00AM H10.00001 Reversible vertical manipulation of Ag atoms on Si(111)-(74×7) at room temperature , FANGFEI MING, KEDONG WANG, SHUAN PAN, JIEPENG LIU, XIEQIU ZHANG, JINLONG YANG, XUDONG XIAO, DEPARTMENT OF PHYSICS, THE CHINESE UNIVERSITY OF HONG KONG, SHATIN, NEW TERRITORY, HONG KONG, CHINA TEAM, HEFEI NATIONAL LABORATORY FOR PHYSICAL SCIENCES AT MICROSCALES, UNIVERSITY OF SCIENCE AND TECHNOLOG TEAM — We have demonstrated a technique to conduct reproducible and reversible vertical manipulation of Ag atoms on the Si(111)-(7×7) surface at room temperature using a scanning tunneling microscope tip. The direction of the transfer of Ag atoms between the sample surface and the tip is simply controlled by the polarity of the bias voltage. Using the 7×7 unit cell as a nanometer size template, complex Ag nano-clusters could be assembled or disassembled by adding or removing Ag atoms in an atom-by-atom manner. With controlled number of Ag atoms filled in a half unit cell, we can construct Ag clusters with up to 25 Ag atoms. The precise control of the number of Ag atoms in the Ag clusters can provide critical information for understanding their physical and chemical properties, and form a fundamental base for the relevant studies of the Ag/Si(111)-(7×7) system and for fabricating nano-devices.

8:12AM H10.00002 Probing surface electronic structure with conductance measurements on Si nanomembranes , WEINA PENG, JAMES ENDRES, SHELLEY SCOTT, DONALD SAVAGE, IRENA KNEZEVIC, MARK ERIKSSON, MAX LAGALLY, University of Wisconsin Madison, MRSEC OF UNIVERSITY OF WISCONSIN MADISON TEAM — The surface electronic structure of nanostructures has a strong, sometimes dominant, influence on their transport properties, because of their large surface to volume ratios. Different surface terminations result in different transport behavior, and therefore conductance measurements on nanostructures can be used to study surface and interface electronic spectra. In our experiments, the conductance of the thin (200nm or less in thickness) top Si layer in silicon-on-insulator is measured as the back gate voltage is varied, for both hydrogen terminations and clean reconstructed surfaces in UHV. Experimental results on samples of different thicknesses are compared systematically with simulations to understand the role of the Si/SiO_2 interface and the electronic structure of the front surface. We explain why the transport behavior of NMs with a clean Si(001) surface is distinct from that with hydrogen termination. Donor type surface states are present in the majority on the hydrogenated surface, and their concentration is on the order of 10^{12} cm^{-2}. On the reconstructed Si surface, instead, pseudo-pinning of the Fermi level occurs because of the high density of states of the clean-surface band (2x1 reconstruction) and the presence of surface defect states.

8:24AM H10.00003 Experimental evidence for trapped volumes in thin Ag films on Si(111)-7x7 , S.T. HAYDEN, YIYAO CHEN, M.W. GRAMLICH, R.S. GARI, G.M. KING, P.F. MICELI, University of Missouri Department of Physics and Astronomy — Thin films of Ag on Si(111)-7x7 were prepared in UHV at room temperature by vapor depositing Ag at a glancing angle with respect to the surface normal. Comparing x-ray reflectivity and atomic force microscopy (AFM) measurements, it is found that both techniques give the same height distribution at the surface. However, for a given deposition angle, x-ray reflectivity measurements reveal that there is a significant portion of trapped volume that goes undetected by the AFM. Also, by increasing the deposition angle from normal to glancing incidence angles, both the roughness and the maximum height distribution profile increase. Experimental evidence for trapped volumes in Ag/Si(111)-7x7 will be discussed. Research funding is supported by NSF DMR-0706278. The Advanced Photon Source Sector 6 beam-line at Argonne National Laboratory is supported by the US-DOE through Ames Lab under Contract No. W-7405-Eng-82.

8:36AM H10.00004 Growth of Iridium and Silver on Ge(111) Studied by STM[1] , MARSHALL VAN ZIJLL, CORY MULLET, EMILIE HUFFMAN, SHIRLEY CHIANG, UC Davis — We have used scanning tunneling microscopy (STM) to characterize the growth of iridium and silver onto Ge(111) as a function of coverage and annealing temperature. Ir was deposited onto the Ge(111) c(2x8) surface at different coverages less than 1ML. The Ir forms islands with a $(\sqrt{3}x\sqrt{3})R30^\circ$ phase and island size increasing with increasing annealing temperature. Stranski-Krastanov growth was observed at most coverages. Ag deposited onto the Ge(111) c(2x8) surface and annealed at 450K forms both a (4x4) phase and a (3x1) phase. The Ge(111) surface reorganizes to a (2x2) phase after deposition of both Ir and Ag. High resolution images have been obtained allowing direct observation of the different phases.

[1]Support from NSF CHE-0719504 and PHY-1004848.

8:48AM H10.00005 One-dimensional Mn atom chains templated on a Si(001) surface[1] , SIGRUN A. KÖSTER, JAMES H.G. OWEN, FRANÇOIS BIANCO, University of Geneva, Switzerland, ALEX M.P. SENA, DAVID R. BOWLER, University College London/London Centre for Nanotechnology, UK, CHRISTOPH RENNER, University of Geneva, Switzerland — Single-atom chains on a wide gap substrate are a very attractive embodiment of a truly one-dimensional system to explore the remarkable physical properties emerging in such low dimensions. We present self-assembled single-atom Mn chains on a Si(001) surface with Bi nanolines, which serve to increase greatly the average length of the Mn chains. They grow perpendicular to the Si(001) dimer rows, at densities which can be adjusted by means of the growth parameter. High resolution scanning tunneling microscopy (STM) micrographs are in perfect agreement with density functional theory (DFT), providing detailed insight into the chain structure. We further discuss low temperature STM spectroscopy and spin dependent DFT modeling suggesting Mn-chains are indeed a suitable candidate to observe electronic and magnetic properties in one-dimension experimentally.

[1]This work was supported by the MaNEP research program via the swiss national science foundation (SNF).

9:00AM H10.00006 Low energy alkali ion-surface charge exchange for Si(111) as a function of doping , REUBEN D. GANN, JORY A. YARMOFF, University of California, Riverside — Alkali ion-surface charge exchange, which can be used to probe surface electronic states, is well understood within the context of the resonant charge transfer (RCT) model. Recent studies have extended the use of alkali ion scattering and the RCT model from metal surfaces to semiconductors and insulators. In the present work, we measure the effect of doping type and concentration on the neutralization probability of alkali ions scattered from semiconductors. Si(111) surfaces were prepared in UHV, and the neutralization probability of scattered Li^+ ions was measured for projectiles that were singly scattered from Si atomic sites. For the clean Si(111)-7×7 surface, the neutralization is determined by the surface electronic states [1] and is independent of doping. Samples were then dosed with atomic hydrogen in order to passivate the surface states and unpin the Fermi level. This affects the neutralization probabilities and reveals differences between n and p-type materials.

[1] Y. Yang and J.A. Yarmoff, Phys. Rev. Lett. 89, 196102 (2002).

9:12AM H10.00007 Binding sites and diffusion barriers of a Ga adatom on the GaAs(001)-$c(4\times 4)$ surface from first-principles computations[1] , J. ROEHL, A. KOLAGATLA, V.K.K. GANGURI, S. KHARE, University of Toledo, R.J. PHANEUF, University of Maryland — The Ga adatom adsorption and diffusion processes on the $\mathrm{GaAs}(001)$-$c(4 \times 4)$ surface were studied using *ab initio* density-functional-theory computations in the local density approximation. Two distinct sets of minima and transition sites were discovered for a Ga adatom relaxing from heights of 3 and 0.5 Å from the surface. These two sets show significant differences in the interaction of the Ga adatom with surface As dimers. An electronic signature of the differences in this interaction was identified. We computed the energetic barriers to diffusion for various adsorption sites. From these, we propose three pathways for diffusion of a Ga adatom on this surface which indicate anisotropic diffusion along different directions.[2]

[1]J.L. Roehl *et al.*, Phys. Rev. B **82**, 165335 (2010).
[2]Supported by NSF DMR 0705464.

9:24AM H10.00008 Surface Structure of Bi-terminated GaAs Grown with Molecular Beam Epitaxy , ADAM DUZIK, JOANNA MILLUNCHICK, University of Michigan — Control of III-V semiconductor surfaces is crucial for high-quality device production. A means of interface control involves the use of Bi as a surfactant, which both smooths the surface and alters the surface reconstruction. We examined the effects of Bi deposition via molecular beam epitaxy on the GaAs(001) surface structure using reflective high energy electron diffraction and scanning tunneling microscopy. After ∼0.2 ML of Bi deposition, scanning tunneling microscopy revealed a disruption in the initial c(4×4) reconstruction. Coverages of ∼0.4 ML and ∼0.6 ML produced a (1×3) and a (2x3) diffraction pattern, respectively, and an atomic surface structure consisting of a disordered row reconstruction, β2(2×4) reconstruction rows, and surface clusters, with 1 ML deep pits at a coverage of ∼0.6 ML. Calculations show these changes in surface structure and morphology are likely not the result of As desorption, but due to the presence of Bi on the surface. These observations may help explain the origin of Bi clusters that give GaAsBi most of its unique properties.

9:36AM H10.00009 Design of carbide thin film coatings from first principles , MIKAEL RÅSANDER, University of California Davis, BIPLAB SANYAL, ULF JANSSON, OLLE ERIKSSON, Uppsala University — Transition metal carbides have many interesting physical properties and have therefore been used in many technological applications, e.g. as thin film metal coatings. A commonly studied thin film coating material is nc-TiC/a-C, where nanocomposites (nc-) of TiC are dispersed in an amorphous (a-) C matrix. An interesting feature of these types of materials is the possibility to design the material to obtain new functionality, e.g. by tuning the C to Ti content. In this talk we will present results obtained by first principles density functional theory calculations of a different approach, where various metals have been alloyed into TiC. Depending on the alloying metals ability to form carbides this will yield different effects. One of these effects is the creation of a driving force for the release of C from the carbide. This C release has been shown to yield favorable lubricating properties of nc-(Ti,Al)C/a-C thin films. We will show that the C release can be tuned by a careful selection of the alloying metal in order to optimize the properties of these types of thin film carbide coatings.

9:48AM H10.00010 THz optical Hall-effect and MIR-VUV ellipsometry characterization of 2DEG properties in HfO_2 passivated AlGaN/GaN HEMT structures[1] , S. SCHÖCHE, A. BOOSALIS, University of Nebraska-Lincoln, C.M. HERZINGER, J.A. WOOLLAM, J.A. Woollam Co. Inc., J. SHI, W.J. SCHAFF, L.F. EASTMAN, Cornell University, M. SCHUBERT, T. HOFMANN, University of Nebraska-Lincoln — We present non-contact, optical measurements of free-charge carrier mobility, sheet density, and effective mass parameters of the 2DEG for different HfO_2 passivated AlGaN/GaN high electron mobility transistor structures at room temperature. Spectroscopic ellipsometry (SE) in the spectral range from THz and Mid-IR to the VUV and THz optical Hall-effect (generalized ellipsometry in magnetic fields) (OHE) are employed. Changes in the HfO_2 layer growth conditions are found to drastically influence the electron density of the channel. The sheet density and the carrier mobility obtained by the optical investigations are in excellent agreement with results from electrical Hall-effect measurements. The electron effective mass parameters determined here using the OHE corroborate previous SdH and cyclotron resonance studies. The surface sensitivity of VUV-SE in combination with OHE allows for correlation of surface passivation and changes in the 2DEG properties.

[1]ARO (W911NF-09-C-0097), NSF (MRSEC DMR-0820521, MRI DMR-0922937, DMR-0907475)

10:00AM H10.00011 Low Temperature Epitaxial Growth of Ge Quantum Dots on Si(100) , ALI ER, HANI ELSAYED-ALI, Old Dominion University — The effect of laser-induced electronic excitations on the self-assembly of Ge quantum dots (QD) on Si(100)-(2x1) grown by pulsed laser deposition is studied. The experiment was conducted in ultrahigh vacuum. A chirped pulse amplified Ti:sapphire laser with ∼60 femtosecond pulse width, center wavelength ∼800 nm, and operating at 1 kHz repletion rate was split into two beams; one used to ablate a Ge target while the other to electronically excite the substrate. *In situ* reflection high-energy electron diffraction (RHEED), scanning tunneling microscopy (STM), and *ex situ* atomic force microscopy (AFM) were used to study the morphology of the grown QDs. For Ge coverage of 12 monolayer, it was observed that the excitation laser reduces the epitaxial growth temperature to 70 $^\circ$C, at which no epitaxy is possible without excitation. By using nanosecond Nd:YAG laser for ablation and excitation, it was shown that applying the excitation laser to the substrate during the growth changes the QD morphology and island density and improves the size uniformity of the QDs at 390 $^\circ$C. RHEED recovery curves show that the excitation laser increases the surface diffusion of the Ge atoms. A purely electronic mechanism of enhanced surface diffusion of the Ge adatoms is involved.

10:12AM H10.00012 Large scale atomic engineering of silicon (100) surfaces , KAI LI, University of Maryland, PRADEEP NAMBOODIRI, SUMANTH CHIKKAMARANAHALLI, JOSEPH FU, RICHARD SILVER, National Institute of Standards and Technology, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY COLLABORATION, UNIVERSITY OF MARYLAND, COLLEGE PARK COLLABORATION — Control of atomic morphology at the micrometer scale has been a long term challenge to enable atomically precise manufacturing. In this presentation we describe our method to pattern micrometer scale, ordered features on a Si surface with subsequent etch and high temperature processing. Following high temperature UHV processing, high quality atomically-ordered surfaces are imaged using atomic-resolution STM. A significant attribute of these surfaces is that the micrometer scale features evolve, but persist, allowing external location of nanometer scale features as well as comprehensive control of atomic terrace sizes and step bunching. A multi step thermal process is used, resulting in surface with symmetric, reproducible step-terrace patterns and very wide atomically flat regions. A kinetic Monte Carlo (KMC) model is used to simulate the current induced electromigration process which is primarily responsible for the long range evolution of surfaces.

10:24AM H10.00013 Theory of Scanning Tunneling Microscopy of Dangling Bonds on Silicon Surfaces , LUCIAN LIVADARU, University of Alberta, JASON PITTERS, NINT, ROBERT WOLKOW, University of Alberta/NINT — Silicon surface dangling bonds (DBs) are electronic gap states with eigenenergy close to the middle of the bandgap of bulk silicon and can be explored as quantum dots. During exploratory fabrication and characterization of DB-structures on H-Si(100) surfaces, scanning tunneling microscopy (STM) imaging showed sharp halo-like features around single DBs that cannot be explained by the standard STM theory. Halo appearance varies with sample doping level and imaging conditions (sample bias and current). Here we investigate the nature of such features in the STM imaging of DBs. We propose a theory of image formation based on non-equilibrium charge transfer balance (via elastic and inelastic channels), from the STM tip to DB on one hand, and from DB to bulk Si on the other. For empty-state imaging mode, in the immediate proximity of a DB (<1nm) tip-induced band bending shifts the DB-level to a value between the Fermi levels of the STM tip and of the sample. Consequently, a steady-state of charge flow is established through the DB state, which dictates the time-average amount of charge on the DB. This in turn affects the total STM current in that proximity leading to the appearance of a halo.

10:36AM H10.00014 The Electronic and Transport Properties of Si(111)-7×7 and Related Reconstructions[1] , MANUEL SMEU, McGill University, WEI JI, Renmin University of China, ROBERT WOLKOW, National Institute for Nanotechnology, HONG GUO, McGill University — The 7×7 reconstruction of Si(111) has the interesting property of being metallic despite bulk Si being a semiconductor. This surface has a complex reconstruction that takes on a dimer-adatom stacking fault (DAS) structure composed of adatoms, rest atoms, and several other key features. It is believed that the conductivity occurs through the dangling bonds of the adatoms, and that it is entirely a surface effect. To elucidate the details of this mechanism, we have investigated a set of related Si(111) reconstructions of increasing complexity in order to resolve the effect of the different DAS features on the electronic and transport properties of the Si(111)-7×7 surface. Density functional theory (DFT) calculations have been carried out on the $\sqrt{3}\times\sqrt{3}$-$R30^\circ$, 2×2, 5×5, and 7×7 reconstructions of Si(111). Additionally, our work is extended to electron transport simulations employing the non-equilibrium Green's function technique coupled with DFT (NEGF-DFT) to calculate the conductance for these systems. Finally, the effect of atomic steps and adsorbates on the conductive properties will also be discussed.

[1]Supported by NSERC, CIFAR, FQRNT and RQCHP.

10:48AM H10.00015 Size dependent superconductivity of Pb islands grown on Si (111) , JIEPENG LIU, XUEFENG WU, FANGFEI MING, XIEQIU ZHANG, KEDONG WANG, BING WANG, XUDONG XIAO, DEPARTMENT OF PHYSICS, THE CHINESE UNIVERSITY OF HONG KONG TEAM, HEFEI NATIONAL LABORATORY FOR PHYSICAL SCIENCES AT MICROSCALES,UNIV. OF SCIENCE AND TECHNOLOGY CHINA TEAM — The superconductivity of nano-sized Pb islands grown on Si (111) with different size at 9 monolayer thickness was studied by low temperature scanning tunneling spectroscopy. By measuring the zero bias conductance as a function of temperature, for larger islands we observed a transition from pseudogap state at high temperature to superconductivity state at low temperature through two distinct slopes, where the superconductivity transition temperature (Tc) of the island can be determined. For island size of $\sim$58 nm^2, a large drop in Tc is found; when the size is further reduced to about 30 nm^2, no superconducting state was observed down to the measured temperature of 3.2 K. By properly subtracting the background and pseudogap effect, information on the temperature dependent superconductivity gap can be obtained. The ratio of $\frac{2\Delta_0}{k_B T_c}$ decreased from 4.5 to 3.3 with the reduction of island size, showing that the electron-phonon coupling becomes weaker as the size decreases.

Tuesday, March 22, 2011 8:00AM - 11:00AM –
Session H11 SPS: SPS Undergraduate Research III D222

8:00AM H11.00001 Nanodynamics of Ferroelectric Ultrathin Films[1] , RYAN HERCHIG, QINGTENG ZHANG, INNA PONOMAREVA, University of South Florida — An active area of research in nanoscale science is the study of ferroelectric ultrathin films. We will report a first-principles-based study of the nanodynamics in ferroelectric $Pb(Zr_{0.4}Ti_{0.6})O_3$ films with thickness 20-192 nm. In our computational experiment we first anneal such films under realistic conditions of partial screening of the surface charge to obtain the ground state nanodomain pattern. After that the films are subjected to ac electric fields with frequencies varying from 0.1 THz to 4.0 THz and close to nanodomain resonance frequency. The domain evolution is then studied as a function of time, electric field frequency, and film thickness in order to quantitatively characterize the laws and parameters associated with it. This allows us to reveal for the first time ever intrinsic high-frequency dynamics of ferroelectric nanostripe domains.

[1]This work is supported by DOE grant DE-SC0005245. The authors would like to acknowledge the use of the services provided by Research Computing, University of South Florida. I. P. acknowledges support from the USF under Grant No. R070699.

8:12AM H11.00002 Thermal Conductivity of Random Multilayer Thin Films , ANTHONY FRACHIONI, B.E. WHITE JR., Binghamton University — Thermoelectric based energy scavenging has tremendous potential for the recovery of waste heat and temperature regulation. Manufactured thermoelectric devices today are limited in efficiency, and therefore widespread use, by high lattice thermal conductivity. In an effort to minimize lattice conductivity with respect to electrical conductivity, opportunities for utilizing the Anderson localization of phonons have been explored. In particular, the thermal conductivity of a model random multilayer thin film with Lennard-Jones bonding has been determined using classical reverse non-equilibrium molecular dynamics as a function of mass induced disorder. Results indicate that the inclusion of random planes in which the atomic mass has been increased by a factor of ten can produce reductions in lattice thermal conductivity by over a factor of one hundred. The dependence of thermal conductivity on the magnitude and nature of this disorder has been measured. Finite size effects have been quantified and a length scale has been determined on which they can be neglected. These results indicate that the pursuit of nanostructured thermoelectric materials in the form of random multilayers may provide a path to efficient and sustainable thermoelectric materials.

8:24AM H11.00003 Controlling the microstructure of binary carbide films with elemental substitutions[1] , K. FELLER, M. HAIDER, A. HODGES, R. SPRENG, E. POSBERGH, H. WOODWARD, S.E. LOFLAND, J.D. HETTINGER, Physics and Astronomy, Rowan University, M. HEON, Y. GOGOTSI, Materials Science and Engineering, Drexel University — We report on experiments to control the microstructure of textured binary carbide thin films deposited by reactive magnetron sputter deposition. Controlling the microstructure in these materials is important as the microstructure of these films provides a template for the resulting carbide-derived carbon (CDC) film and impacts their performance. Specifically, a combinatorial approach is used to add chromium to TiC films creating a compositional gradient as a function of position. We present a measurement of surface roughness as a function of material composition. The resulting materials, $(Ti_{1-x}Cr_x)C$ films, are significantly smoother than their pure TiC counterparts and the resulting CDC's have correlated defects which will improve the performance of the CDC in supercapacitor applications.

[1]This work was supported by Rowan University and NSF under contract DMR-0503711.

8:36AM H11.00004 Polypeptide Chirality Influences Multilayer Thin Film Growth and Structure , ZEPHRA BELL, DHAN KHADKA, DONALD HAYNIE — Polypeptide multilayer thin films are being developed for a variety of applications.These include coatings for implant devices and systems for drug delivery in thebiomedical sciences, and optical coatings. Subsequent polymer adsorption steps involve polymers of opposite polarity. Here, the polymers were polypeptides. This project compared the consequences of changing polypeptide chirality on film growth and structure. The peptides were poly(L-glutamic acid), its right-handed counterpart, poly(D-glutamic acid), and poly(lysine-tyrosine). The first two are negatively charged at neutral pH, the third one is positively charged. Poly(lysine-tyrosine)/poly(L-glutamic acid) films and poly(lysine-tyrosine)/poly(D-glutamic acid) films werefabricated on 1 mm-thick quartz plates. In one experiment, films were grown to 34layers. The UV absorption spectrum was taken after each layer deposited to determinethe rate of polymer self-assembly. Separately, UV or visible wavelength spectra wereobtained for films stained with a dye cooled/heated in the range 4-65 $^\circ$C. In anotherexperiment, a mixture of poly-L-glutamic acid and poly-D-glutamic acid was used as thepolyanion for film buildup. The data show that poly(lysine-tyrosine)/poly(L-glutamicacid) films built up at a higher rate than the corresponding right-handed films.

8:48AM H11.00005 Thermoelectric Properties and Microstructure of $Ca_3Co_4O_9$ thin films on $SrTiO_3$ and Al_2O_3 Substrates[1] , T. PAULAUSKAS, Q. QIAO, A. GULEC, R.F. KLIE, UIC, M. OZDEMIR, C. BOYRAZ, D. MAZUMDAR, A. GUPTA, UA — $Ca_3Co_4O_9$ (CCO), a misfit layered structure exhibiting large Seebeck coefficient at temperatures up to 1000K has attracted increasing attention as a novel high-temperature thermoelectric material. In this work, we investigate CCO thin films grown on $SrTiO_3$ (001) and Al_2O_3 (0001) using pulsed laser deposition. Quality of the thin films was examined using high-resolution transmission electron microscopy and thermoelectric transport measurements. HRTEM images show incommensurate stacks of CdI_2-type CoO_2 layer alternating with rock-salt-type Ca_2CoO_3 layer along the c-axis. Perovskite buffer layer about 10nm thick was found present between CCO and $SrTiO_3$ accompanied by higher density of stacking faults. The CCO grown on Al_2O_3 exhibited numerous misoriented grains and presence of Ca_xCoO_2 phase. Seebeck coefficient measurements yield an improvement for both samples compared to the bulk value. We suggest that thermoelectric properties of CCO increase due to additional phonon scattering at the stacking faults as well as at the film surfaces/interfaces.

[1]This research was supported by the US Army Research Office (W911NF-10-1-0147) and the Sivananthan Undergraduate Research Fellowship.

9:00AM H11.00006 Antireflective Coatings using Layer-by-Layer Self Assembly of Silica and Titania Nanoparticles[1] , RAISA VELASCO CASTEDO, ANITESH ANAND LAL, DAN MAZILU[2], Washington and Lee University — It is known that glass substrates (borosilicate glass) reflect about 4% of light at each air/glass interface and thus, they transmit only 92% of light. For some devices like camera lenses, it is important to maximize the amount of transmitted light. Previous research has demonstrated that it is possible to do so by adding antireflective coatings to the substrates. Our research aimed to deposit thin films on glass substrates that would minimize the reflectance of light and thus, maximize its transmittance. The thin films consisted of multiple alternating layers of silica and titania nanoparticles following the theory behind double-quarter periodic systems and were deposited on the substrates via the ISAM (ionically self-assembled monolayers) technique. Several experiments were conducted in order to investigate the factors that affected the quality of the coatings and some of the significant factors observed were the pH and the molarity of the silica, titania and PDDA solutions. A number of factor-level combinations yielded transmittances in excess of 96%, well above the value for uncoated substrates.

[1]R.E.Lee Summer Research Program at Washington and Lee University
[2]Professor leading the research

9:12AM H11.00007 Compositional dependence of the narrow band emission from zinc oxide nanowires[1] , BRADLEY GOLDER, ERIC DRISCOLL, MARIAN TZOLOV, Lock Haven University of PA — Zinc oxide is a versatile platform thanks to the unique combination of optical, semiconducting, and piezoelectric properties of ZnO. The properties can be further diversified by creating microstructures and by varying the Zn/O ratio in the crystallites. We are illustrating this concept for the case of narrow band emission for ZnO nanostrutures grown through chemical vapor transport. The samples were characterized by photoluminescence spectroscopy (pulsed and continuous wave), scanning electron microscopy, and energy dispersive x-ray spectroscopy. Narrow band emission has been observed in the pulsed excitation mode. The narrowing is intensity dependent suggesting a mechanism of stimulated emission. The emission properties were correlated with the degree of oxidation of the ZnO nanocrystallites and with the presence of optically active defects. The influence of different oxidizing agents on the emission properties of the ZnO nanocrystals will be shown.

[1]This work was partly supported by the NSF grant # 0923047.

9:24AM H11.00008 Dependence of the band gap of highly confined CdSe and PbSe nanocrystals on temperature , AARON ZAUBI, Cornell College, J. BYLSMA, P. DEY, J. REJMAN, S. WITANACHCHI, P. MUKHERJEE, D. KARAISKAJ, University of South Florida, M. BEARD, NREL — We have recorded fluorescence spectra from PbSe and CdSe quantum dots in hexane/toluene respectively between 5K and 300K in order to investigate the temperature dependence of the electronic band gap of these highly confined nanostructures. The band gap for CdSe follows the known blue shift with decreasing temperature. We have measured the temperature dependence of the band gap of PbSe quantum dots for two different diameters below 4 nm and indeed observe a red shift of the band gap with decreasing temperature, which is stronger for the smaller size quantum dots. Such behavior would contradict the expected blue shift of the band gap with decreasing temperature. The origin of this peculiar behavior is not well understood and we are pursuing further theoretical and experimental studies in order to elucidate the mechanism behind it. Using the method of single-nanostructure laser spectroscopy will allow us to observe individual nanostructures while simultaneously removing ensemble averaging effects due to quantum interactions between multiple structures.

9:36AM H11.00009 Synthesis and characterization of ZnO nanocrystals co-doped with Ce^{3+} and Tb^{3+}[1] , KELLY MCCUTCHEON, CHRISTIE LAROCHELLE, Franklin and Marshall College — Rare earth doped zinc oxide nanocrystals produce visible emissions under ultraviolet excitation. Using a sol-gel process, we synthesized a series of ZnO nanocrystals doped with Tb^{3+} and Ce^{3+} in silica glass, keeping the ZnO/SiO_2 ratio constant at 10/90 and doping with 1% rare earth by weight, with varying relative concentrations of Tb^{3+} and Ce^{3+}. The nanocrystals were characterized using photoexitation and emission spectroscopy, time-resolved photoluminescence, UV/VIS spectroscopy, and transmission electron microscopy. We determined that co-doping with cerium enhanced the visible terbium emissions to a point, with the most effective enhancement occurring at mid-range Ce^{3+} concentrations.

[1]Franklin and Marshall College

9:48AM H11.00010 Growth and Morphology of High Mobility Organic Semiconductors[1] , CORTNEY BOUGHER, Appalachian State University, KATELYN GOETZ, Wake Forest University, ZHONG LI, JOHN ANTHONY, University of Kentucky, OANA JURCHESCU, Wake Forest University, BRAD CONRAD, Appalachian State University — We utilize atomic force microscopy (AFM) to image the growth and morphology of chemically modified, solution-deposited anthradithiophene transistors. We discuss the effects of backbone modifications on crystal structure, film properties, and electrical device performance. These devices display a mobility of 0.001 cm^2/Vs to 1 cm^2/Vs. Crystal orientation and film structures, such as film thickness, grain size, and growth modes will be discussed. In addition, AFM images are related to diffraction data and conduction channel crystallographic information is extracted.

[1]This research is supported by ASU, ASU Office of Student Research, the National Science Foundation, and Office of Naval Research.

10:00AM H11.00011 Effect of the polymer concentration on the ON/OFF states of a TN-LCD: polyvinyl alcohol vs. soy lecithin , ROMEO DE COSS MARTINEZ, JOSE LUIS GONZALEZ MURGUIA, Facultad de Ingenieria - UADY — In this work we study the response of a Twisted Nematic Liquid Crystal Display (TN-LCD) by varying both the concentration and the polymer used for the microgroove. We compare the performance of two polymers: polyvinyl alcohol and soy lecithin. In particular, the light transmission for the ON/OFF states is evaluated. The polyvinyl alcohol is a polymer widely used in LCDs while lecithin soy is a natural polymer.

10:12AM H11.00012 Tunable Schottky diodes fabricated from electrospun crossed SnO_2/PEDOT-PSSA nanoribbons[1] , KATHERINE CARRASQUILLO, NICHOLAS PINTO, University of Puerto Rico-Humacao — Hardware in most solid state devices contains at least one interface between a p-type and an n-type semiconductor. Such hetero-junctions are typically fabricated from all inorganic Si based materials. In the past two decades however, devices fabricated from organic-inorganic semiconductors that are not Si based, or from all organic semiconductors have been the focus of much research. Semiconducting n-doped metal oxides are also attractive for use in devices and of particular interest is tin oxide (SnO_2) as it is stable in air and is optically transparent with a band gap of $\sim$3.4 eV. The p-doped conducting polymer PEDOT-PSSA is also stable in air and is widely used in flexible devices. We shall report on the electrospinning technique to fabricate in air Schottky diodes, by simply crossing n-doped SnO_2 and p-doped PEDOT-PSSA nanoribbons. The device parameters could be tuned by a back gate bias and by shining UV light. The diode parameters were calculated using the standard thermionic emission model of a Schottky and was tested as a half wave rectifier.

[1]NSF-RUI and NSF-PREM

10:24AM H11.00013 UV-vis and Transport Characterization of Degradation in Polymer Blend Photovoltaics[1] , EMILEE SENA, JUSTIN PEEL, SHREYA NATHAN, DEVIN WESENBERG, MARIANNE WALLIS, THORSTEINN ADALSTEINSSON, BRIAN MCNELIS, RICHARD BARBER, Santa Clara University — Organic photovoltaic cells are prepared using an active layer containing a functionalized C60 molecule, [6-6]-phenyl C61 butyric acid octadecyl ester (PCBOD); and a conjugated polymer, poly(3-hexylthiophene) (P3HT). PCBOD functions as an electron acceptor in conjunction with P3HT, the electron donor. Both current-voltage (IV) transport data of solar cells and spectroscopic absorption data of the corresponding active layer are collected at regular time intervals for periods up to several days. IV data show changes in power conversion efficiency which are strongly dependent on device preparation (stoichiometry, annealing, etc.). Ultraviolet and visible light absorption exhibits similar time dependence. Recent results show that annealing the active layer up to 200 $^\circ$C substantially improves device performance. Further spectroscopic studies, such as Carbon-13 NMR spectroscopy, are ongoing.

[1]Supported by a Santa Clara University Science, Technology and Society Grant, a grant from IntelliVision and the SCU BIN-REU: funded in part by the UC Santa Cruz BIN-RDI, NASA Grant NNX09AQ44A.

10:36AM H11.00014 Modeling of Quantum Cascade lasers with different waveguide profiles[1] , CHARLES ZHANG, RICHARD CENDEJAS, CLAIRE GMACHL, Princeton University — Quantum Cascade (QC) laser-based sensor systems help us monitor the environment through the detection of trace chemicals that have optical spectra in the mid-infrared. For the laser to become more efficient and usable, the thermal management and the optical and electrical properties of the laser waveguides need to be more closely examined. The performances of QC lasers with different waveguide profiles have so far not been systematically compared and the device optimization for the three design components has not yet been coupled together. Here, we use a finite element solver to calculate the active region peak core temperature, the optical confinement factor and waveguide loss, and the local current density, and compare these for QC lasers with dry- and wet-chemical etch profiles, i.e. with vertical or sloped sidewalls, respectively. Initial results show a preference for wet-etched profiles under thermal conductivity considerations.

[1]This work is supported in part by MIRTHE (NSF-ERC).

10:48AM H11.00015 Photoluminescence studies of WO_3 and WO_{3-x} single crystals , J. EASLEY, Department of Physics, MIT, P. DEY, D. KARAISKAJ, Department of Physics, University of South Florida, S. DEB, NREL, T. CISZEK, Geolite/Siliconsultant, D. DESSAU, University of Colorado, Boulder — WO_3 is an important material to study, not only due to its interesting electronic properties, but also because it has other applications in both electrochromics and energy storage. The mechanism behind the electrochromic effect has been debated for several decades [1]. We have studied two WO_3 single crystals, a transparent and doped WO_{3-x}, in an attempt to understand this effect. A photoluminescence center around 865 nm is observed after sub-band gap excitation at 405 nm with relatively higher intensity in the crystal containing oxygen vacancies. The center appears as a broad transition of 35 nm FWHM and does not appear to be correlated with temperature. However, polarization studies reveal at least two polarization dependent components of the center.

[1] Satyen K. Deb, Solar energy materials and solar cells **92**, 245 (2008), and the references therein

Tuesday, March 22, 2011 8:00AM - 11:00AM –

Session H12 DMP: Focus Session: Dopants and Defects in Semiconductors: Silicon D223/224

8:00AM H12.00001 Isotopic Fingerprints in the Luminescence of Deep Defects in Silicon , MICHAEL L.W. THEWALT, Simon Fraser University — In a series of recent papers [1, 2] we have shown that the dramatic improvements in spectral resolution made possible in highly enriched ^{28}Si can provide surprising new information on the detailed constituents of deep luminescence centers. The 'isotopic fingerprints' reveal the presence, and number, of different chemical species involved in the deep centers. While many of these luminescence centers have been studied for decades, this new technique revealed that *none* of these was what it was thought to be. Armed with this new information, many new centers have been discovered, containing either four or five atoms chosen from among: Cu, Ag, Au, Pt and Li. There is at present no theoretical explanation for the stability and ubiquity of these centers in rapidly thermally quenched silicon.

[1] M. Steger et al., Phys. Rev. B 81, 235217-1-6 (2010).
[2] M. Steger et al., Phys. Rev. Lett. 100, 177402-1-4 (2008).

8:36AM H12.00002 Theoretical study of the Cu_{PL} defect in Si , ALEXANDRA CARVALHO, University of Aveiro, STEFAN K. ESTREICHER, Texas Tech University — Copper is a common contaminant in Si processing. When in supersaturation, a fraction of 1% of the Cu in the sample forms an electrically-active defect easily seen by photoluminescence. This Cu_{PL} defect in Si has a no-phonon line at 1014 meV. It has long been believed to consist of an interstitial copper (Cu_i) weakly bound to a substitutional copper (Cu_s) : The $\{Cu_sCu_i\}$ pair. However, PL studies in isotopically pure ^{28}Si crystals have shown that the defect contains not two but four copper atoms [1]. We examine the possibility that the core of the defect consists of not one but two adjacent substitutional Cu atoms. This core traps two Cu_i atoms, resulting in defect with D_{3d} symmetry. We will discuss its formation mechanism and stability, and show that they are consistent with the conditions at which Cu_{PL} is observed. If this model is correct, then then DLTS lines associated with Cu_s should be re-assigned to $\{Cu_sCu_s\}$.

[1] M. Steger *et al.*, Phys. Rev. Lett. 100, 177402 (2008)

8:48AM H12.00003 EPR parameters of the dangling bond defect in crystalline and amorphous silicon: A DFT-study , GERNOT PFANNER, CHRISTOPH FREYSOLDT, JÖRG NEUGEBAUER, Max-Planck-Institut fuer Eisenforschung, Duesseldorf, Germany — Thin-film a-Si:H solar cells are considered as low-cost alternatives to bulk crystalline silicon (c-Si) solar cells. A disadvantage of these devices is that their efficiency is severely limited by light-induced defects (Staebler-Wronski effect). In this context, electron-paramagnetic resonance (EPR) is a key technique to probe for the local atomic structure of defects with unpaired spins such as the silicon dangling bond. However, the assignment of the EPR signal to a specific defect structure requires comparison to theoretical models. Using density-functional theory, we address structure-property relationships by combining systematic studies for idealized dangling-bond models in c-Si with a statistical analysis of a variety of dangling bonds in a-Si:H supercells. Our studies reveal the influence of the local geometry on sp-hybridization and delocalization. Yet, the structural variability of a-Si:H cannot be captured by these idealized defect models alone. Rather, our calculations indicate that a relatively broad distribution of dangling-bond like structures gives rise to the experimental signal supporting a recent re-evaluation of EPR parameters from multifrequency EPR.

9:00AM H12.00004 Electrically Detected Pulsed ENDOR in Phosphorus-Doped Silicon[1] , FELIX HOEHNE, LUKAS DREHER, Walter Schottky Institut, Technische Universitaet Muenchen, Am Coulombwall 3, 85748 Garching, Germany, HANS HUEBL, Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meissner-Strasse 8, 85748 Garching, Germany, MARTIN STUTZMANN, MARTIN S. BRANDT, Walter Schottky Institut, Technische Universitaet Muenchen, Am Coulombwall 3, 85748 Garching, Germany — We demonstrate the electrical detection of X-band electron nuclear double resonance (ENDOR) in phosphorus-doped silicon at 4 K. A pulse sequence analogous to Davies ENDOR in conventional electron spin resonance is used to measure the nuclear spin transition frequencies of the ^{31}P nuclear spins, where the ^{31}P electron spins are detected electrically via spin-dependent transitions through Si/SiO_2 interface states. In addition, electrical detection of coherent nuclear spin oscillations is shown, demonstrating the feasibility to electrically read out the spin states of possible nuclear spin qubits. Combining the enhanced sensitivity of electrically-detected magnetic resonance and the wide range of applications of pulsed ENDOR, this techniques could be a versatile tool to study paramagnetic defects in semiconductor nanostructures.

[1]This work was supported by the DFG (Grant No. SFB 631, C3).

9:12AM H12.00005 Electroelastic Hyperfine Tuning of Phosphorus Donors in Silicon[1] , LUKAS DREHER, TIMON A. HILKER, Walter Schottky Institut, Technische Universitaet Muenchen, Am Coulombwall 3, 85748 Garching, Germany, ANDREAS BRANDLMAIER, SEBASTIAN T.B. GOENNENWEIN, HANS HUEBL, Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meissner-Strasse 8, 85748 Garching, Germany, MARTIN STUTZMANN, MARTIN S. BRANDT, Walter Schottky Institut, Technische Universitaet Muenchen, Am Coulombwall 3, 85748 Garching, Germany — We demonstrate an electroelastic control of the hyperfine interaction between nuclear and electronic spins opening an alternative way to address and couple spin-based qubits. The hyperfine interaction is measured by electrically detected magnetic resonance in phosphorus-doped silicon epitaxial layers employing a hybrid structure consisting of a silicon-germanium virtual substrate, a piezoelectric actuator, and a loop-terminated coplanar strip line for on-chip microwave magnetic-field generation. By applying a voltage to the actuator, the hyperfine interaction is changed by up to 0.9 MHz, which would be enough to address spin-qubits in isotopically purified ^{28}Si with a sufficient fidelity under optimized conditions.

[1]This work was supported by the DFG (Grant No. SFB 631, C3).

9:24AM H12.00006 Characterizing Individual Group V donors in Silicon , CYRUS F. HIRJIBEHEDIN, PHILIPP STUDER, STEVEN R. SCHOFIELD, VERONIKA BRAZDOVA, DAVID R. BOWLER, NEIL J. CURSON, UCL, UK — The study of dopants in silicon has been rapidly growing in importance because the dimensions of semiconductor devices have now decreased to the point where their functionality relies upon only a few atoms. Group V donors are especially interesting due to their potential application in spintronics and quantum computing. Whereas P dopants have been extensively studied, comparatively little is known about the characteristics of other group V donors. Using a combination of ion implantation and cross-sectional scanning tunneling microscopy (XSTM) and, we study individual Bi and Sb atoms in the cleaved Si(111)2x1 surface. High-resolution STM topography images and scanning tunneling spectroscopy (STS) data allow us to probe the structural and electronic properties of these individual dopants in silicon. Density functional theory (DFT) calculations further support our structural assignments.

9:36AM H12.00007 Ab initio shallow impurity level calculations in semiconductors , GAIGONG ZHANG, UC Davis, ANDREW CANNING, NIELS JENSEN, UC Davis/ LBNL, STEPHEN DERENZO, LIN-WANG WANG, LBNL — Binding energies of B, Al, Ga, In and Tl shallow acceptors in bulk Si were calculated using a GW + Semi-empirical procedure. Within the procedure, both density functional theory calculation within local density approximation (LDA) and GW calculation were performed. In the LDA calculation, a large supercell containing tens of thousands of Si atoms and the center impurity atom was constructed from a potential patching procedure. The central potential of this system was further corrected by 64 atom GW calculations. The folded spectrum method was used to calculate the eigen energies of this large supercell containing the center impurity. The calculated binding energies show good agreement with experimental impurity binding energies. This procedure represents an efficient approach to study shallow impurity levels which are important for semiconductor devices.

9:48AM H12.00008 First principles study of phosphorus and boron defects in Si-XII[1] , BRAD D. MALONE, MARVIN L. COHEN, Department of Physics, University of California, Berkeley, and Materials Science Division, Lawrence Berkeley National Laboratory — We present a first-principles study of phosphorus and boron substitutional defects in Si-XII, a polytype of silicon in the R8 structure. Recent results from nanoindentation experiments reveal that this phase is semiconducting and has the interesting property that it can be doped n- and p-type at room temperature without an annealing step. We examine the formation energies of the B and P defects at the two distinct atomic sites in the R8 structure. We also calculate the thermodynamic transition levels of each defect in its relevant charge states.

[1]This work was supported by National Science Foundation Grant No. DMR10-1006184, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by the Lawrencium cluster at LBNL.

10:00AM H12.00009 Stability of donor-pair defects in $Si_{1-x}Ge_x$ alloy nanowires , JI-SANG PARK, BYUNGKI RYU, K.J. CHANG, Department of Physics, Korea Advanced Institute of Science and Technology — Semiconductor nanowires (NWs) have attracted much attention because of the quantum confinement effect, large surface-to- volume ratio, and compatibility with the existing Si technology. Although impurity doping is important for applications to optoelectronic devices, it is generally difficult to dope nanostructures due to segregation of dopants to the surface, high activation energies induced by the surrounding low dielectric medium, and compensation by defects such as surface dangling bonds. Furthermore, compared with bulk Si, electrically deactivating donor-pair defects are energetically more favorable than isolated shallow donors in NWs. In this work, we perform first-principles density functional calculations to study the stability of donor-pair defects and the doping efficiency in $Si_{1-x}Ge_x$ alloy NWs doped with P impurities. The stability of donor-pair defects is enhanced as the Ge concentration increases. Consequently, the doping efficiency in $Si_{1-x}Ge_x$ alloy NWs is expected to be suppressed by the formation of donor-pair defects, similar to previous calculations for Si NWs with small diameters. The effects of reduced dimensionality, Ge chemical bonding, and strain on the stability of donor-pair defects in alloy NWs are discussed.

10:12AM H12.00010 New electronic effects observed on n-type Si(111)2x1 using cross-sectional STM , NEIL J. CURSON, PHILIPP STUDER, STEVEN R. SCHOFIELD, GREG LEVER, DAVID R. BOWLER, CYRUS HIRJIBEHEDIN, UCL, UK — Cross-sectional scanning tunneling microscopy (XSTM) of in-situ cleaved semiconductor surfaces has two distinct advantages over STM experiments where studies are performed on the surface of the annealed and/or sputtered semiconductor wafers. Firstly, the cleaving process exposes a clean surface without the usual need for high temperature annealing, thus revealing a surface that has not been driven to its thermodynamic minimum energy state. Secondly, the surface being imaged is perpendicular to the surface of the original wafer, which is of particular value for the study of implanted or epitaxially overgrown wafers. We use XSTM measurements, spatially resolved scanning tunneling spectroscopy (STS) and density functional theory (DFT) to study the electronic properties of the cleaved (111)2x1 surface of silicon. We examine bulk-doped, and ion-implanted samples. Our studies reveal new, long range, electronic effects that have implications for future nanoscale devices in silicon.

10:24AM H12.00011 Charged Defects in the Si(001) Surface , STEVEN SCHOFIELD, London Ctr. Nanotech. and Dept. Phys. & Astron., UCL, London, UK, PHILIPP STUDER, London Ctr. Nanotech. and Dept. Electron. & Elec., UCL, London, UK, CYRUS HIRJIBEHEDIN, London Ctr. Nanotech., Dept. Phys. & Astron. and Dept. Chem., UCL, London, UK, NEIL CURSON, London Ctr. Nanotech. and Dept. Electron. & Elec., UCL, London, UK, GABRIEL AEPPLI, DAVID BOWLER, London Ctr. Nanotech. and Dept. Phys. & Astron., UCL, London, UK — The Si(001) surface has been the subject of intense research for decades due to its ubiquitous use in the semiconductor industry, its applicability as a model semiconductor surface, and proposals for its use in novel quantum devices. Surprisingly, atomic-scale investigations using scanning tunneling microscopy and spectroscopy (STM/STS) continue to produce new insights into the structural and electronic properties of this deceptively simple semiconductor surface. Tip- and charge-induced band bending are generally considered to play only minor roles in measurements of silicon surfaces due to Fermi level pinning by surface states and defects. However, such effects become important when investigating charged defects and/or surfaces that have had their surface states removed through chemical passivation. We present high resolution STM images and spectroscopy data of defects in the Si(001) surface. We include band bending and charge state in the discussion of the results.

10:36AM H12.00012 Near surface dopant depletion in UHV prepared H-Si(100): spectroscopic and imaging effects , JASON PITTERS, NINT-NRC, ROBERT WOLKOW, University of Alberta — Dangling bonds (DBs) have been shown to be useful in directing chemical reactions on silicon and for atom scale electronics such as quantum cellular automata. One enabling aspect of DBs is that they can assume various charge states depending on the type and level of crystal doping. We have found that for degenerately doped n-type silicon, the scanning tunneling spectroscopy (STS) and imaging characteristics H-Si(100) surfaces and DBs varies depending on the preparation method. Samples heated to 1050°C were found to have a consistent level of doping throughout the bulk and near surface regions. Samples heated to 1250°C showed a reduced dopant concentration in the near surface region. STS showed shifted I/V spectra. The loss of degeneracy was indicated by the loss of tunneling through dopant states in the band gap. These results show that UHV prepared silicon does not have a consistent dopant profile and that the bulk dopant density should not be assumed in the near surface region. This has important ramifications for DB imaging and modeling.

10:48AM H12.00013 Ab initio study of water molecule dissociation on the hydrogenated Si(100) surface[1] , MARILIA J. CALDAS, REGINA LELIS-SOUSA, Institute of Physics, University of Sao Paulo — The reaction mechanisms for the H_2O molecule dissociation at the Si surface, and the resulting oxidation sites, are still object of debate. Here, we present a detailed theoretical investigation of the reaction pathways for the dissociation of water on the Si(100)(2x1):H surface, starting from different initial "attack" sites and leading to different final, oxidized configurations. We use extended-surface (slab) models, working within DFT, with pseudo-potentials and plane wave basis set in the quantum-espresso code. The pathways were mapped using the CI-NEB method with both local and gradient corrected exchange-correlation functionals in order to obtain a fair estimate of energy barriers. Our results indicate that the oxidation routes suggested by earlier experimental works are not favored. We propose two new oxidation routes, with simultaneous release of one H2 molecule: one related to chemisorption of the oxygen atom on the Si-Si dimer bond, and another related to the absorption on the back-bond. Analysis of energy barriers showed that these two new possibilities are both kinetically and energetically viable. We also present analyses of the profiles obtainable through STM for the investigated structures, which should help experimental identification.

[1]We acknowledge support from CNPq and FAPESP, Brazil.

Tuesday, March 22, 2011 8:00AM - 11:00AM –
Session H13 GSNP: Focus Session: Jamming Theory and Experiment I D225/226

8:00AM H13.00001 Jamming in Disordered and Ordered States: From RLP to FCC[1] , LEONARDO SILBERT, Southern Illinois University — The concept of jamming was originally introduced in the context of zero-temperature, frictionless sphere packings through which the jamming transition was identified with the more familiar idea of random close packing. More recently, the jamming behaviour for particles with friction has led to a practical definition of the less well-defined random loose packed limit. However, there are a number of subtleties associated with jamming that extend these concepts further. Here we implement a range of protocols to generate jammed packings both with and without friction, and find that the jamming transition actually consists of a finite region in packing fraction depending on the protocol used to create the jammed state. Furthermore, we examine how it is possible to tune the structural properties of jammed packings from the disordered regime through to the ordered face centred cubic lattice, and the subsequent changes in the jamming properties as the structure is manipulated.

[1]Supported by NSF CBET-0828359

8:36AM H13.00002 Long wavelength behavior of the static structure factor in jammed packings , JAIME BOHORQUEZ-BALLEN, LEONARDO SILBERT, Southern Illinois University Carbondale — There are several features associated with the jamming transition in monodisperse sphere packings. One recently reported property is the anomalous long wavelength behavior of the static structure factor, $S(k)$. An unusual linear dependence with the wavenumber k, becomes increasingly pronounced on approach to the jamming transition. However, it remains unclear how polydispersity and force model affect this behavior. Here, we study the structure factor of jammed disordered bidisperse sphere packings using computer simulations, especially its behavior in the long wavelength regime ($k \to 0$). We evaluated the structure factor using an appropiate formalism for polydisperse systems and extract information on the susceptibility in the low-k limit.

8:48AM H13.00003 Topology of the force field in a jammed granular systems exposed to an intruder[1] , LOU KONDIC, XIAONI FANG, NJIT, MIROSLAV KRAMAR, KONSTANTIN MISCHAIKOW, Rutgers, COREY O'HERN, Yale, JIE ZHANG, ROBERT BEHRINGER, Duke — It is well known that the structure of forces and stresses in granular systems goes through significant changes close to jamming. In this talk, we will present precise and objective measures of these changes based on topological properties of the force field in granular systems exposed to compression and shear. Then, we will discuss how these measures evolve in granular systems during an impact of a large intruder. We will particularly concentrate on the role of packing, polydispersity, and friction on structure of the force field.

[1]Supported by NSF Grant. No. DMS-0835611 and DTRA Grant No. 1-10-1-0021

9:00AM H13.00004 Critical Scaling of Shearing Rheology at the Jamming Transition of Soft Core Frictionless Disks[1]

, STEPHEN TEITEL, University of Rochester, PETER OLSSON, Umeå University — We perform numerical simulations to determine the shear stress and pressure of steady-state shear flow in a soft-disk model in two dimensions at zero temperature in the vicinity of the jamming transition ϕ_J. We use critical point scaling analyses to determine the critical behavior at jamming, and we find that it is crucial to include *corrections to scaling* for a reliable analysis. We find that the relative size of these corrections are much smaller for pressure than for shear stress. We furthermore find a superlinear behavior for pressure and shear stress above ϕ_J, both from the scaling analysis and from a direct analysis of pressure data extrapolated to the limit of vanishing shear rate.

[1]Supported by DOE Grant No. DE-FG02-06ER46298, Swedish Research Council Grant No. 2007-5234, and a grant from the Swedish National Infrastructure for Computing (SNIC) for computations at HPC2N.

9:12AM H13.00005 Glassiness, Rigidity and Jamming of Frictionless Soft Core Disks[1]

, STEPHEN TEITEL, University of Rochester, DANIEL VÅGBERG, PETER OLSSON, Umeå University — The jamming of frictionless bi-disperse soft core disks is considered, using a variety of different protocols to produce the jammed state. We find, consistent with earlier works, that cooling and compression can lead to a broad range of jamming packing fractions ϕ_J, depending on cooling or compression rate and on initial configuration. Such ϕ_J show no clear upper bound as the cooling or compression rate decreases. In contrast, we show that shearing leads to a jamming transition to a disordered solid, with a well-defined, non-trivial, value of ϕ_J as the shearing rate vanishes. We show that shearing breaks up the particle clustering (the precursor to phase separation) that can lead to increasing values of ϕ_J under slow cooling or compression, and argue that the process of shearing creates a well-defined ensemble that is independent of the starting configuration.

[1]Supported by DOE Grant No. DE-FG02-06ER46298, Swedish Research Council Grant No. 2007-5234, a grant from the Swedish National Infrastructure for Computing (SNIC) for computations at HPC2N and the Univer. of Rochester Center for Research.

9:24AM H13.00006 Exact tools for 2D granular packings

, ERIC DEGIULI, NEIL BALMFORTH, Dept. of Mathematics, University of British Columbia — Building on the loop force formulation of Ball and Blumenfeld[1], a new, exact potential formulation is given for two dimensional, static packings of frictional, monodisperse disks. Using degree-of-freedom counting and explicit constructions, it is shown that the natural graph for analysis of stress distribution in such packings is the Delaunay triangulation. Edges of this graph which do not correspond to contacts yield "virtual contact" vectors, which are shown to be of great physical importance. In particular, the new potential satisfies force and torque balance identically and is subject only to the Coulomb constraint and a new set of physically transparent constraints on the "virtual contacts." Using the new coordinates, previous results on the contact force distribution are rationalized, and a unified framework is presented for understanding the sources of correlation between contact forces. A new maximum-entropy argument is presented to derive the contact force distribution, and the dependence on shear, friction, and coordination number is discussed.

[1]PRL 88 115505, 2002

9:36AM H13.00007 Particle-to-Particle Dynamics in a Granular Pile Subject to Cyclic Shear

, STEVEN SLOTTERBACK, WILLIAM UPDEGRAFF, University of Maryland, MARTIN VAN HECKE, Universiteit Leiden, WOLFGANG LOSERT, University of Maryland — We report a study of the particulate motions of a granular pile under cyclic shear and how they relate to the bulk rheological properties of the pile. Using a laser sheet scanning technique, we track the trajectories of all of the particles within a section of a split-bottom shear cell. We shear the pile quasistatically to ensure rate independence of shear stress. Immediately after reversal of the shear direction, we observe a transient drop in shear stress of the pile over a characteristic strain. We construct a network of nearest neighbors that roll or slide past one another between frames. We find that, for strain amplitudes less than the aforementioned characteristic strain, rolling/sliding links are extinguished with higher frequency than for larger amplitudes. We also report other particle level measures, such as mean squared displacements, for various amplitudes of oscillatory shear.

9:48AM H13.00008 Ratio of effective temperature to pressure controls the dynamics of sheared hard spheres

, THOMAS HAXTON, Molecular Foundry, Lawrence Berkeley National Laboratory, ANDREA LIU, Department of Physics and Astronomy, University of Pennsylvania — Using molecular dynamics simulations, we calculate the effective temperature, $T_{\rm eff}$, and the pressure, p, of steadily sheared mixtures of hard spheres of mass m and diameters σ and 1.4σ in contact with a thermal reservoir at temperature T. We vary the packing fraction, ϕ, and the shear stress, Σ. We define $T_{\rm eff}$ from the ratio of correlations to response and show that different correlation-response relations yield a consistent numerical value $T_{\rm eff} \geq T$ that reduces to $T_{\rm eff} = T$ when $\Sigma = 0$. We show that the effective temperature represents the limiting value of the effective temperature for soft spheres in the limit $p\sigma^3/\epsilon \to 0$, where ϵ is the repulsive energy scale. We find that the dimensionless ratio $T_{\rm eff}/p\sigma^3$ controls the dynamic jamming transition that occurs with decreasing shear stress and increasing packing fraction. In particular, we find that the dependence of the dimensionless relaxation time, $\tau\sqrt{p\sigma/m}$, on $T_{\rm eff}/p\sigma^3$ as shear stress is varied is quantitatively similar to the dependence of $\tau\sqrt{p\sigma/m}$ on $T/p\sigma^3$ in equilibrium.

10:00AM H13.00009 Shear-jammed states in granular materials[1]

, DAPENG BI, Brandeis University, JIE ZHANG, Indiana University - Purdue University Fort Wayne, R.P. BEHRINGER, Duke University, BULBUL CHAKRABORTY, Brandeis University — For frictionless particles with purely repulsive interactions, there is a critical packing fraction ϕ_J below which no jammed states exist. Experiments by Zhang & Behringer on physical granular systems show jammed states in the regime of $\phi < \phi_J$ can be created by the application of shear stress. Compared to the states above ϕ_J, the shear-jammed states are mechanically more fragile, but they resist shear. These shear-jammed states cannot exist under isotropic stress. Rather, their formation require the anisotropic contact network as a backbone which is created by an applied shear stress. The anisotropic components of the stress tensor and contact network fabric tensor form a classic hysteresis loop suggesting an analogy to ferromagnetic behavior and critical phenomena. These new states must be incorporated into a more general jamming picture. We also carry out extensive analysis on shear-jammed states and find local stress fluctuations are controlled by their respective global pressures. To explain the scaling of local stress fluctuations, we construct a mean-field model based on the entropy of stress configurations.

[1]Supported by NSF-DMR0905880 and NSF-DMR0906908.

10:12AM H13.00010 Quasistatic flows near jamming: The role of inertia and dissipation

, CRAIG MALONEY, Carnegie Mellon University, Department of Civil and Environmental Engineering, PETER TROCHA, Carnegie Mellon Univeristy, Department of Civil and Environmental Engineering — We perform massively parallel computer simulations of granular particles at fixed shearing rate and density near the onset of jamming. The microscopic dynamical model contains two types of damping; one which damps the *absolute* motion of a particle with respect to a homogeneously shearing background (as in SLLOD type approaches) and another which damps the *relative* motion of a particle with respect to its near-neighbors (as in discrete element approaches). We study how the damping mechanism and its strength affects the collective particle dynamics through the statistics of local particle displacements and local strains. In particular, we show that for strong, *absolute* damping, the single particle displacement statistics can be similar for systems at different distances from jamming while the short-time plastic activity can vary dramatically.

10:24AM H13.00011 Viscoelastic response near the jamming transition[1] , BRIAN TIGHE, Lorentz Institute, Leiden University — We use numerical and theoretical methods to investigate oscillatory rheology in soft sphere packings, which serve as a minimal model for foams, emulsions, and other complex fluids that undergo a jamming transition. Although the zero frequency (elastic) properties of jammed media are well documented, far less is known about their viscoelastic response. We demonstrate that the frequency-dependent storage and loss moduli display critical scaling with distance to the jamming point. This behavior is governed by a diverging time scale that separates quasistatic response from a critical regime in which viscous and elastic forces contribute equally to the stress. We provide scaling arguments for all of the relevant critical exponents.

[1]Supported by the Dutch Organization for Scientific Research.

10:36AM H13.00012 Phase transition kinetics in the site dilute Ising model[1] , KANG LIU, CHRISTOPHER SERINO, Boston University, RANJIT CHACKO, Clark University, WILLIAM KLEIN, Boston University — We consider the phase transition kinetics of a quenched site dilute Ising model. To date, most studies of this model have focused on dilution-averaged quantities, such as the critical temperature and the associated critical exponents. In this talk we study how the spatial distribution of the dilution affects the local growth of the stable phase after an instantaneous quench. For an off critical quench, we find growth occurs most rapidly in areas of increased dilution for both unstable state decay and nucleation. Conversely, growth after a critical quench is accelerated in environments with relatively few vacant sites. Additionally, we consider the role of the range of interaction in these processes.

[1]The authors wish to thank the DOE for support through grant DE-FG02-95ER14498.

10:48AM H13.00013 A first-order phase transition defines the random close packing of hard spheres , YULIANG JIN, HERNAN MAKSE, The City College of New York — Randomly packing spheres of equal size into a container consistently results in a static configuration with a density of ∼64%. The ubiquity of random close packing (RCP) rather than the optimal crystalline array at 74% begs the question of the physical law behind this empirically deduced state. Indeed, there is no signature of any macroscopic quantity with a discontinuity associated with the observed packing limit. Here we show that RCP can be interpreted as a manifestation of a thermodynamic singularity, which defines it as the "freezing point" in a first-order phase transition between ordered and disordered packing phases. Despite the athermal nature of granular matter, we show the thermodynamic character of the transition in that it is accompanied by sharp discontinuities in volume and entropy. This occurs at a critical compactivity, which is the intensive variable that plays the role of temperature in granular matter. This approach is useful since it maps out-of-equilibrium problems in complex systems onto simpler established frameworks in statistical mechanics.

Tuesday, March 22, 2011 8:00AM - 11:00AM –

Session H14 DMP GSNP DCOMP: Focus Session: Friction, Fracture and Deformation Across Length Scales I: Sliding Friction and Asperities D227

8:00AM H14.00001 Nanoscale friction anisotropy controlled by interface inhomogeneous slip and lattice defects[1] , SHUNFANG LI, Zhengzhou U., U. of Tennessee, ZHENYU ZHANG, Oak Ridge Nat. Lab, U. of Tennessee, YANFEI GAO, U. of Tennessee, Oak Ridge Nat. Lab — Stick-slip behavior observed from nanoscale asperity friction experiments is often simulated by the one-degree-of-freedom Tomlinson model, which is unable to explain well the effects of lattice structure and interface defects, particularly the friction anisotropy. Using our recently developed Rice-Peierls framework, we study the relative sliding of two elastic half-spaces with a circular contact for two types of interplanar potential: i) triangular lattice potential (3-fold); ii) rectangle potential (2-fold). Our major findings are as follows: first, one can construct friction anisotropy from the interface interaction potential; second, one can modulate the friction anisotropy by controlling the sliding direction and the ratio of contact radius to lattice spacing. We identify that for both cases, when a/b is small, the frictional behavior approaches the Tomlinson limit, while, when a/b is large, the frictional behavior is governed by interface defects. The latter case and its resulting friction anisotropy are very sensitive to the degree of interface incommensurability.

[1]Sponsored by USNSF, DMSE/BES of USDOE, and NSF of China.

8:12AM H14.00002 Frictional Sliding of Amorphous Contacts over Six Decades of Velocity[1] , MICHAEL FALK, Johns Hopkins University, WOO KYUN KIM, University of Minnesota — Our understanding of the nanoscale origins of sliding friction primarily arises from theories of idealized crystalline surfaces in contact. However, many if not most tribological interactions involve one or more surfaces that are disordered in structure. The role that the amorphous nature of these surfaces plays in mediating friction is poorly understood. We apply an emerging simulation methodology, hyperdynamics, for the first time to friction, examining sliding between an oxidized silicon tip and surface over a previously inaccessibly wide range of sliding velocities. The simulations replicate interesting temperature dependent change in the velocity dependence of the friction force observed in this system experimentally, and reveal the nature of the intermediate state-switching transitions responsible for this behavior. A theory based on these transitions is developed and used to describe the experimental and simulated data. We conclude that this type of transition must be quite common in frictional sliding when one or more of the involved surfaces are not perfectly crystalline.

[1]Supported by NSF ENG CMMI-0926111

8:24AM H14.00003 Sliding Over a Phase Transition[1] , ERIO TOSATTI, SISSA, ICTP, CNR-IOM-Democritos, Trieste, Italy, ANDREA BENASSI, CNR-IOM-Democritos, Trieste, Italy, ANDREA VANOSSI, SISSA and CNR-IOM-Democritos, Trieste, Italy, GIUSEPPE E. SANTORO, SISSA, ICTP, CNR-IOM-Democritos, Trieste, Italy — The frictional response experienced by a stick-slip slider when a phase transition occurs in the underlying solid substrate is a potentially exciting, poorly explored problem. We show, based on 2-dimensional simulations modeling the sliding of a nanotip, that indeed friction may be heavily affected by a continuous structural transition. First, friction turns nonmonotonic as temperature crosses the transition, peaking at the critical temperature T_c where fluctuations are strongest. Second, below Tc friction depends upon order parameter directions, and is much larger for those where the frictional slip can cause a local flip. This may open a route towards control of atomic scale friction by switching the order parameter direction by an external field or strain, with possible application to e.g., displacive ferroelectrics such as $BaTiO_3$, as well as ferro- and antiferro-distortive materials.

[1]Supported by project ESF FANAS/AFRI sponsored by the Italian Research Council (CNR).

8:36AM H14.00004 Onset of Sliding in Single Asperity Contacts[1] , VINCENT LIGNERES, MARK ROBBINS, Johns Hopkins University — Continuum models of friction often assume that sliding initiates at the edge of a contact, and gradually spreads across the contact. However these partial slip models make simple assumptions about friction laws and must break down at atomic scales. Molecular dynamics simulations are used to analyze the nature of atomistic effects and the variation of partial slip with length scale. In continuum theory there are singularities in tangential force at the edge of the contact that initiate slip. The discrete spacing between atoms and interfacial elasticity reduce these singularities in small contacts. Elastic coupling within the contact also limits partial slip and favors coherent slip across the interface. The variation of these effects with length scale, atomic geometry and the presence of adsorbed monolayers is described.

[1]This material is based upon work supported by the Air Force Office of Scientific Research under Grant No. FA9550-0910232

8:48AM H14.00005 Finite size effects at high speed frictional interfaces[1] , J.E. HAMMERBERG, R. RAVELO, T.C. GERMANN, B.L. HOLIAN, Los Alamos National Laboratory — Non-Equilibrium Molecular Dynamics simulations have exhibited characteristic velocity weakening for the tangential frictional force at smooth single crystal interfaces for velocities greater than a critical velocity, v_c. This behavior has been seen in a number of material pairs including Cu-Ag, Ta-Al and Al-Al. Expressions for v_c that characterize this behavior depend on system size. We discuss the size dependence for Al-Al single crystal interfaces for two cases: an Al(111)/Al(001) interface sliding along [1-10],N=1.5M, and an Al(110)[001]/Al(110)[1-10] interface sliding along [001], N=$7.5\text{x}10^6$ corresponding to a three-fold increase in system size normal to the sliding direction. We find agreement with an inverse size scaling for v_c. We discuss the similarities in behavior for a highly defective plastically deformed sample with Al(110)[001]/Al(110)[1-10] orientation having the same normal dimension and N= $16.0\text{x}10^6$.

[1]This work supported by the U.S. Department of Energy under contract DE-AC52-06NA25396.

9:00AM H14.00006 The Tribological Properties of Nanocrystalline Metals , MICHAEL CHANDROSS, SHENGFENG CHENG, Sandia National Laboratories — Materials that perform well in electrical contacts usually exhibit high adhesion during frictional contacts. An excellent example of this phenomenon is pure gold, which has extremely low electrical contact resistance, but generally has a high friction coefficient. The exception to this, however, is nanocrystalline gold alloyed with minute amounts of Ni or Co, which in addition to its low contact resistance can also show low friction. The mechanism for this remains poorly understood. We carried out large scale molecular dynamics (MD) simulations to study the tribological response of both single crystal and nanocrystalline gold or silver films in contact with curved probe tips or flat slabs under a variety of sliding conditions. Results show that grain reorientation and coalescence across the contact interface under compressive load or during shearing are responsible for the observed high friction in these contacts. In metallic alloys of silver, the addition of other elements such as copper introduces lattice mismatch and hinders the grain coalescence, which reduces friction during sliding.

9:12AM H14.00007 Tribo-induced melting transitions at sliding tungsten/gold-nickel asperity contacts , LIMING PAN, Department of physics, North Carolina State University, DANIEL LICHTENWALNER, Department of Materials Science and Engineering, North Carolina State University, ANGUS KINGON, Brown University, JACQUELINE KRIM, Department of Physics, North Carolina State University — Tribo-induced nanoscale surface melting mechanisms have been investigated by means of a combined QCM-STM technique [1] for a range of Au and Au-Ni alloys with varying compositional percentages and phases. A transition from solid- solid to solid-"liquid like" contact[1] was observed for each sample at sufficiently high asperity sliding speeds. Pure gold, solid-solution and two-phase Au-Ni (20 at.% Ni) alloys were compared, which are materials of great relevance to MEMS RF switch technology [2]. The transition points agree favorably with theoretical predictions for their surface melting characteristics. We acknowledge NSF and AFOSR support for this research.

[1] B. D. Dawson, S. M. Lee, and J. Krim, Phys. Rev. Lett. 103, 205502 (2009)
[2] Zhenyin Yang; Lichtenwalner, D.J.; Morris, A.S.; Krim, J.; Kingon, A.I, Journal of Microelectromechanical Systems, April 2009, Volume: 18 Issue:2, 287-295

9:24AM H14.00008 *In-situ* study of AFM tip wear by contact resonance force microscopy , JASON KILLGORE, ROY GEISS, DONNA HURLEY, National Institute of Standards & Technology — The size and shape of an atomic force microscope (AFM) tip strongly influence the resolution and accuracy of the instrument. Here we present a new means to directly measure tip wear *in situ* during contact-mode AFM scanning. Tip wear is observed from changes in contact radius determined by contact resonance force microscopy (CR-FM). In CR-FM, a flexural eigenmode of the cantilever is excited and tracked while the tip is in contact with a sample. As the tip wears, the resonant frequency increases, corresponding to increased contact radius. We demonstrate excellent agreement between quantitative tip wear results from CR-FM and from established *ex-situ* techniques such as scanning electron microscope imaging. Even for compliant cantilevers scanned at very low forces, we are able to resolve subnanometer changes in contact radius. Overall, benefits of our wear-monitoring approach are that CR-FM provides quantitative values of contact radius, allows continuous measurements, affords high spatial resolution, and does not adversely influence the wear rate.

9:36AM H14.00009 A physical basis for frictional ageing using single-asperity measurements , QUNYANG LI, University of Pennsylvania, DAVID GOLDSBY, TERRY TULLIS, Brown University, ROBERT CARPICK, University of Pennsylvania — Rate and state friction laws are widely used to model laboratory data and reproduce a variety of phenomena in earthquake modeling, and in other multi-asperity contacts. However, these laws lack a physical basis. To identify mechanisms underlying the time dependence of friction, especially the ageing effect, atomic force microscopy (AFM) was employed to probe friction for nanometer-scale single asperity contacts between oxidized silicon AFM tips and a set of substrates. Similar to macroscopic rock friction experiments, 'slide-hold-slide' (SHS) experiments on silica revealed a linear increase in friction with the log of the hold time. However, SHS experiments on chemically inert substrates showed little to no ageing. This indicates that the ageing mechanism is related to interfacial chemical reactions, and not plastic deformation of asperities. Ageing in silica-silica contacts is more than an order of magnitude higher than for macroscopic interfaces. However, modeling of slip in multi-asperity contacts suggests that the single- and multi-asperity results agree, since the magnitude of the ageing effect in multi-asperity contacts is reduced by asperity interactions. These results provide the first asperity-level insights into possible mechanisms behind rate and state friction laws.

9:48AM H14.00010 Friction at the nanoscale:theory and experiment , MICHAEL MARDER, The University of Texas at Austin — Bowden and Tabor established more than 50 years ago that friction is due to populations of asperities. In recent years, increasingly detailed experiments have begun to document the dynamics of these asperities during sliding, and to show that several different modes of motion are possible. I will discuss experiments that probe slipping motion of macroscopic samples down to the nanoscale, and show that the small slow slipping motions are described by the rate and state theory of friction that was developed for very different length and time scales.

10:24AM H14.00011 Stiffness of Contacts of Self-Affine Surfaces[1] , TRISTAN A. SHARP, MARK O. ROBBINS, SREEKANTH AKARAPU, Johns Hopkins University — The presence of roughness on a wide range of scales has a profound effect on the contact area and interfacial stiffness between contacting surfaces. In turn, the interfacial stiffness dominates the response of many macroscopic systems. Molecular dynamics simulations are used to characterize contacts between self-affine fractal surfaces with different roughness exponents. A unified framework describes the relation between roughness, system size, surface separation, stiffness, and contact area for a wide variety of systems. The contact area and normal stiffness rapidly approach Persson's continuum theory with increasing system size [1]. The lateral stiffness and friction are much more sensitive to atomic-scale effects. Atomic scale displacements at the interface can greatly reduce lateral stiffness and may explain the low lateral stiffness observed in some experiments.

[1] B. N. J. Persson Phys. Rev. Lett. 99, 125502 (2007).

[1]This material is based upon work supported by the Air Force Office of Scientific Research under Grant No. FA9550-0910232

10:36AM H14.00012 Stick-Slip and the Transition to Sliding in a 2D Granular Medium and a Fixed Particle Lattice[1] , ROBERT BEHRINGER, Duke University, JACKIE KRIM, NC State University — We report an experimental study of stick-slip to steady sliding for a solid object pulled via a spring across 2D granular substrates of photoelastic disks that are either fixed in a solid lattice or unconstrained, i.e. a disordered granular bed. We observe a progression of friction regimes with increasing sliding speed: single, mixed, and double slip-stick regimes, steady sliding, and inertial oscillations. For the granular bed, we characterize frictional behavior for the low speed stick-slip regime, including spring and elastic energy dependencies. For the granular solid, we explore friction with/without externally applied vibrations, and compare to sliding on a granular bed. We find that external vibration reduces transition values for both the single to double slip transition and the stick-slip to steady sliding transition. Moreover, we observe that the effect of packing disorder on granular friction appears similar to the effect of vibration induced disorder, a result that to our knowledge has not been reported previously in the experimental literature.

[1]Support from US ARO grant W911NF-07-1-1031 and NSF grant DMR0906908

10:48AM H14.00013 A simple model fault system[1] , CHRISTOPHER SERINO, WILLIAM KLEIN, Boston University — The Gutenberg-Richter distribution, which characterizes the frequency-magnitude statistics collected over earthquake fault systems, has lead seismologists as well as physicists and geophysicists to propose various simple models to explain this empirical scaling relation. To date, these models have been limited to the description of a single fault. We discuss a model of an earthquake fault system made up of non-interacting faults that are represented as damaged, Olami-Feder-Christensen models. The frequency-magnitude statistics do not, in general, scale on a single fault with some realization of damage; however, these statistics follow a simple distribution that can also be used to describe the data collected from actual earthquake faults. What is more, by varying the amount of damage on each fault in the system, as well as the relative frequency with which a fault with a given amount of damage occurs within the system, we obtain a one-parameter family of models, all of which produce Gutenberg-Richter-like statistics. This parameter is a measure of the stress dissipation within the fault system, a quantity known to vary with various geological properties, and offers an explanation for the range of b-values observed by seismologists.

[1]The authors wish to thank the DOE for support through grant DE-FG02-95ER14498.

Tuesday, March 22, 2011 8:00AM - 10:48AM –

Session H15 DMP GMAG FIAP: Focus Session: Spins in Semiconductors - Ferromagnetic Semiconductors D171

8:00AM H15.00001 Interplay of confinement and spin-orbit interaction in ferromagnetic semiconductors , TOMASZ DIETL, Institute of Physics, PAS; University of Warsaw, Poland — We review experimental and theoretical works which show a surprising influence of confinement on properties of III-V ferromagnetic semiconductors related to the spin-orbit interaction. In particular, according to SQUID studies, magnetization of (Ga,Mn)As thin films show two distinct components of orthogonal in-plane easy axes, whose relative strength can be controlled by the gate voltage [M. Sawicki et al. Nature Phys. 6, 22 (2010)]. Furthermore, in high T_C structures a confinement leads to an unanticipated collapse of the anomalous Hall effect [D. Chiba et al. Phys. Rev. Lett. 104, 106601 (2010)]. A possibility of a non-trivial interplay of confinement and spin orbit interaction is further highlighted by the theoretical prediction of a non-collinear spin arrangement in thin films of (Ga,Mn)As [A. Werpachowska and T. Dietl, Phys. Rev. B 82, 085204 (2010)]. Finally, we show how a large energy separation between the heavy and light hole subbands in compressively strained gated InAs:Mn quantum wells leads to hysteretic behavior even in the single Mn impurity limit [U. Wurstbauer et al. Nature Phys. (2010) doi:10.1038/nphys1782].

8:36AM H15.00002 Room Temperature Ferromagnetism in GaN-AlN Quantum Confined Heterostructures[1] , T.F. KENT, J. YANG, L. YANG, S.D. CARNEVALE, B. NILES, Department of Materials Science and Engineering, The Ohio State University, D.R. HOY, Y.-H. CHIU, E. JOHNSTON-HALPERIN, Department of Physics, The Ohio State University, M.J. MILLS, R.C. MYERS, Department of Materials Science and Engineering, The Ohio State University — GaN and AlN two dimensional electron gas heterostructures were grown by plasma assisted molecular beam epitaxy. During growth, a δ-doped layer of Gd was introduced at a controlled distance from the interface of the GaN and AlN layers. Resulting magnetic and structural properties were characterized by a variety of complementary methods including X-ray diffractometry, atomic force microscopy, transmission electron microscopy, superconducting quantum interference device magnetometry, photoluminescence spectroscopy and measurement of the anomalous Hall effect. Doping with Gd was observed to give rise to a colossal magnetic moment of 200$\mu_{\rm B}$/Gd with a Curie point in excess of 300K. To elucidate the mechanism by which introduction of Gd results in such a large moment, a wide variety of heterostructure geometries and growth conditions have been explored.

[1]Work supported by the Institute for Materials Research at The Ohio State University.

8:48AM H15.00003 Digital magnetic heterostructures based on GaN , LUIZ G. FERREIRA, Universidade de São Paulo, Brazil, MARCELO MARQUES, JOÃO P. T. SANTOS, LARA K. TELES, Instituto Tecnologico de Aeronautica, Brazil — Delta doped heterostructures based on GaN are possible wide band gap spintronic material with high temperature ferromagnetic transition [Hory et al, Physica B 324, 142 (2002); Reed et al, Appl. Phys. Lett. 79, 3473 (2001)]. They are formed by a thin magnetic layer or submonolayer, embedded into thick semiconductor layers [Marques et al, Phys. Rev. B 73, 224409 (2006)]. In this work we studied digital magnetic heterostructures with isolated magnetic monolayers of V, Cr, Mn, Fe, Co, Ni, or Cu embedded in GaN. We performed first-principles calculations within the density functional theory with self-energy, to account for excitation energies [Ferreira et al, Phys. Rev. B 78, 125116 (2008)]. The technique allowed us to calculate the GaN band gap as $E_{gap}^{calculated} = 3.53eV$ with no adjustable parameters. GaN:V and GaN:Cr do have ferromagnetic ground states with high Curie temperatures, as predicted by a mean-field approximation. GaN:Cr presents a 2D half-metallic ground state with 100% spin polarization. GaN:V has an unusual ground state, with a 2.0μ_B magnetic moment, no states at the Fermi energy, a minority spin gap of 3.0eV, and a majority spin gap of only 0.3eV.

9:00AM H15.00004 Intrinsic ferromagnetism at AlN-MgB_2 interfaces , YOSHIHIRO GOHDA, SHINJI TSUNEYUKI, Univ. of Tokyo — Spin polarization without magnetic elements is possible utilizing dangling bonds. In particular, nitrogen-dangling bonds of cation vacancies are responsible for spin polarization in nitride semiconductors. Enhancement of ferromagnetism due to cation vacancies by Gd dopants has also been found [1], which is consistent with colossal magnetic moments per Gd observed in experiments. However, randomness of point-defect distribution is not feasible to control magnetisation. In this situation, ordered structures of spin sites are highly desirable for the control of magnetization. In this study, we demonstrate by means of first-principles calculations that nitride-boride interfaces could be a candidate for such ordered spin sites. Partially occupied N p states at AlN-MgB_2(0001) interfaces exhibits two-dimensional spin polarization, which cannot be anticipated from the atomic structure because the N dangling bonds are apparently saturated by Mg. Hund's coupling of the two N $p_{||}$ orbitals as well as high density of spin-unpolarized states at the Fermi energy contribute to strong itinerant ferromagnetism. Roles of metal-induced gap states [2] will also be discussed.

[1] Y. Gohda and A. Oshiyama, Phys. Rev. B 78, 161201(R) (2008).
[2] Y. Gohda, S. Watanabe, and A. Groß, Phys. Rev. Lett. 101, 166801 (2008).

9:12AM H15.00005 Room temperature ferromagnetism in cluster free, Co doped Y_2O_3 dilute magnetic oxide , C.N. WU, S.Y. HUANG, W.C. LIN, T.S. WU, Y.L. SOO, Dept. of Physics, National Tsing Hua Univ., Taiwan, W.C. LEE, Y.J. LEE, Y.H. CHANG, M. HONG, Dept. of Materials science and Engineering, National Tsing Hua Univ., Taiwan, J. KWO, Dept. of Physics, National Tsing Hua Univ., Taiwan; Center for Condensed Matter Sciences, National Taiwan Univ, Taiwan — Diluted magnetic oxides (DMO) displaying the ferromagnetic behavior far above room temperature has attracted much attention for potential spintronic applications. Our study using low temperature co-deposition has produced uniformly doping of transitional metal (TM) Co (2-10 at.%) in Y_2O_3 films without formation of clusters or second phases, stable up to 450°C anneals under most ambient. This was confirmed by EXAFS local structural analysis, XANES, and XMCD measurement. Ferromagnetic behavior of magnetic moment was observed at 300K, and the Co saturation magnetization was modulated by the concentration of oxygen vacancies under various post treatments. The observation is consistent with the impurity band exchange model to account for apparent ferromagnetism in these nearly insulating DMO films. One surprising implication from this model is the occurrence of ferromagnetic insulator behavior in TM doped HfO_2 is more likely than the widely studied TM doped ZnO, TiO_2, and SnO_2 systems of smaller band gaps for doping concentrations kept under cation percolation threshold.

9:24AM H15.00006 No role of magnetic impurities in observed ferromagnetism in $Ti_{1-x}Ta_xO_2$ thin film[1] , MALLIKARJUNA RAO MOTAPOTHULA, Graduate Student, A. ROY BARMAN, N.L. YAKOVLEV, S. DHAR, M.B.H. BREESE, T. VENKATESAN, NANOCORE, NATIONAL UNIVERSITY OF SINGAPORE TEAM, CIBA, DEPARTMENT OF PHYSICS, NATIONAL UNIVERSITY OF SINGAPORE COLLABORATION, ELECTRICAL AND COMPUTER ENGINEERING, NATIONAL UNIVERSITY OF SINGAPORE COLLABORATION — Recently, the idea of cationic-vacancy-induced FM in wide band-gap semiconducting oxides was proposed on theoretical grounds. Experimentally, we observed ferromagnetism in thin films of anatase $Ti_{1-x}Ta_xO_2$ grown by PLD. Ta incorporation gives rise to cationic defects, acting as magnetic centers and free charge carriers as detected by various spectroscopic and transport measurements. To confirm that the ferromagnetism is an intrinsic property of $Ti_{1-x}Ta_xO_2$ and to rule out any impurity issues such as presence of magnetic elements and clustering, we carried out in-depth analysis based on Rutherford backscattering spectroscopy (RBS), Proton induced X-Ray Emission spectroscopy (PIXE) and Secondary Ion Mass Spectroscopy (SIMS). Form these results we concluded that the observed FM was not due to magnetic impurities. Rather it is an intrinsic property of $Ti_{1-x}Ta_xO_2$ thin film.

[1]NanoCore, National University of Singapore

9:36AM H15.00007 Magnetism of DMS SnO_2:Co Thin Films Grown by RF Sputtering[1] , GRATIELA STOIAN, Florida State University, PATRICIA STAMPE, ROBIN KENNEDY, Florida A&M University, STEPHAN VON MOLNAR, Florida State University — SnO_2:Co thin films with dopant concentrations ranging from 2-15at% were deposited on r-cut sapphire substrates via RF sputtering, to examine the origin of the room temperature ferromagnetism (RTFM) observed in such materials. Films deposited with 9:1 Ar/O_2 partial pressure ratio have a saturation moment of $\sim 0.34 \mu_B$/Co. Utilizing Coey's generalized grain boundary model [1], this implies that only $\sim(2 \pm 0.5)$% of the sample is FM. Furthermore, XPS studies reveal that the cobalt valance is 2+, suggesting it exists in the form of an oxide, either Co substitutional or as CoO clusters. Furthermore, angle dependent measurements indicate no sign of phase segregation. We speculate that the FM is due to the spontaneous magnetization of uncompensated spins at the surface of the CoO antiferromagnetic nanocrystals [2] in the host SnO_2. This model may also explain the large anisotropy observed in some of our films.

[1] Coey et. al IEEE Trans. Magn. (2010)
[2] Dietl et. al PRB **76**, 155312 (2007)

[1]This work was supported by NSF DMR-0605734.

9:48AM H15.00008 Observation of room-temperature ferromagnetism in Cu:ZnO films part I; soft X-ray Magnetic Circular Dichroism , C. SANCHEZ-HANKE, Brookhaven National Laboratory, T.S. HERNG, D.-C. QI, National University of Singapore, T. BERLIJN, Brookhaven National Laboratory, J.B. YI, K.S. YANG, National University of Singapore, Y. DAI, Shandong University, Y.P. FENG, I. SANTOSO, X.Y. GAO, A.T.S. WEE, National University of Singapore, W. KU, Brookhaven National Laboratory, J. DING, A. RUSYDI, National University of Singapore — We report direct evidence of room-temperature ferromagnetic ordering in O-deficient Cu:ZnO films by using soft x-ray magnetic circular dichroism and x-ray absorption [1]. Our measurements have revealed unambiguously two distinct features of Cu atoms associated with (i) magnetically ordered Cu ions present only in the oxygen-deficient samples and (ii) magnetically disordered regular Cu^{2+} ions present in all the samples. We find that a sufficient amount of both oxygen vacancies and Cu impurities is essential to the observed ferromagnetism, and a non-negligible portion of Cu impurities is uninvolved in the magnetic order.

[1] T.S. Herng et al, Phys. Rev. Lett. **105**, 207201 (2010)

10:00AM H15.00009 Observation of room-temperature ferromagnetism in Cu:ZnO films part II; a theoretical study , T. BERLIJN, W. KU, Brookhaven National Laboratory, T.S. HERNG, D.-C. QI, J.B. YI, K.S. YANG, National University of Singapore, Y. DAI, Shangdong University, Y.P. FENG, I. SANTOSO, National University of Singapore, C. SANCHEZ-HANKE, Brookhaven National Laboratory, X.Y. GAO, A.T.S. WEE, J. DING, A. RUSYDI, National University of Singapore — To better understand the observation of room-temperature ferromagnetic ordering in O-deficient Cu:ZnO films [1], we calculated the configuration-averaged spectral function $\langle A(k,\omega)\rangle$ of ZnO with 2% Cu impurities and 1% O vacancies within the "LDA+U" approximation, solving the Hamiltonian only within the low energy Hilbert space, defined via the first-principles Wannier functions [2]. Based on these first principles results we proposed a microscopic "indirect double-exchange" model for the FM in Cu:ZnO that explains our main experimental findings.

[1] T.S. Herng et al, Phys. Rev. Lett. **105**, 207201 (2010)
[2] T. Berlijn et al, arXiv:1004.1156 (2010)

10:12AM H15.00010 Electrodeposition of Co-doped Cu_2O layers with high Curie temperature[1] , ANDRE A. PASA, IURI S. BRANDT, ALEXANDRE D.C. VIEGAS, MILTON A. TUMELERO, JOSE J. S. ACUNA, Departamento de Fisica, Universidade Federal de Santa Catarina, Florianopolis, Brazil, ENIO LIMA JR., ROBERTO D. ZYSLER, Centro Atomico Bariloche and Instituto Balseiro, Argentina — In this work, we have studied the magnetic properties of room temperature electrodeposited Cu_2O layers doped with Co. These layers were growth from electrolytes containing lactic acid and copper sulfate, with the addition of cobalt sulfate for the doping process. The layers are considered as a diluted magnetic semiconductor, showing ferromagnetic behavior above room temperature and saturation magnetization proportional to the concentration of cobalt sulfate. The decrease of lattice parameter and resistivity with the increase of the band gap for doped samples were results that pointed out to the Co incorporation to the growing layers as individual atoms. In addition, no evidences for the existence of superparamagnetic particles were observed from ZFC and FC curves, hysteresis loops and HRTEM images. The magnetic behavior is associated to Co atoms diluted in the Cu_2O lattice and a promising Curie temperature for spintronic application of 550 K was determined.

[1]CNPQ, CAPES, FAPESC, FINEP, ANPCyT (PICT2007-832), CONICET (PIP2008-1333) and UNCuyo

10:24AM H15.00011 The spin polarized electronic structures and magnetic properties of Co doped and Ga codoped ZnO , M.-H. TSAI, T.-Y. JIANG, C.-Y. HUANG, National Sun Yat-Sen University — The understanding of the magnetic property of Co doped ZnO (ZnO:Co) has been inconclusive with confusing experimental observations. Here, spin-polarized first-principles calculations have been performed for ZnO:Co to better understand its magnetic property. Without O and Zn vacancies, the total energy per Co ion in ZnO:Co in the ferromagnetic (FM) state was found to be only 6meV lower than that in the antiferromagnetic (AFM) state, which suggests that at room or higher temperature ZnO:Co is in the spin glass state. O vacancies and co-doping with Ga ions were found to enhance Co-Co FM coupling by induced delocalized states in the vicinity of Co 3d bands. The O vacancy was found to have a greater effect of FM enhancement than the co-doped Ga ion. While Zn vacancies were found to lower the Fermi level and enhance hybridization between Co 3d and valence-band O 2p states, which enhances super-exchange coupling and renders ZnO:Co to be in the AFM state. The opposite effects of O and Zn vacancies imply that the magnetic property of ZnO:Co depends strongly on the relative concentrations of O and Zn vacancies.

10:36AM H15.00012 Magnetotransport in the amorphous Ge(1-x)Mn(x) with self-assembled nanostructures[1] , WENJING YIN, University of Virginia, JAN JAROSZYNSKI, National High Magnetic Field Lab, JIWEI LU, University of Virginia, COPELAND KELL, LI HE, Rensselaer Polytechnic Institute, MELISSA DOLPH, JERROLD FLORO, STUART WOLF, University of Virginia — Mn ions have been reported to segregate into intermetallic precipitates or form coherent clusters in crystalline Ge(1-x)Mn(x) thin films. In this study, we investigated the microstructure of amorphous Ge(1-x)Mn(x) synthesized using low temperature molecular beam epitaxy, and observed the self-assembly of Mn rich nanostructures in Ge matrix with both cluster and column shapes by varying the Mn concentration. The magnetotransport properties were found to closely correlate with the magnetism. Negative magnetoresistance (MR) showed a dominant effect in as-grown materials, and required a very high magnetic field to saturate, whereas only positive MR was observed in post-annealed Ge(1-x)Mn(x). The anisotropic behavior in magnetism and magnetoresistance will also be discussed.

[1]Supported by NSF/NRI

Tuesday, March 22, 2011 8:00AM - 11:00AM –

Session H16 GMAG DMP: Focus Session: Spins in Carbon-Based Materials– Spin Valves and Interfaces D173

8:00AM H16.00001 Spin filtering effect of ferromagnetic metal-organic interfaces , MIRKO CINCHETTI, Department of Physics and Research Center OPTIMAS, University of Kaiserslautern — The study of the spin properties of organic semiconductors (OSC) is recently receiving great attention. Being characterized by moderate spin-relaxation lengths, one of the most promising routes to employ OSC for spintronics applications is probably to exploit the high spin injection achievable across ferromagnetic metal-organic interfaces [1,2]. Combined with the extreme flexibility and tunability of OSC, it is expected that such hybrid interfaces will constitute a fundamental building block for advanced spintronics devices, where spin-injection is controlled by fine-tuning of the interface physical ad chemical properties. An example has been recently presented in [3], where doping of the OSC copper phthalocyanine (CuPc) has been successfully used to tune the spin functionality of a cobalt-CuPc interface. In particular, the presence of a spin-polarized hybrid interface state, acting as a spin-filter at the interface, has been used to enhance the efficiency of spin injection to values above 100%. In order to exploit such great potential of hybrid organic-inorganic interfaces, fundamental knowledge about their spin-dependent properties is essential. Besides the cobalt-CuPc interface, we have studied the iron-CuPc, cobalt- tris[8-hydroxyquinoline]aluminium (Alq3) and iron-Alq3 interfaces. We applied several complementary experimental techniques, namely spin polarized scanning tunnelling microscopy and spectroscopy together with spin polarized ultraviolet photoemission spectroscopy and spin- and time-resolved two-photon photoemission. We found evidence for spin-polarized interface states and show that they act as a spin-filter for electrons crossing the interface between the ferromagnetic metal and the OSC. Correspondingly, we observed a pronounced spin-dependency of the lifetime of electrons injected in the above mentioned hybrid spin-polarized interface states.

[1] M. Cinchetti et al., Nature Materials 8, 115-119 (2009);
[2] H. Ding et al., Phys. Rev. B 78, 075311 (2008);
[3] M. Cinchetti et al., Phys. Rev. Lett. 104, 217602 (2010).

8:36AM H16.00002 Spin valve effect and high field magnetoresistance in hybrid magnetic tunnel junction of V(TCNE)$_{x\ 2}$/rubrene/ $La_{2/3}Sr_{1/3}MnO_3$[1] , JUNG-WOO YOO, BIN LI, C.Y. CHEN, V.N. PRIGODIN, A.J. EPSTEIN, The Ohio State University, H.W. JANG, C.W. BARK, C.B. EOM, University of Wisconsin — Molecule/organic-based magnets, that allow chemical tuning of electronic and magnetic properties, are a promising new class of magnetic materials for future spintronics [1]. V (TCNE:tetracyanoethylene)$_x$ ($x \sim 2$) is the room temperature organic-based magnetic semiconductor ($T_c \sim 400$ K). It has ferrimagnetic coupling between the spins in the $TCNE^-$ anions and spins in V^{II} leading highly spin- polarized valence and conduction bands. In this talk, we present realization of an organic-based magnetic as an electron spin polarizer in the standard spin valve device geometry [2]. The room temperature organic-based magnet, V(TCNE)$_x$ was successfully incorporated into the standard magnetic tunnel junction devices in tandem with LSMO ($La_{2/3}Sr_{1/3}MnO_3$) film. Beside spin valve effect, the device exhibits large negative high-field magnetoresistance, which may be associated with anomalous field dependent Fermi level shift in LSMO.

[1] A.J. Epstein, MRS Bull. 28, 492 (2003)
[2] Yoo et al., Nature Materials 9, 638 (2010)

[1]This work was supported in part by the AFOSR, DOE, and NSF.

8:48AM H16.00003 Organic Spin Valves with Characteristics of Inelastic Tunneling and Hopping Transport , MINN-TSONG LIN, KAI-SHIN LI, YIN-MING CHANG, SANTHANAM AGILAN, JHEN-YONG HONG, JUNG-CHI TAI, Dept. of Physics, National Taiwan University, WEN-CHUNG CHIANG, Dept. of Physics, Chinese Culture University, KEISUKE FUKUTANI, P.A. DOWBEN, Dept. of Physics and Astronomy, University of Nebraska — We report on the inelastic scattering characteristics of an organic-based spin valve with a thin organic barrier of 3,4,9,10-perylene-teracarboxylic dianhydride (PTCDA) dusted with alumina at organic/ferromagnetic interfaces. Spin injection with magnetoresistance up to 12% at room temperature was achieved. In the inelastic tunneling spectrum, the observation of characteristic vibrational loss peak of organic spacer provides direct evidence of the interplay between the spin-polarized electrons and the organic molecules. The spin-dependent transport mechanism can be further described with a model of combined tunneling and hopping processes as verified by experiments as a function of organic layer thickness.

9:00AM H16.00004 Coulomb blockade magnetoresistance in organic spin transport device[1] , DALI SUN, X.-G ZHANG, PAUL C. SNIJDERS, Oak Ridge National Laboratory, HANGWEN GUO, The University of Tennessee / Oak Ridge National Laboratory, ZHENG GAI, T. ZAC WARD, Oak Ridge National Laboratory, JIAN SHEN, The University of Tennessee / Fudan University — Using buffer-layer-assisted growth, we successfully fabricated organic spin transport devices with a discontinuous granular magnetic layer centered in an organic spacer film. The Coulomb blockade magnetoresistance (MR) effects were observed, as predicted by X.-G. Zhang *et al* (Phys. Rev. B. 81, 155122, 2010). The spin-dependent Coulomb blockade voltage arises from the coupled magnetic dots inside the organic material and correlate with the observed MR effect.

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

9:12AM H16.00005 Spin-polarized tunnel injection and extraction effects on magneto-resistance in organic semiconductor spin valves[1] , MOHAMMAD YUNUS, P. PAUL RUDEN, University of Minnesota, DARRYL L. SMITH, Los Alamos National Lab. — Experimental evidence of large magneto-resistance has been reported for organic spin valves. An organic spin valve consists of a conjugated hydrocarbon semiconductor sandwiched between two ferromagnetic contacts. Tunnel injection of charge carriers from a ferromagnetic contact can be strongly spin-polarized. The process is modeled as tunneling through a thin interfacial layer into localized molecular states of the organic semiconductor near the equilibrium Fermi level, and subsequent thermally activated hopping of the charge carriers out of these localized states into the bulk of the semiconductor, where the transport can be described by macroscopic device equations. The extraction of charge carriers follows an analogues process at the collecting contact. We explore the consequences of parallel or anti-parallel alignment of contact magnetizations on the spin-polarization and the magneto-resistance associated with the spin-polarized current in the device.

[1]Supported by NSF ECCS under grant #0724886.

9:24AM H16.00006 Spin-orbit coupling, spin relaxation, and spin diffusion in organic solids: applications to Alq_3 and CuPc[1] , ZHI-GANG YU, SRI International — We develop a systematic approach of quantifying spin-orbit coupling (SOC) and a rigorous theory of carrier spin relaxation caused by the SOC in disordered organic solids. The SOC mixes up- and down-spin in the polaron states and can be characterized by an admixture parameter γ^2. The spin mixing effects spin flips as polaron hops from one molecule to another even through the interaction that facilitate hopping is spin-indepdent. The spin relaxation time is $\tau_{sf} = \bar{R}^2/(16\gamma^2 D)$ and the spin diffusion length is $L_s = \bar{R}/4|\gamma|$, where $\bar{R}$ is the mean polaron hopping distance and D the carrier diffusion constant. We show that the SOCs in tris-(8-hydroxyquinoline) aluminum (Alq_3) and in copper phthalocyanine (CuPc) are particularly strong, due to the orthogonal arrangement of the three ligands in the former and Cu $3d$ orbitals in the latter. The theory quantitatively explains the recent observed spin diffusion lengths in Alq_3 from muon measurements and in CuPc from two-photon photoemission.

[1] This work was partly supported by the Office of Basic Energy Sciences, US Department of Energy.

9:36AM H16.00007 Triplet exciton controlled current in an organic semiconductor , WILLIAM BAKER, University of Utah, DANE MCCAMEY, University of Sydney, KIPP VAN SCHOOTEN, University of Utah, JOHN LUPTON, Universität Regensburg, CHRISTOPH BOEHME, University of Utah, BOEHME GROUP COLLABORATION, LUPTON GROUP COLLABORATION — Organic materials like MEH-PPV have relatively low spin-orbital coupling leading to long spin lifetimes and good spin-selection rules. As a result, the rates of recombination of an ensemble of polaron pairs can be changed by resonant manipulation of either the P^+ or the P^- spins, leading to a flopping between the singlet to triplet manifolds - this can be observed as a small change in the device current [1]. In this study we have used pulsed electrically detected magnetic resonance with electron-rich OLED devices to investigate the possibility of other spin-dependent processes like an exciton-polaron interaction. We expect that devices with excess electrons will show signals from free electrons interacting with long lived triplet excitons. Coherent Rabi nutation experiments were carried out from room temperature down to 5K. At room temperature only a single polaron-pair resonance is observed at g$\sim$2.003. However, as the temperature is decreased a signal at g$\sim$4(triplet exciton resonance) is observed along with a second signal at g$\sim$2.003 corresponding to the rotation of a single polaron.

[1] D. R. McCamey, *et. al.* Nature Mater. **7**, 723, (2008)

9:48AM H16.00008 STM studies of Lanthanide Phthalocyanine molecules on metallic and thin-insulating surfaces , FADI EL HALLAK, BEN WARNER, UCL, UK, MICHAEL WATERS, U. Nottingham, UK, JORIS VAN SLAGEREN, U. Nottingham, UK; U. Stuttgart, Germany, CYRUS F. HIRJIBEHEDIN, UCL, UK — Molecules deposited onto surfaces are of interest because of their potential use as nano-scale electronic components. More recently, the magnetic properties of these systems have also become accessible. Using scanning tunneling microscopy (STM), it is possible to study both sets of properties, and to examine the local environment of the molecules. For example, large magnetic anisotropies have been observed for transition metal Phthalocyanine (Pc) molecules on thin insulators, which decouple the spin from the underlying metal. We present STM imaging and spectroscopy data on lanthanide double-decker Pcs. We explore the different binding configurations and study how these can influence the properties of these molecules on surfaces.

10:00AM H16.00009 STM Studies of Iron Phthalocyanine on Fe(110) Films[1] , ANDREAS SANDIN, DAN DOUGHERTY, J. E. (JACK) ROWE, NC State University — We have observed molecular-scale-resolution arrays of Iron Phthalocyanine (FePc) molecules which we adsorbed at room temperature on thin ($\sim$5-10 ML) films of Fe(110). These molecular layers were grown in a UHV Omicron/AFM/STM/ multi-probe system at NC State in the Physics Department at pressures of $\sim 10^{-10}$ torr. Our results indicate a strong inter-molecular interaction that produces well-ordered films at monolayer coverage. For lower coverage ($\sim$0.2 – 0.6 ML) the FePc-Fe substrate interaction strongly dominates and the STM image morphology has only small clusters of 2-6 molecules. Our data clearly shown that the FePc molecules are lying flat on the surface in the ordered $\sim$1 ML samples since we see evidence of the carbon-ring ligands in some images. We discuss the possibility of spin-dependent effects between the molecular Fe and the substrate Fe as an example of potential molecular-modified spin-based devices. Initial STM-spectroscopy including both I vs. V and Z vs. V results are consistent with our structural observations.

[1]Supported in part by the NSF Chemical Centers for Innovation program (Grant CHE-0943975).

10:12AM H16.00010 Scanning Tunneling Microscopy and Spectroscopy Studies of a Model Organic Spintronic Interface: Alq3 on Cr(001) , ZHENGANG WANG, ALEX PRONSCHINSKE, DANIEL DOUGHERTY, NC State University, SURFACE SCIENCE TEAM — Scanning tunneling microscopy was used to observe coverage-dependent structure during growth of the first monolayer of Alq3 on a Cr(001) surface. No long range molecular ordering is observed, though molecules tend to form randomly oriented chain-like aggregates even at the lowest coverages. This illustrates that the well-known amorphous nature of Alq3 films begins even in the first layer, but that the disorder in films have subtle local correlations relevant to electronic and spintronic device modeling. Scanning tunneling spectroscopy was used to locate the LUMO-derived transport state above the Fermi level and correlate its position with local film structure.

10:24AM H16.00011 STM studies of a novel organic/inorganic interface: TCNE/GaAs(110)[1] , N.M. SANTAGATA, J.A. GUPTA, The Ohio State University — Recent efforts in the field of spintronics have focused on the integration of organic molecular magnets with inorganic semiconductors. Little is known, however, about the interfacial chemistry and physics that occurs between the organic spin injector and the inorganic device structure. We are therefore studying tetracyanoethylene/GaAs(110) as a model system to gain a basic understanding of the properties that emerge upon integration of these materials. Utilizing low temperature (7 K) ultrahigh vacuum scanning tunneling microscopy we are able to identify both bonding geometries and bonding sites for isolated TCNE molecules on the unreconstructed GaAs(110) surface. Scanning tunneling spectroscopy can provide a detailed look at the interfacial electronic structure, including alignment of individual molecular orbitals with respect to the band structure of the underlying substrate. Single transition metal–TCNE complexes can be realized and investigated via atomic/molecular manipulation.

[1]Funding by: NSF CAREER Award (DMR-0645451) and the Center for Emergent Materials, an NSF-funded MRSEC (DMR-0820414)

10:36AM H16.00012 Magnetic Field Effects Generated by Inter-molecular Excited States in Organic Semiconductors , LIANG YAN, MING SHAO, BIN HU, University of Tennessee — It has experimentally found that an external magnetic field can change electroluminescence, electric current, and photocurrent, generating magnetic field effects (MFEs) in non-magnetic organic semiconductors. Our photoluminescence studies have found that the intermolecular excited states are accountable for the MFEs while the intra-molecular excited states exhibit negligible MFEs. Our experimental studies further indicated that inter-molecular excited states can exhibit tunable spin-orbital coupling and exchange interaction based on materials mixing. We observed that tuning inter-molecular spin-orbital coupling and exchange interaction can largely modify the MFEs through spin-dependent formation and intersystem crossing in inter-molecular excited states. Therefore, the use of inter-molecular excited states presents a new mechanism to generate magnetic responses in non-magnetic organic semiconductors.

10:48AM H16.00013 Charge transport through single alkanedithiol molecules on an ultrathin insulating film: Influence on an atomic Kondo resonance , TAEYOUNG CHOI, JAY GUPTA, ohio state university — Studies of charge/spin transport through single molecules are important for understanding organic-based electronic and memory devices. We have realized a single molecule wire comprising an alkanedithiol molecule and a single Co atom contact using a low temperature scanning tunneling microscope. This wire is formed on an ultrathin insulating layer (Cu2N on Cu(100)). A Kondo resonance observed on isolated Co atoms on Cu2N indicates minimal contact to the Cu substrate. However, increased contact to Cu is achieved by connecting the Co atom via the alkanedithiol molecule. A change in the Kondo lineshape on the Co atom indicates an open conduction channel through the molecule. This result provides an opportunity to study charge/spin transport through single molecules with atomically precise contacts. We acknowledge financial support from NSF CAREER Award No. DMR-0645451 and NSF MRSEC-0820414. http://www.physics.ohio-state.edu/∼jgupta.

Tuesday, March 22, 2011 8:00AM - 10:48AM –

Session H17 DMP GMAG: Focus Session: Bulk Properties of Complex Oxides - Ferrites D174

8:00AM H17.00001 Inelastic neutron scattering measurements on the triangular lattice antiferromagnet CuFe1-xGaxO2 in the paraelectric and multiferroic phases , FENG YE, Oak Ridge National Laboratory — The intensive efforts to study multiferroic materials in recent years have led to a better understanding of the fundamental physical processes and interactions leading to the complex behavior in those compounds. In this talk, I will focus on the recent neutron scattering measurements and calculations of the spin dynamics of the triangular lattice antiferromagnet $CuFe_{1-x}Ga_xO_2$. In pure $CuFeO_2$ a low-temperature collinear spin structure is stabilized by long range magnetic interactions. The spin wave spectra show dynamics precursory to the multiferroic phase. When this system is doped with a few percent of nonmagnetic gallium, its low-temperature phase has a complex noncollinear (CNC) spin order and becomes multiferroic. The CNC phase appears to have distorted screw-type magnetic configuration that is stabilized by the displacement of the oxygen atoms. The spin dynamics and the spin order in this material, as well as their implications to the origin of the ferroelectricity will be discussed [1,2].

[1] J. T. Haraldsen, et al., *Phys. Rev. B*, **82**, 020404 (2010).
[2]. Research was sponsored by the U.S. DOE/BES, Division of Materials Sciences and Engineering and the Division of Scientific User Facilities.

8:36AM H17.00002 Investigating the spin dynamics of the non-collinear magnetic phase of 3.5% Ga-doped $CuFeO_2$[1] , T. KIMURA, Division of Materials Physics, Osaka University, J.T. HARALDSEN, Theoretical Division, Los Alamos National Laboratory, F. YE, Neutron Scattering Science Division, Oak Ridge National Laboratory, R.S. FISHMAN, Materials Science and Technology Division, Oak Ridge National Laboratory, J.A. FERNANDEZ-BACA, Neutron Scattering Science Division, Oak Ridge National Laboratory and Department of Physics and Astronomy, The University of Tennessee, Y. YAMAGUCHI, K. KIMURA, Division of Materials Physics, Osaka University — We examine the evolution of the non-collinear phase of a hexagonal lattice antiferromagnet to help understand the inelastic neutron scattering measurements for the multiferroic ground state of 3.5% Ga-doped $CuFeO_2$. With the complex ground state stabilized by the displacement of the oxygen atoms, the multiferroic coupling is explained by the predicted "spin-driven" model. By comparing the observed and calculated spectrum of spin excitations for multiple spin configurations, we conclude that the magnetic ground state is a distorted screw-type spin configuration with a distribution of turn angles produced by lattice distortions.

[1]Research sponsored by the Division of Materials Sciences and Engineering, U.S. DOE under contract with UT-Battelle, LLC.

8:48AM H17.00003 Long-period solitonic lattice in the rare earth orthoferrite TbFeO3 , NIELS JENSEN, Riso National Laboratory, Roskilde, Denmark, SERGEY ARTYUKHIN, University of Groningen, ANDREY MALJUK, Helmholtz-Zentrum Berlin, KIM LEFMAN, University of Copenhagen, MAXIM MOSTOVOY, University of Groningen, DIMITRI ARGYRIOU, European Spallation Source ESS AB — Rare earth orthoferrites show a variety of magnetic transitions and spectacular magneto-electric effects originating from the coupling between the iron and rare earth magnetic sublattices. Our recent single-crystal neutron diffraction measurements revealed the presence of an unusual incommensurate phase in TbFeO3, which is induced by the magnetic field along the c axis and has a period of about 100 unit cells. We also present the results of model calculations, which explain the origin of this novel phase and reproduce the magnetic phase diagram of TbFeO3.

9:00AM H17.00004 Magnetic and Raman spectroscopic studies of yttrium substituted $BiFeO_3$, R. NAIK, S. TALEBI, AMBESH DIXIT, Wayne State University, V. NAIK, University of Michigan, Dearborn, G. LAWES, Wayne State University — As a room temperature multiferroic $BiFeO_3$is attractive for a number of applications. However the relatively weak magnetism limits its suitability for applications. $Bi_{1-x}Y_xFeO_3$ (x=0, 0.05, 0.10, 0.15 and 0.20) ceramic samples have been prepared by sol-gel technique and thin films by metalorganic decomposition. X-ray diffraction, X-ray photoelectron and Raman spectroscopy measurements confirm that these ceramic and thin film samples are of single phase. More remarkably these Y modified $BiFeO_3$ samples exhibit enhanced room temperature magnetic and magnetodielectric properties, with the saturation magnetization approaching 25 emu cm^{-3} for x=0.20. We discuss the correlation between the enhanced room temperature magnetization and two-phonon Raman modes in the context of investigating the origin of the magnetic properties in $Bi_{1-x}Y_xFeO_3$.

9:12AM H17.00005 ABSTRACT WITHDRAWN –

9:24AM H17.00006 Relation between electric phase and magnetic ordering of Y-type Hexaferrite , WOO-SUK NOH, H. JANG, K.-T. KO, J.-H PARK, c-CCMR & Dept. of Physics, POSTECH, S.H. CHUN, K.H KIM, XMPL, Seoul National University, B.-G PARK, J.-Y KIM, PAL, POSTECH — Y-type hexaferrite $Ba_{0.5}Sr_{1.5}Zn_2Fe_{12}O_{22}$(BSZFO), one of multiferroic materials, we could acquire magnetic field-induced commensurate phase, changing of magnetic phase of BSZFO and $Ba_{0.5}Sr_{1.5}Zn_2(Fe_{1-x}Al_x)_{12}O_{22}$ (x = 0.08)(BSZFAO) using resonant soft X-ray scattering(RSXS) experiment. Also we could confirm that magnetic ordering changing has some relation with electric phase transition, q=1.5 at ferroelectric phase not only BSZFO but also BSZFAO. This research results were acquired by using 2A EPU beamline at PAL.

9:36AM H17.00007 Magnetic Spectra on Charge Ordering in $R_{1/3}Sr_{2/3}FeO_{3-\sigma}$ (R = La, Pr, and Nd) , JIE MA, JIAQIANG YAN, SOULEYMANE OMAR DIALLO, REBECCA STEVENS, ANNA LLOBET, FRANS TROUW, DOUGLAS ABERNATHY, MATTHEW STONE, ROBERT MCQUEENEY, AMES LABORATORY, AMES, IA 50011 COLLABORATION, DEPARTMENT OF PHYSICS AND ASTRONOMY, IOWA STATE UNIVERSITY, AMES, IA 50011 COLLABORATION, OAK RIDGE NATIONAL LABORATORY, PO BOX 2008, OAK RIDGE, TN 37831, USA COLLABORATION, LOS ALAMOS NATIONAL LABORATORY, LOS ALAMOS, NM 87545 COLLABORATION — $R_{1/3}Sr_{2/3}FeO_{3-\sigma}$ (R = La, Pr, and Nd) compounds are reported to have the same charge ordering (CO) and Neel temperatures. Inelastic neutron scattering is applied to study the magnetic energy effect on the CO state in this system. Based on the ratio of the ferromagnetic exchange energy (J_F) and antiferromagnetic exchange energy ($|J_{AF}|$), the magnetic exchange energy can stabilize the CO state in $La_{1/3}Sr_{2/3}FeO_{3-\sigma}$ and $Pr_{1/3}Sr_{2/3}FeO_{3-\sigma}$ alone; with the smaller R^{3+} substitution, $|J_{AF}|$ increases a lot from $La_{1/3}Sr_{2/3}FeO_{3-\sigma}$ to $Nd_{1/3}Sr_{2/3}FeO_{3-\sigma}$, but the CO of Fe ions could still be driven by magnetic energy itself with the correction on magnetic energy ratio.

9:48AM H17.00008 First-principles calculations for XAS of infinite-layer iron oxides , MITSURU KODERA, ISIR, Osaka University, TATSUYA SHISHIDOU, ADSM, Hiroshima University, TAMIO OGUCHI, ISIR, Osaka University — The oxygen defect perovskite $SrFeO_{3-x}$ shows various properties such as the giant magnetoresistance effect and the thermoelectric effect. It had been believed that the oxygen content in $SrFeO_{3-x}$ changes up to $x = 0.5$. Recently, Tsujimoto *et al.* have succeeded in synthesizing the infinite-layer iron oxide $SrFeO_2$. $SrFeO_2$ has a square-planar oxygen coordination, while the iron oxides usually have the tetrahedral and octahedral coordination. $CaFeO_2$ has also infinite layer structure and the same magnetic ordering as $SrFeO_2$. However, it is suggested that the oxygen coordination of $CaFeO_2$ is different from that of $SrFeO_2$. In order to investigate the electronic structure of iron in (Ca, Sr)FeO_2, the x-ray absorption spectroscopy (XAS) spectrum has been measured. In this work, we perform the calculation for XAS spectrum near the Fe-K edge of (Ca, Sr)FeO_2 using the first-principles calculations. We compare the results with the experiment and discuss the electronic structure of iron in (Ca, Sr)FeO_2.

10:00AM H17.00009 Canted-spin-caused electric dipoles: a local symmetry theory , THOMAS A. KAPLAN, SUBHENDRA D. MAHANTI, Michigan State University — A pair of magnetic atoms with canted spins $\mathbf{S}_a$ and $\mathbf{S}_b$can give rise to an electric dipole moment **P.** Several forms for the dependence of **P** on the spins have been derived from various microscopic models, some of which have been invoked to explain experimental results found in some multiferroic materials. The forms are $\mathbf{P}_1 \propto \mathbf{R} \times (\mathbf{S_a} \times \mathbf{S}_b)$, $\mathbf{P}_2 \propto \mathbf{S_a} \times \mathbf{S}_b$, $\mathbf{P}_3 \propto \mathbf{S_a}(\mathbf{S_a} \cdot \mathbf{R}) - \mathbf{S}_b(\mathbf{S}_b \cdot \mathbf{R})$, where **R** is the relative position of the atoms. To unify and generalize these various forms we consider **P** as the most general quadratic function of the spin components that vanishes whenever $\mathbf{S_a}$ and $\mathbf{S}_b$are collinear. The study reveals new forms. We generalize to the vector **P**, Moriya's symmetry considerations on the (scalar) DM energy $\mathbf{D} \cdot \mathbf{S_a} \times \mathbf{S}_b$(which led to restrictions on **D**). This provides a rigorous proof that $\mathbf{P}_1$ is allowed no matter how high the symmetry of the atoms plus environment, and gives restrictions for all other contributions. The analysis leads to the suggestion of new terms omitted in the existing microscopic models, and predicts an unusual antiferroelectric ordering in the antiferromagnetically and ferroelectrically ordered phase of $RbFe(MoO_4)_2$.

10:12AM H17.00010 Structural and magnetic ordering in bulk Sr2FeMoO6 synthesized by planetary ball mill: The effects of grinding.[1] , J.M. LUCY, A.J. HAUSER, B. PETERS, F.Y. YANG, The Ohio State University — The standard solid-state synthesis procedure has been widely used to make bulk complex oxides, including half-metallic double perovskite Sr2FeMoO6. However, although it is generally recognized that multi-step grinding and heating are crucial for synthesis of high quality materials, little has been done to quantitatively characterize the effect of grinding on the quality of the final products. We systematically varied the level of grinding, ranging from poor grinding by hand for a short period of time (∼10 min) to very fine grinding and mixing by a planetary ball mill for many hours which produces uniform sub-micron particles. XRD, SEM and VSM were used to characterize the structural and magnetic properties. The Sr2FeMoO6 samples made by different grinding methods exhibit drastically different structural and magnetic ordering. The highest quality Sr2FeMoO6 is from the most thorough grinding and gives a close to ideal Fe/Mo ordering and magnetic moment close to 4 Bohr magneton per formula unit.

[1]This work is supported by the Center for Emergent Materials, a NSF MRSEC at OSU (DMR-0820414).

10:24AM H17.00011 Theory of ferromagnetic double perovskites[1] , OINAM NGANBA MEETEI, ONUR ERTEN, ANAMITRA MUKHERJEE, MOHIT RANDERIA, NANDINI TRIVEDI, PATRICK WOODWARD, The Ohio State University — We derive and validate an effective classical spin model which describes the magnetic properties of double perovskites (DP) like Sr_2FeMoO_6, including the effects of disorder and carrier concentration. This model generalizes the Anderson-Hasegawa model for manganites to DP's. We validate our effective spin model by making detailed comparisons with the results obtained from a quantum Hamiltonian of itinerant electrons interacting with spins on the Fe-sites. We show that the conduction electron polarization at the chemical potential $P(T)$ tracks the temperature-dependence of the total magnetization $M(T)$. We point out the importance of Coulomb correlation U on Mo-sites and of direct Mo-Mo hopping t' on stabilizing the ferromagnetic phase as a function of electron doping (by La substitution of Sr). We show how the small parameters U and t' are crucial in understanding the experimental results for T_c as a function of carrier concentration. We predict how the ferromagnetic T_c can be raised substantially (up to 40%), without sacrificing the polarization P, by a combination of excess Fe and La-doping.

[1]Supported by the NSF-MRSEC grant DMR-0820414

10:36AM H17.00012 Role of disorder and doping in ferromagnetic double perovskites[1] , ANAMITRA MUKHERJEE, OINAM NGANBA MEETEI, ONUR ERTEN, MOHIT RANDERIA, NANDINI TRIVEDI, PATRICK WOODWARD[2], The Ohio State University — We use an effective classical spin model, which we have recently derived and validated, to examine the effect of disorder on the magnetic properties of double perovskites like Sr_2FeMoO_6 (SFMO). We compute the effects of excess Fe, excess Mo, and anti-site disorder on the magnetization $M(T)$ and the ferromagnetic transition temperature T_c, and show that our results are quantitatively consistent with available experiments. We then use these results to propose routes to increase the ferromagnetic T_c above that of pure SFMO (420K). We predict that, by adding excess Fe on Mo sites and compensating for the change in conduction electron density by La substitution on the Sr sites, we can raise T_c by as much as 40%, without substantially sacrificing the conduction electron polarization P at the chemical potential.

[1]Supported by the NSF-MRSEC grant DMR-0820414
[2]Dept. of Chemistry

Tuesday, March 22, 2011 8:00AM - 11:00AM –
Session H18 DCOMP: Electronic Structure II D172

8:00AM H18.00001 Spectral element solution of the Kohn-Sham atom , KRISTOPHER ANDERSEN, High Performance Technologies, Inc / Naval Research Laboratory, NOAM BERNSTEIN, Naval Research Laboratory, JOHN PASK, Lawrence Livermore National Laboratory — Electronic structure calculations of atoms are important in nuclear physics, and are necessary input for most methods to construct first-principles effective potentials (i.e., pseudopotentials and projector augmented wave potentials). The standard method to solve the atomic problem within Kohn-Sham density functional theory is the shooting method. In this work, the more robust spectral element method is applied to the 1D atomic radial equation. The spectral element method provides a strict, upper-bound on the absolute error in the Kohn-Sham eigenvalues and wavefunctions enabling the solution to be converged to a well controlled accuracy. The results of this method are compared to the extensive "NIST Atomic Reference Data for Electronic Structure Calculations" database for elements H to U, providing a more rigourous assessment of this dataset than previously available.

8:12AM H18.00002 Ab initio calculations of optical absorption spectra: Solution of the Bethe-Salpeter equation within density matrix perturbation theory[1] , DARIO ROCCA, UC Davis, DEYU LU, Brookhaven National Laboratory, HUY-VIET NGUYEN, GIULIA GALLI, UC Davis — We present an approach to compute optical absorption spectra from first principles, which is suitable for the study of large systems and gives access to spectra within a wide energy range. In this approach, the quantum Liouville equation is solved iteratively within first order perturbation theory, with a Hamiltonian containing a static self-energy operator [1]. This is equivalent to solving the Bethe-Salpeter equation. Explicit calculations of single particle excited states and inversion of dielectric matrices are avoided using techniques based on Density Functional Perturbation Theory [1,2]. The calculation and inclusion of GW quasi-particle corrections within this framework are discussed. The efficiency and accuracy of our approach are demonstrated by computing optical spectra of solids, nanostructures and dipeptide molecules exhibiting charge transfer excitations.

[1] D.Rocca, D.Lu and G.Galli, J. Chem. Phys. 133, 164109 (2010).
[2] H. Wilson, F. Gygi and G. Galli, Phys. Rev. B , 78, 113303, (2008).

[1]Work supported by NSF CHE-0802907 and DOE BES-FG02-06ER46262 grants.

8:24AM H18.00003 Ab-initio calculations of absorption spectra of nanowires by solving the Bethe-Salpeter Equation[1] , YUAN PING, DARIO ROCCA, Department of Chemistry, University of California, Davis, DEYU LU, Brookhaven National Laboratory, GIULIA GALLI, Department of Chemistry and Department of Physics, University of California, Davis — A first principle approach to the solution of the Bethe Salpeter equation without empty electronic states has been recently developed [1], which makes possible the calculations of absorption spectra of relatively large systems (with several hundreds of electrons). We present applications of this approach to quasi-one dimensional systems, including chains of hydrogen molecules and Si nanowires. We discuss techniques to further improve the performance of absorption spectra calculations, and present a general scheme to accurately integrate the divergence in the screened exchange integrals. Finally, in the case of Si nanowires, we discuss the effect of surface reconstruction in shaping optical absorption spectra.

[1] D. Rocca, D. Lu and G. Galli, J. Chem. Phys. 133, 164109 (2010)

[1]NSF-Chem CALTECH 68D-1086057 and DOE-BES DE-FG02-06ER46262.

8:36AM H18.00004 Efficient GW calculations using eigenvalue-eigenvector decomposition of the dielectric matrix[1] , HUY-VIET NGUYEN, T. ANH PHAM, DARIO ROCCA, GIULIA GALLI, University of California-Davis — During the past 25 years, the GW method [1] has been successfully used to compute electronic quasi-particle excitation spectra of a variety of materials. It is however a computationally intensive technique, as it involves summations over occupied and empty electronic states, to evaluate both the Green function (G) and the dielectric matrix (DM) entering the expression of the screened Coulomb interaction (W). Recent developments have shown that eigenpotentials of DMs can be efficiently calculated without any explicit evaluation of empty states [2]. In this work, we will present a computationally efficient approach to the calculations of GW spectra by combining a representation of DMs in terms of its eigenpotentials [3] and a recently developed iterative algorithm [4]. As a demonstration of the efficiency of the method, we will present calculations of the vertical ionization potentials of several systems. [1] L. Hedin, Phys. Rev. 139, A796 (1965). [2] H.-V. Nguyen and S. de Gironcoli, Phys. Rev. B 79, 205114 (2009); H. F. Wilson, D. Lu, F. Gygi, and G. Galli, Phys. Rev. B 79, 245106 (2009). [3] D. Lu, F. Gygi, and G. Galli, Phys. Rev. Lett. 100, 147601 (2008). [4] P. Umari, G. Stenuit, and S. Baroni, Phys. Rev. B 81, 115104 (2010)

[1]Work was funnded by SciDAC-e DE-FC02-06ER25777

8:48AM H18.00005 A TDLDA+U approach on strongly hybridized Frenkel excitons in Mott insulators and implications to TDDFT and GW+BSE[1] , CHI-CHENG LEE, Academia Sinica, Taiwan, H.C. HSUEH, Tamkang University, Taiwan, WEI KU, Brookhaven National Laboratory — The applicability of nowadays first-principles approach on local excitations of strongly correlated systems is unknown. We therefore derived the dynamical linear response of LDA+U functional within the framework of TDDFT.[2] The strength and weakness of LDA+U functional in describing charge excitations of strongly interacting Mott insulators is examined via this TDLDA+U method. Formulated using real-space Wannier functions, a computationally inexpensive framework gives detailed insights into the formation of tightly bound Frenkel excitons with reasonable accuracy. Specifically, a strong hybridization of multiple excitons is found to significantly modify the exciton properties. Furthermore, our study exposes a significant generic limitation of adiabatic approximation in TDDFT with hybrid functionals and in existing Bethe-Salpeter-equation approaches, advocating the necessity of strongly energy-dependent kernels in future development. Finally, a superatom approach beyond TDLDA+U will also be discussed.

[1]This work is supported by DOE CMSN of USA, and NSC of Taiwan.
[2]Chi-Cheng Lee et al., Phys. Rev. B 82, 081106(R) (2010).

9:00AM H18.00006 Level alignment at covalently bonded metal-organic interfaces within the GW approximation , JEFFREY NEATON, ISAAC TAMBLYN, Molecular Foundry, LBNL, SU YING QUEK, Institute of High Performance Computing (IHPC) and Physics and Applied Physics in Nanyang Technological University, STANIMIR BONEV, LLNL and Dalhousie University, PIERRE DARANCET, Molecular Foundry, LBNL — Accurate calculations of orbital energies for molecules chemisorbed on metal surfaces are important for understanding energy conversion, molecular scale transport, and charge transfer events at metal electrodes. Here, using density functional theory (DFT) and many-body perturbation theory within the GW approximation (GWA), we report the orbital energies of a well-studied molecule, benzene diamine (and derivatives), covalently bonded to aluminum and gold surfaces. For chemisorbed derivatives on Al surfaces, we predict a shift in the highest occupied molecular orbital resonance energy greater than 1 eV relative to the DFT result. We discuss our GWA results in the context of a model self-energy approach based on prior work [1], which can be applied to larger systems at greatly reduced computational cost.

[1] J. B. Neaton, M.S. Hybertsen, and S.G. Louie, PRL, 97, 216405 (2006)

9:12AM H18.00007 GW approach to degenerate systems[1] , JOHANNES LISCHNER, JACK DESLIPPE, STEVEN G. LOUIE, UC Berkeley — Many-body perturbation theory based on the GW approximation to the electron self energy describes accurately in first-principles calculations the electronic (quasiparticle) excited states of solids, clusters and molecules. However, despite the multitude of important systems with degenerate ground states, ranging from open-shell atoms and molecules to magnetic defects in solids, the GW approach has been applied almost exclusively to closed-shell systems. In this talk, we discuss some of the problems with existing GW calculations for degenerate systems, such as spin contamination, the multiplet problem, and the proper definition of the Green function in open-shell systems. Different formulations to overcome these problems are explored.

[1]This work was supported by National Science Foundation Grant No. DMR10-1006184, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at Lawrence Berkeley National Laboratory's NERSC facility

9:24AM H18.00008 Ab-initio theory of spin fluctuations in magnets , VLADIMIR ANTROPOV, LIQIN KE, Ames Laboratory, MARK VAN SCHILFGAARDE, Arizona State University, MIKHAEL KATSNELSON, Radboud University of Nijmegen — We propose a framework for a true ab initio theory of magnetism, based on many-body perturbation theory (MPBT). It fits in naturally with methods based MPBT such as the GW approximation; but the approach can be implemented as an extension to any existing static method for electronic structure such as the local spin density approximation to density functional theory, to include spin fluctuations. Initially we calculated the spin fluctuation contributions using random phase approximation. The self consistency procedure similar to the one used in Moryia-Kawabata theory can be naturally implemented. The fluctuation dissipation theorem is used to calculate the reduction of the mean field magnetic moment in itinerant magnets. The applications of the technique includes traditional 3d ferromagnetic metals, their alloys and compounds and 5f systems.

9:36AM H18.00009 A GW-based many-body perturbation theory approach for investigating materials with strong spin-orbit coupling , BRADFORD BARKER, JACK DESLIPPE, OLEG YAZYEV, STEVEN LOUIE — Spin-orbit coupling is an essential ingredient in understanding the electronic properties of materials of recent interest. We have developed a means of incorporating spin-orbit coupling to the quasiparticle excitations in solids within the GW approach. We apply our method to the properties of materials with heavy ion cores. This work was supported by National Science Foundation Grant No. DMR10-1006184, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by NERSC.

9:48AM H18.00010 Self-consistent band-structure calculations at GW quality and DFT expense[1] , STEPHAN LANY, P. GRAF, M. D'AVEZAC, A. ZUNGER, Natl. Renewable Energy Lab., CO — GW provides rather accurate quasi particle energies where approximate DFT methods tend to fail, yet are too computer intensive for complex inorganic materials (large systems or dense Brillouin zone sampling) that are currently of interest, e.g. for energy conversion. We explore the possibility that the trends of the GW quasi-particle energy corrections due to the non-local and energy dependent self-energy Σ(r,r',E) can be captured by atomic potentials that do not significantly increase the computational effort of a standard DFT calculation. We proceed in 4 steps: (i) Perform GW reference calculations for II-VI and III-V semiconductors (ii) Define atomic potentials that are added to the DFT Hamiltonian. Here we extend the concept of the non-local external potentials (NLEP) of Ref. [1], now allowing for two parameters per atom type and angular momentum. (iii) Fit the NLEP parameters to the GW test set. (iv) Finally, we test transferability by applying the potentials to the III_2-VI_3 and II_3-V_2 compounds that were not included in the fitting set.

[1] S. Lany, H. Raebiger, A. Zunger, Phys. Rev. B 77, 241201(R) (2008).

[1]This work was supported through the Center for Inverse Design, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

10:00AM H18.00011 The sc-COHSEX+GW and the static off-diagonal GW approaches to quasiparticle wavefunctions and energies , JACK DESLIPPE, MANISH JAIN, GEORGY SAMSONIDZE, MARVIN COHEN, STEVEN LOUIE, University of California at Berkeley and Lawrence Berkeley National Lab — Within the conventional GW approach, density functional theory (DFT) is typically used as a mean-field starting point; the self-energy operator is evaluated to 1st order in the DFT Green's function G_0 and screened Coulomb interaction W_0. The quasiparticle energies are calculated from diagonal elements of Σ in the DFT orbital basis. This approach works extraordinarily well for many materials but has limitations when the DFT states are far from the quasiparticle wavefunctions. In such cases, off-diagonal elements of Σ in the mean-field basis are large and the full Σ matrix is needed. The slow convergence of the off-diagonal elements make approaches requiring the explicit construction of this matrix prohibitively expensive. We present two alternative approaches based on the static (COHSEX) approximation that efficiently include the mean-field off-diagonal matrix element effects: a sc-COHSEX+GW approach where a renormalized basis is obtained from a self-consistent evaluation of quasiparticle wavefunctions in the static approximation and a less intensive treatment of just the off-diagonal elements within the COHSEX approximation. We show examples of the approaches for molecules and crystalline systems. Support by NSF DMR10-1006184, DOE DE-AC02-05CH11231.

10:12AM H18.00012 Constructing unoccupied states for G_0W_0 quasiparticle calculations from plane-waves , GEORGY SAMSONIDZE, MANISH JAIN, JACK DESLIPPE, MARVIN L. COHEN, STEVEN G. LOUIE, Department of Physics, University of California, Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 — Standard methods of first-principles calculations of the quasiparticle energies within the G_0W_0 scheme require summing over large numbers of unoccupied states. The generation of these states within the ab initio pseudopotential plane-wave density functional theory (DFT) quickly becomes a bottleneck of the calculation with increasing system size, especially in low-dimensional systems. In this work, we propose a method for approximating the high-energy continuum and resonant states in low-dimensional systems. The continuum and resonant states above a chosen energy are replaced with symmetrized plane-waves and localized DFT states computed with short-range localized basis functions (such as in the SIESTA code), respectively. The Gram-Schmidt process is used to orthogonalize these constructed high-energy unoccupied states. The method opens a route towards precise G_0W_0 quasiparticle calculations in large low-dimensional systems using a small number of unoccupied DFT states. This work was supported by NSF Grant No. DMR10-1006184, the U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by NSF through TeraGrid at NICS and DOE at LBNL's NERSC.

10:24AM H18.00013 On-site screened Coulomb interactions for localized electrons in transition metal oxides and defect systems , BI-CHING SHIH, Department of Physics, University at Buffalo, State University of New York, PEIHONG ZHANG, Department of Physics, University at Buffalo, State University of New Your, DEPARTMENT OF PHYSICS TEAM — Electronic and structural properties of strongly correlated material systems are largely determined by the strength of the on-site Coulomb interaction. Theoretical models devised to capture the physics of strongly correlated materials usually involve screened Coulomb interactions as adjustable parameters. We present first-principles results for the screened on-site Coulomb and exchange energy for transition metal oxides. The dielectric screening is calculated within the random phase approximation and the localized electrons are represented by maximally localized Wannier functions. We further extend our study to calculate on-site Coulomb interactions for localized defect states in semiconductors. We acknowledge the computational support provided by the Center for Computational Research at the University at Buffalo, SUNY. This work is supported by the National Science Foundation under Grant No. DMR-0946404 and by the Department of Energy under Grant No. DE-SC0002623.

10:36AM H18.00014 Optimizing Generalized Norm-Conserving Pseudopotentials , D.R. HAMANN, Dept. of Physics & Astronomy, Rutgers University — The "generalized" method permits the construction of norm-conserving pseudopotentials at energies that do not correspond to bound atomic states, giving added flexibility in the treatment of angular-momentum channels for which no bound states exist.[1] An effective method for optimizing the convergence of pseudopotential calculations with plane-wave-basis cutoff energy requires atomic wave functions with decaying tails, and has not been applicable to such "generalized" states.[2] By introducing a potential well outside the core radius for selected angular-momenta, an artificial decaying tail can be produced for positive-energy states. This permits the application of the optimization method, and we find convergence behavior comparable to that for ordinary bound states. In practice, we terminate the positive-energy all-electron wave function smoothly with an exponential or Gaussian tail, and never need to treat the implied well potential explicitly. The projectors to form fully-nonlocal operators[3] can be terminated at the core radii as usual, despite differences of the semi-local potentials outside the well radii.

[1]D. R. Hamann, Phys. Rev. B **40**, 2980 (1989).
[2]A. M. Rappe, *et al.*, Phys. Rev. B **41**, 1227 (1990).
[3]L. Kleinman and D. M. Bylander, Phys. Rev. Lett. **48**, 1425 (1982).

10:48AM H18.00015 Development of a Semi-empirical Hamiltonian for Phosphorus for Quantum Mechanics Based Simulations of Phosphorous-based Nanostructures , PAUL TANDY, CHRISTOPHER LEAHY, MING YU, C.S. JAYANTHI, S.Y. WU, University of Louisville — We have developed a parameterized semi-empirical Hamiltonian for phosphorous for simulation studies of phosphorous-based nanostructures including phosphorous-doped silicon nanowires.This Hamiltonian models the environment-dependent electron-ion and ion-ion interactions and electron-electron correlations, by capturing the salient features of *ab initio* Hamiltonians/*ab initio* methods, (*e.g.*, electron screening and charge self-consistency).Such a semi-empirical Hamiltonian has been shown to be successful in predicting the properties of intermediate-sized silicon, boron, and carbon clusters and extended structures of boron and silicon [1-4]. We optimized the parameters of our Hamiltonian for phosphorous by fitting the properties of bulk (black phosphorous) and small clusters (P_2 to P_{10}) as obtained by our method to *ab initio* calculations. It is expected that such a Hamiltonian will have the predictive power to enable the study of larger phosphorous based nanostructures that are not possible via *ab initio* studies.

[1] C. Leahy, et al, Phys. Rev. B 74,155408 (2006). [2]P. Tandy, et al, Bulletin of the APS,2009 APS March Meeting Vol. 54, Num.1, Sess. D26, [3] Ming Yu, et al, J. Chem. Phys. 130,184708 (2009). [4] Ming Yu, S.Y. Wu, and C.S. Jayanthi, Physica E 42, 1 (2009).

Tuesday, March 22, 2011 8:00AM - 11:00AM –

Session H19 GMAG DMP: Focus Session: Spin Transport & Magnetization Dynamics in Metals III D170

8:00AM H19.00001 Large and inverted spin signals in nonlocal spin valves , YI JI, HAN ZOU, SIU-TAT CHUI, XIAOJUN WANG, University of Delaware — For a metallic nonlocal spin valve (NLSV), usually the nonlocal resistance value is high for the parallel (P) state of spin injector and detector and the value is low for the antiparallel (AP) state. The difference between two states is known as the spin signal. We show that a 6 miliohms spin signal was observed in a typical NLSV device. However, in another NLSV device with apparently similar structure and dimensions as the previous one, we found a very large spin signal of 90 milliohms with an inverted sign, meaning that the P state yields a low value and the AP state yields a high value. The resistance between the spin detector and the Cu channel is extremely large, exceeding mega-ohms. We conclude that a break-junction is formed at the detector/Cu interface due to static discharge. The large magnitude of the spin signal is due to the spin-charge coupling at the low-conductance break-junction interface. The inverted sign is due to a very different spin-dependent density of states near the break-junction. Work supported by DOE grant No. DE-FG02-07ER46374.

8:12AM H19.00002 Spin transfer effects in non-local spin valves with sustained d.c. currents , HAN ZOU, YI JI, University of Delaware — We utilized pure spin current in a nonlocal spin valve (NLSV) for spin-transfer. The submicron lateral device consists of a Py spin injector (80 nm wide), a Py spin detector (60 nm wide), and a Cu nonmagnetic channel (100 nm wide). The thickness of the spin detector is 3.5 nm, and a nanoscale magnetic domain (60 nm by 100 nm) in the detector underneath the Cu channel can be switched by spin-transfer. We explore reversible spin-transfer switching over a wide temperature range and using both d.c. current pulses and sustained dc currents. Since a d.c. current changes the baseline of the nonlocal resistance, spin-transfer in NLSV has only been explored by d.c. current pulses. In this work, we achieved NLSV spin-transfer with sustained d.c. currents. The hysteresis of nonlocal resistance as a function of the sustained current is clearly observed, despite the baseline variations. High field and polarity-dependent features in the nonlocal MR curves indicate evidence of spin-transfer induced magnetization dynamics. Work supported by US DOE grant No. DE-FG02-07ER46374.

8:24AM H19.00003 Spin injection into ferromagnetic insulators , SABURO TAKAHASHI, Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan, JUN-ICHIRO OHE, HIROTO ADACHI, SADAMICHI MAEKAWA, Advanced Science Research Center, Japan Atomic Energy Agency, Tokai 319-1195, Japan — Spin current in a junction of a normal metal and a ferromagnetic insulator is theoretically studied. At the interface, spins of conduction electrons in a normal metal interact with localized spins in ferromagnetic insulator through the exchange interaction. When a spin accumulation is present in the normal metal, accumulated spins decay into magnons via spin-flip scattering of conduction electrons at the interface, thereby creating a magnon spin current in the ferromagnet. Using the linear response theory, we calculate the spin current across the interface and find that spin accumulation plays a role of spin voltage for generating the spin current thorough the junction. Using the spin Hall effect, the spin current injection from a normal metal into a ferromagnetic insulator is demonstrated. We also discuss the spin current in the presence of temperature difference between the normal metal and the ferromagnetic insulator.

8:36AM H19.00004 Quantifying Spin Hall Effects in Nonmagnetic Metals[1] , AXEL HOFFMANN[2], Materials Science Division, Argonne National Laboratory — Spin Hall effects intermix spin and charge currents even in nonmagnetic materials and, therefore, offer the possibility to generate and detect spin currents without the need for using ferromagnetic materials. In order to gain insight into the underlying physical mechanism and to identify technologically relevant materials, it is important to quantify the spin Hall angle γ, which is a direct measure of the charge-to-spin (and vice versa) conversion efficiency. Towards this end we utilized non-local transport measurements with double Hall bars fabricated from gold and copper.[3] In principle, this geometry permits the study of spin currents both generated and detected via spin Hall effects. We observe an unusual non-local resistivity that changes sign as a function of temperature. However, this results is quantitatively similar in gold and cooper, indicating that the non-local signals are not due to spin transport. An analysis of the data based on a combination of diffusive and quasi-ballistic transport leads to an upper limit of $\gamma < 0.027$ for gold at room temperature. Therefore we developed an approach based on spin pumping, which enables us to quantify even small spin Hall angles with high accuracy. Spin pumping utilizes microwave excitation of a ferromagnetic layer adjacent to a normal metal to generate over a macroscopic area a homogeneous *dc* spin current, which can be quantified from the line-width of the ferromagnetic resonance. In this geometry voltages from spin Hall effects scale with the device dimension and therefore good signal-to-noise can be obtained even for materials with small spin Hall angles. We integrated ferromagnet/normal metal bilayers into a co-planar waveguide and determined the spin Hall angle for a variety of non-magnetic materials (Pt, Pd, Au, and Mo) at room temperature. Of these materials Pt shows the largest spin Hall angle with $\gamma = 0.013 \pm 0.002$.[4]

[1]Financial support was through U.S. Department of Energy, Office of Science under Contract no. DE-AC02-06CH11357.

[2]It is a great pleasure to acknowledge my excellent collaborators: O. Mosendz, G. Mihajlović, V. Vlaminck, H. Schultheiß, J. E. Pearson, F. Y. Fradin, S. D. Bader, M. A. Garcia, T. Hirahara, and G. E. W. Bauer.

[3]G. Mihajlović, J. E. Pearson, M. A. Garcia, S. D. Bader, and A. Hoffmann, Phys.Rev. Lett. **103**, 166601 (2009).

[4]O. Mosendz, V. Vlaminck, J. E. Pearson, F. Y. Fradin, G. E. W. Bauer, S. D. Bader, and A. Hoffmann, arXiv:1009.5089; O. Mosendz, J. E. Pearson, F. Y. Fradin, G. E. W. Bauer, S. D. Bader, and A. Hoffmann, Phys. Rev.Lett.**104**, 046601 (2010).

9:12AM H19.00005 Giant spin Hall effect of Au films with Pt impurities: Surface-assisted skew scattering , BO GU, Japan Atomic Energy Agency, TIMOTHY ZIMAN, Institut Laue Langevin, GUANG-YU GUO, National Taiwan University, NAOTO NAGAOSA, University of Tokyo, SADAMICHI MAEKAWA, Japan Atomic Energy Agency — We show theoretically a novel route to obtain giant room temperature spin Hall effect (SHE) using surface-assisted skew scattering. By a combined approach of density functional theory and the quantum Monte Carlo (QMC) method, we have studied the SHE due to a Pt impurity in different Au hosts. We show that the spin Hall angle (SHA) could become larger than 0.1 on the Au (111) surface, and decreases by about a half on the Au (001) surface, while it is small in bulk Au. The QMC results show that the spin-orbit interaction (SOI) of the Pt impurity on the Au (001) and Au (111) surfaces is enhanced, because the Pt 5 levels are lifted to the Fermi level due to the valence fluctuations. In addition, there are two SOI channels on the Au (111) surface, while only one for Pt either on the Au (001) surface or in bulk Au.

9:24AM H19.00006 Spin Hall angle in Pd below the spin diffusion length[1] , V. VLAMINCK, H. SCHULTHEISS, J. PEARSON, F. FRADIN, S. BADER, A. HOFFMANN, Argonne National Laboratory, O. MOSENDZ, Hitachi San Jose Research Center — The spin-orbit coupling gives rise to an inter-conversion of spin and charge currents. A pure spin current is accompanied by a charge accumulation perpendicular to both the spin polarization and spin current, so-called inverse spin Hall effect (ISHE). We report measurements of the ISHE in a permalloy/palladium (Py/Pd) bilayer integrated with a coplanar wave-guide by pumping a pure spin current via ferromagnetic resonance (FMR) [1]. The magnetization precession creates a spin accumulation at the Py/Pd interface that diffuses into the normal metal and partially scatters back into the permalloy when the Pd thickness is smaller than the spin diffusion length. We observe an increasing broadening of the FMR linewidth with increasing thickness of Pd from which we extract the spin diffusion length in Pd and an average spin mixing conductance. The resultant pure spin current induces, in turn, a spin Hall voltage that is measured across the metallic layer. The spin Hall angle obtained from fitting the dc voltage [1] remains fairly constant even for thickness smaller than the spin diffusion length.

[1] O. Mosendz et al., Phys. Rev. B (in press). arXiv: 1009.5089

[1]U.S. Department of Energy, contract No. DE-ACOZ-06CH11357.

9:36AM H19.00007 Spin Torque Ferromagnetic Resonance Induced by the Spin Hall Effect , LUQIAO LIU, TAKAHIRO MORIYAMA, DAN RALPH, ROBERT BUHRMAN, CORNELL UNIVERSITY TEAM — We demonstrate that the spin Hall effect in a thin film with strong spin-orbit scattering can excite magnetic precession in an adjacent ferromagnetic film. The flow of alternating current through a Pt/NiFe bilayer generates an oscillating transverse spin current in the Pt, and the resultant transfer of spin angular momentum to the NiFe induces ferromagnetic resonance (FMR) dynamics. The Oersted field from the current also generates an FMR signal but with a different symmetry. The ratio of these two signals allows a quantitative determination of the spin current. As an independent check, we also apply a DC charge current to the Pt/NiFe bilayer while measuring the FMR signal. The effective damping of the NiFe layer can be increased or decreased depending on the relative angle between the magnetic moment and the injected spin. The amplitude of spin current extracted from this measurement agrees quite well with that obtained from the FMR lineshape. The self-calibration nature of this new technique makes it an excellent solution for a quantitative measurement of the SHE in a ferromagnetic/non-magnetic metal bilayer.

9:48AM H19.00008 Spin-orbit dichroism in SX-ARPES of Pt(111)[1] , JUN MIYAWAKI, ASHISH CHAINANI, YASUTAKA TAKATA, MASAKI OURA, RIKEN SPring-8 Center, YASUNORI SENBA, HARUHIKO OHASHI, JASRI/SPring-8, SHIK SHIN, RIKEN SPring-8 Center, ISSP Univ. Tokyo — We study the bulk electronic structure of Pt(111) using polarization dependent soft x-ray (SX)-ARPES ($h\nu$=450–610 eV). Pt is known to exhibit the largest spin Hall conductivity of all metals, which is derived from its large spin orbit coupling [1,2]. We have measured band dispersions along Γ-K-X ($h\nu$=466 eV) with clockwise and counterclockwise circularly polarized x-rays and obtained circular dichroism (CD) in the valence band of Pt. A comparison with calculated band dispersions including spin-orbit coupling gives a very good match with the experimental results [3,4], thus establishing the role of spin-orbit coupling in the electronic structure of Pt. Our results also identify (i) a hybridization gap with symmetry switching dichroism and (ii) strong CD of bands at the Fermi level, which provide the carriers responsible for SHE.
[1] T. Kimura, *et al.*, Phys. Rev. Lett. **98**, 156601 (2007). [2] M. Morota, *et al.*, arXiv:1008.0158v1. [3] G. Y. Guo, *et al.*, Phys. Rev. Lett. **100**, 096401 (2008). [4] A. D. Corso and A. M. Conte, Phys. Rev. B **71**, 115106 (2005).

[1]The present work has been performed under the approval of RIKEN (Proposal No. 20100055).

10:00AM H19.00009 Anisotropic Spin Hall Effect from First Principles[1] , FRANK FREIMUTH, STEFAN BLÜGEL, YURIY MOKROUSOV, Institut fuer Festkoerperforschung & Institute for Advanced Simulation, Forschungszentrum Juelich and JARA, 52425 Juelich, Germany — We present first principles calculations [1] of the intrinsic non-dissipative spin Hall conductivity (SHC) for $3d$, $4d$ and $5d$ transition metals focusing in particular on the anisotropy of the SHC in nonmagnetic hcp metals and in antiferromagnetic Cr. For the metals of this study we generally find large anisotropies. We derive the general relation between the SHC vector and the direction of spin-polarization and discuss its consequences for hcp metals. Especially, it is predicted that for systems where the SHC changes sign due to the anisotropy the spin Hall effect may be tuned such that the spin polarization is parallel either to the electric field or to the spin current. Additionally, we describe our computational method [2,3] emphasizing the Wannier interpolation technique and the definition of the conserved spin current.

[1] e-print: http://arxiv.org/abs/1011.2714
[2] F. Freimuth et al. Phys. Rev. B **78**, 035120 (2008)
[3] www.flapw.de

[1]This work is supported by the DFG Project MO 1731/3-1 and HGF-YIG grant VH-NG-513.

10:12AM H19.00010 Detection of the transverse voltage associated with the spin Seebeck effect in ferromagnetic thin films , AZURE D. AVERY, RUBINA SULTAN, DAIN BASSETT, University of Denver, MATTHEW R. PUFALL, National Institute of Standards and Technology, Boulder, CO, BARRY L. ZINK, University of Denver — The spin Seebeck effect, the generation of spin current in response to an applied thermal bias across a sample, is a novel effect involving spin current that is being researched in nanostructures for advances in spin caloritronics. Understanding the fundamental physics governing heat transport at the nanoscale is challenging because thermal properties of nanostructures are often difficult measurements to make. We present a novel technique for detecting the presence of a thermally generated spin current based on a micromachined thermal isolation platform. Our technique offers advantages including the ability to measure this effect in a reduced dimension sample, to reverse the thermal gradient, and to generate a large $\triangle T$ across the sample. We present results for a range of thin films and compare to previously reported similar larger scale structures. We discuss future experiments to probe the local nature of the spin Seebeck effect, additional thermal properties including the traditional Seebeck effect and thermal conductivity, and the application of our technique to an array of nanowires.

10:24AM H19.00011 Gigantic enhancement of spin Seebeck effect by phonon drag , HIROTO ADACHI, Japan Atomic Energy Agency, KEN-ICHI UCHIDA, EIJI SAITOH, Tohoku University, JUN-ICHIRO OHE, Japan Atomic Energy Agency, SABURO TAKAHASHI, Tohoku University, SADAMICHI MAEKAWA, Japan Atomic Energy Agency — We investigate both theoretically and experimentally a gigantic enhancement of the spin Seebeck effect [K. Uchida et al., Nature 455, 778 (2008); C. M. Jaworski et al., Nature Mater. 9, 898 (2010); K. Uchida et al., Nature Mater. 9, 894 (2010)] in a prototypical magnet $LaY_2Fe_5O_{12}$ at low temperatures. Our theoretical analysis sheds light on the important role of phonons; the spin Seebeck effect is enormously enhanced by nonequilibrium phonons that drag the low-lying spin excitations. We further argue that this scenario gives a clue to understand the observation of the spin Seebeck effect that is unaccompanied by a global spin current, and predict that the substrate condition affects the observed signal.

10:36AM H19.00012 Two Exponentials Associated with Temperature in Spin-Seebeck Effect Geometry[1] , WAYNE SASLOW, MATTHEW SEARS, Texas A&M University — Recent experiments report the observation of a Spin-Seebeck effect, where an applied thermal gradient along (x) a very thin (z), narrow (y) ferromagnetic sample F is associated with a spin current.[2] In present geometries this spin current is measured indirectly via a Pt bar above (z) the sample; a voltage difference V along y is measured and interpreted as being due to a spin current j_s into (z) the Pt, which then causes an inverse Spin Hall effect (j_s causes transverse V). Measured voltages often show a $\sinh(x/s)$ dependence, where s is long compared to any relevant spin-diffusion length.[3] The spin current has been interpreted as accompanying a temperature disequilibrium between the phonons and magnons in F.[4] The present work uses irreversible thermodynamics to include magnon-phonon equilibration in F and the thermal properties of the (non-magnetic) substrate S. We find two exponentials describing the overall thermal response along x, the second one associated with equilibration between F and S. If the thermal coupling between F and S is poor, then the second length can be rather long.

[1]Supported by Department of Energy grant DE-FG02-06ER46278.
[2]K. Uchida et al, Nature 455, 778 (2008).
[3]C. M. Jaworski et al, Nature Materials 9, 898 (2010).
[4]J. Xiao et al, Phys. Rev. B 81, 214418 (2010).

10:48AM H19.00013 Dissipationless mechanism of skyrmion Hall effect in two-dimensional double-exchange ferromagnets , SHIGEKI ONODA, Condensed Matter Theory Laboratory, RIKEN, KI-SEOK KIM, Asia Pacific Center for Theoretical Physics and Department of Physics, Pohang University of Science and Technology — We revisit a theory of nonequilibrium single-skyrmion transport in two-dimensional double-exchange ferromagnets with the Rashba spin-orbit interaction. Combining the collective-coordinate approach with the Keldysh formalism and an effective U(1) gauge theory, the velocity of a skyrmion core is calculated under the electric field. Then, it is found that the emergent Chern-Simons term and the associated intrinsic anomalous Hall can produce a dissipationless skyrmion Hall current through the coupling between electrons and localized spins, which takes the form of the spin transfer torque. In metals, this is additive to the conventional dissipative motion of magnetic vortices, which relies on phenomenological damping terms in the Landau-Lifshitz-Gilbert equation.

Tuesday, March 22, 2011 8:00AM - 11:00AM –

Session H20 FIAP/DMP GERA/DCOMP: Focus Session: Physics of Energy Storage Materials III – Hydrogen Storage Adsorbents D168

8:00AM H20.00001 Strategies for Hydrogen Storage in Nanoporous Metal-Organic Framework Materials , RANDALL SNURR, Northwestern University — Storing hydrogen by physisorption in porous materials is a challenging problem of great interest for future vehicle technology. Metal-organic frameworks (MOFs) are a new class of nanoporous materials that have demonstrated exciting potential for solving this problem. MOFs are synthesized by the self-assembly of metal nodes and connecting organic linker molecules to create stable, porous frameworks. The synthetic chemistry opens the possibility to create an almost unlimited number of MOFs and to tailor them for particular applications, such as hydrogen storage. The diversity of MOFs also creates an opportunity to learn more about the fundamentals of hydrogen adsorption in porous materials. We have used a combination of classical Monte Carlo simulations and quantum mechanical approaches to investigate fundamental questions about hydrogen storage in MOFs and to design new materials with improved storage capabilities. Relationships have been elucidated between hydrogen uptake and properties such as the MOF surface area, void volume, degree of catenation, enthalpy of adsorption, and cation content. Introduction of cations is a promising strategy to improve hydrogen uptake at room temperature, and different metal cations and different strategies for introducing them into MOFs have been screened computationally.

8:36AM H20.00002 Increased hydrogen uptake of MOF-5 by powder densification , DONALD SIEGEL, JUSTIN PUREWAL, Mechanical Engineering Department, University of Michigan, DONG'AN LIU, ANDREA SUDIK, JUN YANG, Ford Motor Company, STEFAN MAURER, ULRICH MULLER, BASF SE — The metal-organic framework MOF-5 has attracted significant attention due to its ability to store large quantities of H_2 by mass, up to 10 wt.% absolute at 70 bar at 77K. On the other hand, since MOF-5 is typically obtained as a bulk powder, it exhibits a low volumetric density and poor thermal conductivity—both of which are undesirable characteristics for a hydrogen storage material. Here we explore the extent to which powder densification can overcome these deficiencies, as well as to characterize the impact of densification on crystallinity, pore volume, surface area, and crush strength. MOF-5 powder was processed into cylindrical tablets with densities up to 1.6 g/cm^3 by mechanical compaction. We find that optimal hydrogen storage properties are achieved for $\rho \sim 0.5$ g/cm^3, yielding a 350% increase in volumetric H_2 density with only a modest 15% reduction in gravimetric H^2 excess in comparison to the powder. Higher densities result in larger reductions in gravimetric excess. Total pore volume and surface area decrease commensurately with the gravimetric capacity, and are linked to an incipient amorphization transformation. Nevertheless, a large fraction of MOF-5 crystallinity remains intact in densities up to 0.75 g/cm^3, as confirmed from powder XRD.

8:48AM H20.00003 First-principles study of hydrogen adsorption in metal-doped COF-10 , M.M. WU, Q. WANG, Q. SUN, P. JENA, Y. KAWAZOE, DEPARTMENT OF ADVANCED MATERIALS AND NANOTECHNOLOGY, PEKING UNIVERSITY TEAM, DEPARTMENT OF PHYSICS, VIRGINIA COMMONWEALTH UNIVERSITY COLLABORATION, INSTITUTE FOR MATERIALS RESEARCH, TOHOKU UNIVERSITY COLLABORATION — Covalent organic frameworks (COFs), due to their low-density, high-porosity, and high-stability, have promising applications in gas storage. In this study we have explored the potential of COFs doped with Li and Ca metal atoms for storing hydrogen under ambient thermodynamic conditions. Using density functional theory we have performed detailed calculations of the sites Li and Ca atoms occupy in COF-10 and their interaction with hydrogen molecules. The binding energy of Li atom on COF-10 substrate is found to be about 1.0 eV and each Li atom can adsorb up to three H2 molecules. However, at high concentration, Li atoms cluster and, consequently, their hydrogen storage capacity is reduced due to steric hindrance between H2 molecules. On the other hand, due to charge transfer from Li to the substrate, O sites provide additional enhancement for hydrogen adsorption. With increasing concentration of doped metal atoms, the COF-10 substrate provides an additional platform for storing hydrogen. Similar conclusions are reached for Ca doped COF-10.

9:00AM H20.00004 Enhanced Dihydrogen-Metal Interaction in Transition Metal Exposed Paddle-Wheel Frameworks , YONG-HYUN KIM, KAIST, JOONGOO KANG, SU-HUAI WEI, National Renewable Energy Laboratory, JI HYUN BAK, KAIST — The experimentally observed enhancement of hydrogen adsorption in Cu_2-tetracarboxylate paddle-wheel frameworks is investigated by first-principles density-functional theory calculations [1]. We reveal that the puzzling enhancement is due to the effective orbital coupling between the occupied H_2 σ and the unoccupied Cu 4s-derived states. The nontrivial dihydrogen-metal σs interaction is enabled by a strong localization of the Cu 4s orbital after hybridizing with the neighboring oxygen 2p orbitals. Based on this understanding, we predict that the dihydrogen-metal interaction can be further increased by alloying Cu with s-orbital element Zn or Mg. We will also discuss on the enhanced dihydrogen adsorption on other 3d-transition-metal paddle wheel frameworks.

[1] Y.-H. Kim, J. Kang, and S.-H. Wei, Phys. Rev. Lett., in press (2010).

9:12AM H20.00005 Iron decorated - functionalized MOF for high-capacity hydrogen storage: First-principles calculations , MOON-HYUN CHA, JISOON IHM, Department of Physics and Astronomy, Seoul National University — We perform electronic structure calculations for the Fe-decorated, OH-functionalized isoreticular metal organic framework 16 (IRMOF16) to investigate the hydrogen storage capacity. Because of the relatively strong Kubas interaction between Fe and H_2, hydrogen molecule can be adsorbed on the proposed MOF even at room temperature. The reversibly usable storage capacity under ambient conditions reaches 6.0 wt%. Fe has a much lower oxidation tendency than other metals (e.g., Ti, Ca, or Li) used for decorating backbone structures and therefore far more convenient in practical implementation. We also find that the spin flip, which comes from the competition between exchange field splitting and ligand field splitting, plays a significant role in the interaction between Fe and H_2.

9:24AM H20.00006 Study on Ca32C60 Cluster for Hydrogen Storage[1] , PING CUI, ZHILING DUN, MENG YE, RAN TAO, HAIPING LAN, U of Science and Technology of China, ZHENYU ZHANG, Oak Ridge National Laboratory, U of Tennessee-Knoxville, U of Science and Technology of China — Using first-principles calculations within density functional theory (DFT), we study the assembly of Ca32C60, the most desirable metal-coating fullerene as hydrogen storage medium. We first explore possible structures of Ca32C60 dimer with different initial configurations, and find a surprisingly large binding energy up to 2.8 eV. Our further analysis on electronic structures indicates that such a large binding strength stems from the enhanced chemical reactivity of Ca due to the Ca-3s valence electrons partially transferred to the fullerene. We then systematically investigate the alkali and alkali earth elements coated on fullerene, and find that the chemical reactivity of these metal elements can be tuned due to the large electron affinity of C60. Based on this finding, we then extend our studies to the bulk form and two-dimensional structures of Ca32C60, and propose an optimum assemble structure for hydrogen storage. These results shall facilitate designing and optimizing carbon-based materials for hydrogen storage.

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

9:36AM H20.00007 Interaction potential and IR absorption of endohedral H_2 in C_{60}[1] , TOOMAS ROOM, MIN GE, D. HUVONEN, U. NAGEL, Nat. Inst. of Chem. Phys. Biophys., Estonia, S. MAMONE, M.H. LEVITT, M. CARRAVETTA, Southampton Uni., UK, Y. MURATA, K. KOMATSU, Kyoto Uni., Japan, J.Y.-C. CHEN, N.J. TURRO, Columbia Uni. — We measured the IR spectra of a H_2 molecule trapped inside a C_{60} cage at temperatures from 6 to 300 K and analyzed the spectra by using a model of a vibrating rotor in a spherical potential. The electric dipole moment of IR transitions is induced by the translational motion of H_2. The rotation of H_2 is unhindered but coupled to the translational motion. The isotropic and translation-rotation coupling part of the potential are anharmonic and different in the ground and excited vibrational states of H_2. The vibrational frequency and the rotational constant of endohedral H_2 are smaller than in the gas phase. The assignment of IR lines to ortho- and para-H_2 is confirmed by measuring spectra of a para enriched $H_2@C_{60}$ and is consistent with the earlier interpretation of the low temperature IR spectra [S. Mamone *et al.*, J. Chem. Phys. **130**, 081103 (2009)].

[1]Support by the Estonian Ministry of Education and Research grant SF0690029s0 and SF grants ETF7011, ETF8170 and JD187 is acknowledged.

9:48AM H20.00008 Metallacarboranes: Towards promising hydrogen storage metal organic framework , ABHISHEK SINGH, Materials Research Centre, Indian Institute of Science, Bangalore 560012, India, ARTA SADRZADEH, BORIS YAKOBSON, Department of Mechanical Engineering and Materials Science, Rice University, Houston, Texas 77005, USA — Using first principles calculations we show the high hydrogen storage capacity of metallacarboranes,[1] where the transition metal (TM) atoms bind hydrogen via Kubas interaction. The average binding energy of ∼0.3 eV/H favorably lies within the reversible adsorption range The Sc and Ti are found to be the optimum metal atoms maximizing the number of stored H_2 molecules. Depending upon the structure, metallacarboranes can adsorb up to 8 wt% of hydrogen, which exceeds DOE goal for 2015. Being integral part of the cage, TMs do not suffer from the aggregation problem. Furthermore, the presence of carbon atom in the cages permits linking the metallacarboranes to form metal organic frameworks (MOF), thus able to adsorb hydrogen via Kubas interaction, in addition to van der Waals physisorption.

[1]A. K. Singh, A. Sadrzadeh, and B. I. Yakobson, Metallacarboranes: Toward Promising Hydrogen Storage Metal Organic Frameworks, JACS 132,14126 (2010).

10:00AM H20.00009 Anomalous Characteristics of a PVDC Carbon Adsorbant[1] , CARLOS WEXLER, MATTHEW BECKNER, JIMMY ROMANOS, TYLER RASH, PETER PFEIFER, RAINA OLSEN, University of Missouri Columbia — Nanoporous carbon produced by the pyrolisis of poly(vinylidene chloride-co-vinyl chloride) shows remarkably high adsorption of molecular hydrogen despite its relatively low surface area. In particular, its room temperature volumetric storage is significantly higher than other carbons with surface areas four times higher. In this talk we will present experimental hydrogen adsorption isotherms (and low-temperature isosteric heats of adsorption), subcritical nitrogen adsorption, real space images (TEM), and inelastic neutron scattering. In all cases, the sample characteristics are quite unusual. Whereas the sample under consideration is quite unusual in its high hydrogen sorption capacity, other samples in the literature also show similar unusual characteristics, suggesting the presence of phenomena not fully understood by standard adsorption theory.

[1]This material is based upon work supported in part by the Department of Energy under Award Nos. DE-FG02-07ER46411, DE-FG36-08GO18142, and DE-AC02-06CH11357.

10:12AM H20.00010 ABSTRACT WITHDRAWN –

10:24AM H20.00011 Inelastic Neutron Scattering from Hydrogen Adsorbed in Carbon[1] , RAINA OLSEN, MATTHEW BECKNER, HASKELL TAUB, PETER PFEIFER, CARLOS WEXLER, University of Missouri — Inelastic neutron scattering (INS) from adsorbed hydrogen offers a powerful tool to probe the local adsorption environment of storage material. We will show recently measured INS spectra of hydrogen adsorbed on four different carbon samples and discuss the interpretation of their spectral features, using previous theoretical calculations [1]. Both rotational and vibrational transitions can be observed, along with free recoil scattering parallel to the adsorption plane. The spectra from carbon nanotubes and activated carbon are well explained by theory. However, the spectra from PVDC carbon is quite unusual.

[1] R. Olsen, L. Firlej, B. Kuchta, H. Taub, P. Pfeifer, and C. Wexler; Sub-Nanometer Characterization of Activated Carbon by Inelastic Neutron Scattering; Carbon (under review).

[1]This material is based upon work supported in part by the Department of Energy under Award Nos. DE-FG02-07ER46411, DE-FG36-08GO18142, and DE-AC02-06CH11357.

10:36AM H20.00012 Analysis of hydrogen sorption characteristics of boron-doped activated carbons[1] , M. BECKNER, J. ROMANOS, D. STALLA, E. DOHNKE, A. SINGH, M. LEE, G. SUPPES, M.F. HAWTHORNE, P. YU, C. WEXLER, P. PFEIFER, U of Missouri — There is significant interest in the properties of boron-doped activated carbons for their potential to improve hydrogen storage.[2] Boron-doped activated carbons have been produced using a novel process involving the pyrolysis of a boron containing compound and subsequent high-temperature annealing. In this talk we will present a systematic study of the effect of different boron doping processes on the samples' surface area, micropore structure, and hydrogen sorption. Experimental results include boron content from prompt gamma neutron activation analysis, boron-carbon chemistry from Fourier transform infrared spectroscopy (FTIR), nitrogen subcritical adsorption, and 80K and 90K hydrogen adsorption isotherms which allow us to evaluate the hydrogen binding energy for each sorptive material.

[1]This material is based on work supported by the US Department of Defense under Awards No. N00164-07-P-1306 and N00164-08-C-GS37, the US Department of Energy under Awards No. DE-FG02-07ER46411 and DE-FG36-08GO18142.
[2]See http://all-craft.missouri.edu

10:48AM H20.00013 The effect of KOH:C and activation temperature on hydrogen storage capacities of activated carbons[1] , TYLER RASH, MATT BECKNER, JIMMY ROMANOS, ERIC LEIMKUEHLER, ALI TAKEEI, GALEN SUPPES, CARLOS WEXLER, PETER PFEIFER, University of Missouri — The Alliance for Collaborative Research in Alternative Fuel Technologies (ALL-CRAFT[2]) has been producing high surface area activated carbons. Here we will investigate the effect of the ratio of activating agent to carbon and activation temperature on hydrogen sorption characteristics and sample structure. Results show that a ratio of 3:1 KOH:C and an activation temperature of 790 C are the ideal activation conditions for hydrogen storage applications. Hydrogen sorption measurements are completed using a volumetric instrument that operates at pressures up to 100 bar and at temperatures of 80 K, the sublimation temperature of dry ice (-78.5 C), and room temperature. Specific surface area and pore size distributions are measured using subcritical nitrogen isotherms.

[1]This material is based on work supported by the US Department of Defense under Awards No. N00164-07-P-1306 and N00164-08-C-GS37, the US Department of Energy under Awards No. DE-FG02-07ER46411 and DE-FG36-08GO18142.
[2]See http://all-craft.missouri.edu

Tuesday, March 22, 2011 8:00AM - 11:00AM –

Session H21 GIMS: Focus Session: Advances in Scanned Probe Microscopy II – High Frequencies and Optical Techniques D161

8:00AM H21.00001 Rapid Serial Prototyping and Analysis of Nanomagnet-Tipped Attonewton-Sensitivity Cantilevers for Magnetic Resonance Force Microscopy[1] , JOHN MAROHN, ERIC MOORE, JONILYN LONGENECKER, Cornell Univ., Ithaca, NY 14853 — Magnetic resonance force microscopy offers exciting possibilities for imaging protons and electrons in native and spin-labeled biomolecules. The central component of a magnetic resonance force microscope experiment is a custom-fabricated attonewton-sensitivity cantilever with an overhanging magnetic-nanorod tip. We have recently developed a method for making precision tips which involves 1) fabricating overhanging magnetic tips on shortened mock cantilevers, 2) using focused ion beam milling and deposition (FIB/FID) to cut the mock cantilever (and attached tip) free from the substrate, and then 3) attaching the released structure to a full-length high-sensitivity cantilever. The resulting magnets have been characterized by cantilever magnetometry, high-resolution transmission electron microscopy (HR-TEM), and nanometer-resolution electron energy loss spectroscopy (EELS). This approach to fabrication and analysis is allowing us to optimize tips for proposed single-electron-spin imaging experiments in a very short time. Rapid access to such high-quality tips will significantly advance our ability to image individual biomolecules and macromolecular complexes.

[1]Funded by ARO, NIH, and NSF.

8:12AM H21.00002 Development of Magnet-on-Oscillator Low Temperature NMR Force Microscopy[1] , J.W. PASTER, J.T. MARKERT, Department of Physics, The University of Texas at Austin — We report recent advances for our nuclear magnetic resonance force microscopy (NMRFM) experiment. Force detection of nuclear spins is made possible by coupling NMR spin flip sequences to a mechanical oscillator. Periodic inversion of the spins in a magnetic field gradient provides the ac coupling force. The force sensitivity for NMRFM improves with decreasing distance between a small gradient magnet and the spins in a sample. Adapting a perpendicular oscillator orientation allows us to decrease the magnet-to-sample distance, providing increased sensitivity. We've also adapted a magnet-on-oscillator design. With this approach, we can perform experiments using oscillating cantilever-driven adiabatic reversal, a technique which has been used to detect single electron spins below the surface of a solid [1]. We've integrated an optical fiber interferometer to measure an oscillator's motion with sub nanometer precision. We can routinely measure the resonance frequencies, quality factors, and spring constants of various oscillators.

[1] Rugar D et al. Nature. 2004;430:329–332

[1]We acknowledge support from NSF DMR-0605828 and Welch F-1191

8:24AM H21.00003 Correlation of Noise in Multiple Cantilever Modes , DORAN SMITH, DIMITRI ALEXSON, US Army Research Lab — The ultrasensitive cantilevers utilized in frequency detection MRFM schemes are susceptible to noncontact interactions between the cantilever tip and the sample. Large efforts have been undertaken to comprehensibly understand the surface related dissipation mechanisms. We propose that sample dielectric fluctuations near DC frequencies should effect all the driven cantilever's oscillatory modes similarly. Utilizing the fundamental and second harmonic mode of the cantilever we have demonstrated this. The correlation between the frequency deviations of the two modes of a driven cantilever increases as the tip-to-sample distance decreases and the measured 1/f noise due to dielectric fluctuations becomes manifest. This result provides additional support for the theory developed by Yazdanian, Marohn and Loring, J. Chem. Phy. 128, 224706 (2008) explaining the origins of noncontact friction and frequency jitter.

8:36AM H21.00004 Nanoscale scanning probe ferromagnetic resonance imaging using localized modes[1] , P. CHRIS HAMMEL, Ohio State University — We report the demonstration of scanned probe ferromagnetic resonance imaging (FMRI), a new technique based on Magnetic Resonance Force Microscopy that offers a window into nanoscale properties of buried ferromagnets. Images have been obtained with a current resolution of 200 nm, and significant improvements are straightforwardly possible. Ferromagnetic Resonance (FMR) is a powerful spectroscopic tool for studying internal magnetic fields, interactions and dynamic magnetic properties of ferromagnetic systems, but conventional FMR measures global properties of an entire sample. In FMRI the "magnetic field well" created by the probe tip field confines the spin wave modes; these can then be scanned to obtain FMR images. This new microscope is unique in its ability to map internal magnetic fields in buried ferromagnets with spectroscopic precision and nanoscale resolution. First images in permalloy films reveal the ability to image inhomogeneities in magnetic properties with field resolution of approximately 1 Gauss/$\sqrt{\mathrm{Hz}}$. We report a first application to imaging the internal exchange bias field in exchange-biased films.

[1]Supported by the U.S. DOE through Grant No. DE-FG02-03ER46054.

9:12AM H21.00005 MRFM based spectroscopy of GaAs , DIMITRI ALEXSON, DORAN SMITH, US Army Research Lab — The apparent contradiction of how to perform NMR spectroscopy given the large magnetic field gradients present in MRFM is resolved by removing the magnetic field gradient while RF based NMR spectroscopic pulses are applied to the sample. This is accomplished by 1) shuttling (move) the sample away from the magnetic particle mounted on the cantilever, 2) apply RF spectroscopic pulse sequences to the sample, 3) store a component of the free induction decay along the z-axis, 4) shuttle the sample back to the cantilever, and 5) read out the magnetization stored on the z-axis with MRFM using an adiabatic rapid passage protocol (ARP). We will describe our progress on performing shuttle based spectroscopy of GaAs using MRFM. We will describe our measurements of T1 of Ga69 in GaAs with an inversion-recovery experiment. Using a single ARP sweep, the polarization is inverted and its recovery is monitored with a driven cantilever using the CERMIT protocol.

9:24AM H21.00006 Development of Variable Temperature NMR Force Microscopy[1] , ISAAC V. MANZANERA ESTEVE, JOHN T. MARKERT, University of Texas. Physics Department — We report our progress on the construction of a variable temperature NMR force microscopy probe and the development of its control system for three dimensional nanoscale scanning. The probe contains two 3-axis piezo-driven slip-stick motion stages for fiber interferometer and for gradient magnet positioning. The control station is a LabView software based control system capable to perform signal generation and data acquisition. Preliminary scan position dependent NMR Force measurements on ammonium sulfate $(NH_4)_2SO_4$ were performed at room temperature in a sample-on-oscillator configuration. Both piezo-driven and thermal noise cantilever motion have been analyzed to determine resonant frequencies ω_c, quality factor Q, and spring constants k; a typical cantilever yielded $\omega_c = 1494.40 \pm 0.10$Hz, $k = 0.039 \pm 0.004 N/m$, $Q = 93$. RF frequency-modulation-driven artifact effects have been observed and measured during analysis.

[1]We acknowledge support from DMR-0605828 and Welch F-1191

9:36AM H21.00007 Nitrogen Impurities in Diamond Studied using Magnetic Resonance Force Microscopy , MICHAEL HERMAN, PALASH BANERJEE, DENIS PELEKHOV, P. CHRIS HAMMEL, The Ohio State University — Spin-bearing defects and impurities in diamond have attracted much attention in recent years, with the N-V center defect being a good example. A related defect in the diamond lattice is comprised of a substitutional nitrogen alone and is known as the P1 center with an electron spin S = 1/2 localized on a N-C bond with a strong hyperfine coupling to the ^{14}N nuclear spin I = 1. We have used Magnetic Resonance Force Microscopy (MRFM) to study the properties of a small collection of P1 centers in diamond. By operating with large field gradients approaching a few Gauss per nanometer, we are able to couple fewer than 100 spins and probe their relaxation properties with a sensitivity approaching a few spins. We have seen that spin lifetimes in the rotating frame are dependent on impurity concentration. We'll show long spin lifetimes (>2 s) while undergoing tens of thousands adiabatic spin flips. We also show that spin lifetimes are shorter in diamond implanted with nitrogen ions to create P1 centers. This work was supported by The Army Research Office under W911NF-07-1-0305 and the National Science Foundation under DMR-0807093.

9:48AM H21.00008 Parametric Amplification Protocol for Frequency-Modulated Magnetic Resonance Force Microscopy Signals , LEE HARRELL, Department of Physics and Nuclear Engineering, U.S. Military Academy, West Point, NY, ERIC MOORE, SANGGAP LEE, STEVEN HICKMAN, JOHN MAROHN, Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY — We present data and theoretical signal and noise calculations for a protocol using parametric amplification to evade the inherent tradeoff between signal and detector frequency noise in force-gradient magnetic resonance force microscopy signals, which are manifested as a modulated frequency shift of a high- Q microcantilever. Substrate-induced frequency noise has a $1/f$ frequency dependence, while detector noise exhibits an f^2 dependence on modulation frequency f. Modulation of sample spins at a frequency that minimizes these two contributions typically results in a surface frequency noise power an order of magnitude or more above the thermal limit and may prove incompatible with sample spin relaxation times as well. We show that the frequency modulated force-gradient signal can be used to excite the fundamental resonant mode of the cantilever, resulting in an audio frequency amplitude signal that is readily detected with a low-noise fiber optic interferometer. This technique allows us to modulate the force-gradient signal at a sufficiently high frequency so that substrate-induced frequency noise is evaded without subjecting the signal to the normal f^2 detector noise of conventional demodulation.

10:00AM H21.00009 Nonlinear Near-Field Microwave Microscopy for RF Defect Localization in Nb-Based Superconducting Radio Frequency Cavities[1] , TAMIN TAI, University of Maryland — Niobium Superconducting Radio Frequency (SRF) cavities are very sensitive to localized defects that give rise to quenches at high accelerating gradients. In order to identify these defects via scanning microscopy, and to further understand the origins of the quench under high radio frequency excitation (1-3 GHz), a scanning probe with localized and up to ∼200 mT RF magnetic field is required for low temperature microscopy to achieve sub-micron resolution. For this purpose, we developed a micro loop probe on silicon substrate with outer diameter 20 μm and inner diameter 17 μm and successfully fabricated it by lithography. The probe has been used to identify a signal arising from the nonlinear Meissner effect in a Nb thin film. In addition, a magnetic write head is another promising candidate to achieve this goal of understanding localized defect behavior under high RF magnetic field at low temperatures [1]. We will discuss and compare both types of probe for nonlinear scanning microscopy and RF defect localization in superconductors.

[1] Tamin Tai, X. X. Xi, C. G. Zhuang, Dragos I. Mircea and Steven M. Anlage, "Nonlinear Near-Field Microwave Microscope For RF Defect Localization in Superconductors" (http://arxiv.org/abs/1008.2948)

[1]We acknowledge the support of DOE/HEP.

10:12AM H21.00010 Super-rolloff electron tunneling transduction of nanomechanical motion using frequency downmixing , MENG KAN, MARK FREEMAN, WAYNE HIEBERT, National Institute for Nanotechnology, National Research Council of Canada and Department of Physics, University of Alberta, Edmontonton, Canada — Electron tunneling transduction has high sensitivity for detecting the motion of nanomechanical devices, but the relatively low detection bandwidth of a few 10's of kHz has limited its development. Here we demonstrate a novel downmixing transduction scheme which eliminates the detection bandwidth problem of electron tunneling transduction. With this technique, the high frequency vibration modes (∼ 1 MHz) of a MEMS doubly clamped beam are measured. This measurement is 2 orders of magnitude above the electronic bandwidth of our readout circuitry with no fundamental limitation anticipated up to microwave frequencies. The displacement sensitivity is 40 fm/Hz$^{1/2}$ comparable to state-of-the-art low finesse free-space optical interferometry. The back-action force induced by the STM tip on the MEMS device is also explored and is shown to have a small effect on the measurement resonance frequency, causing slight resonance frequency shifts of order 1%.

10:24AM H21.00011 ABSTRACT WITHDRAWN –

10:36AM H21.00012 Toward Atomic-Scale Optical Probes with UHV STM[1] , ÖZGÜN SÜZER, LI GAO, JOSEPH A. SMERDON, JONGWEON CHO, NATHAN P. GUISINGER, JEFFREY R. GUEST, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL 60439, USA — We present the details of a variable temperature ultra-high vacuum (UHV) scanning tunneling microscopy (STM) apparatus with optical access for the investigation of optically active materials at the atomic scale. Local field enhancement in close proximity to the ultra-sharp STM tip enables the observation of optical signals from a very small number of surface adsorbates and even single molecules, which, combined with the electronic sensitivity and high spatial resolution of STM, allows the simultaneous optical, electronic, and topographic analysis of nanoscale systems. A high-numerical-aperture (NA) optic is integrated into the STM to achieve sharp and stable focusing of the laser excitation while maintaining polarization integrity and high collection efficiency. The initial findings of investigations carried out on epitaxial graphene grown on SiC and operational characteristics of the apparatus are discussed. A next-generation optically accessible 4K UHV STM apparatus under development is also introduced.

[1]This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-06CH11357 and "SISGR" Contract No. DE-FG02-09ER16109.

10:48AM H21.00013 Protecting TERS Probes While Keeping Extreme Enhancement , REBECCA AGAPOV, ANDREY MALKOVSKIY, The University of Akron, Dept. of Polymer Science, Akron, OH, ALEXEI SOKOLOV, Chemical Sciences Division, ORNL and Dept. of Chemistry, University of Tennessee, Knoxville, TN, MARK FOSTER, The University of Akron, Dept. of Polymer Science, Akron, OH — Protecting the probes used for tip enhanced Raman spectroscopy (TERS) with alumina coatings reduces chemical, mechanical and thermal degradation that otherwise limit the applicability of this emerging technique. Protected plasmonic structures are of interest for surface enhanced Raman spectroscopy (SERS) generally, especially for SERS-based sensors, but we focus particularly on the special case of TERS. Most recently we have focused on the detailed effect of the protective coating for cases in which the enhancement is particularly strong. "Blinking," which is characteristic of extreme enhancement, has been observed with TERS on polymer films for the first time. An Al_2O_3 coating prolongs the duration of blinking from 20 minutes to 2 days without significant detriment to the extreme enhancement. The fact that blinking has been observed in the presence of the alumina coating allows us to eliminate chemical enhancement as a major mechanism of the extreme enhancement evidenced by blinking.

Tuesday, March 22, 2011 8:00AM - 11:00AM –
Session H22 DCMP: Heavy Fermions D163

8:00AM H22.00001 Field-induced Spin Fluctuations in Intermetallic CeX_2Ge_2(X= Cu, Ag, Au) , DEEPAK SINGH, National Institute of Standard and Technology, A. THAMIZHAVEL, Tata Institute of Fundamental Research, SUNG CHANG, JEFFREY LYNN, National Institute of Standard and Technology — Intermetallic rare-earth compounds containing a lattice of 4 f or 5 f- electrons are prototypical systems to study the magnetic quantum phase transition which mainly results from the fluctuation of the antiferromagnetic moment at T= 0 K. Therefore, understanding the mechanism behind spin fluctuations is important towards a meaningful universal formulation of the QPT phenomena. We have performed magnetic, thermodynamic and neutron scattering measurements on CeX_2Ge2 (X = Cu, Ag, Au) compounds in single crystal form to further understand the mechanism behind spin fluctuations. CeX_2Ge_2 crystallize in a $ThCr_2Si_2$-type tetragonal crystal structure and undergo antiferromagnetic transitions at T_N = 4.2 K (Cu), 4.6 K (Ag) and 13.5 K (Au). Detail measurements of Q-vectors associated with the long-range order and the numerical modeling of the data revealed the propagation of amplitude modulated spin density wave in $CeCu_2Ge_2$ and $CeAg_2Ge_2$ with the propagation vectors of (0.29,0.29,0.52) and (0,0.705,0.11) respectively. Dynamic measurements of CeX_2Ge_2 compounds in applied magnetic field, exhibiting the varying nature of spin fluctuations as X changes, will be discussed and compared with other Ce-based intermetallic compounds.

8:12AM H22.00002 Growth and properties of heavy fermion thin films and superlattices[1] , YIZE LI, MAO ZHENG, BRIAN MULCAHY, L.H. GREENE, JAMES N. ECKSTEIN, University of Illinois at Urbana-Champaign — We have grown thin films of the heavy fermion phases $CeCu_2Ge_2$ (CCG) and $CeFe_2Ge_2$ (CFG) on MgO and DySrO3 substrates using molecular beam epitaxy. We find that the growth begins via island nucleation leading to a granular morphology, since there are two equivalent registrations of the film with the substrate. After nucleating, the grains grow flat with c-axis orientation. These single phase films show similar temperature(T) dependent transport behavior as seen in single crystals of the materials, including for CCG Kondo scattering and the emergence of coherent coupling of the heavy fermion transport channel at low T and for CFG a monotonic decrease in resistivity as the temperature is lowered. Superlattices combining CCG and CFG in different supercell architectures were also grown. In transport, they show a systematic evolution with composition between the distinct R(T) behavior of the two parent phases. A correlation between spectroscopic measurements and resistivity was found and details will be presented.

[1]This work is supported by DOE under Award No.DE-AC02-98CH10886.

8:24AM H22.00003 Neutron Scattering Study of the Field Induced Non-Fermi-Liquid Behavior in $CeAuSb_2$, SUNG CHANG, DEEPAK SINGH, NIST Center for Neutron Research, ARUMUGAM THAMIZHAVEL, Tata Institute of Fundamental Research — The modestly heavy Fermion compound $CeAuSb_2$ ($\gamma = 90$ mJ/K^2 mol) was reported to exhibit highly anisotropic magnetic properties with an antiferromagnetic transition temperature $T_N \approx 5$ K [1]. In addition, the unconventional temperature dependence of the resistivity and specific heat, observed when an external magnetic field suppresses T_N to 0 K, has lead to the identification of $CeAuSb_2$ as a system showing possible magnetic field-induced quantum critical behavior [2]. Here we report on neutron scattering measurements of $CeAuSb_2$ in magnetic fields up to 9 T applied along the $\langle h, h, 0\rangle$ direction. Both elastic and inelastic measurements were carried out to track the evolution of the magnetic structure and spin fluctuations as a function of applied field.

[1] A. Thamizhavel et al., Phys. Rev. B **68**, 054427 (2003).
[2] L. Balicas et al., Phys. Rev. B **72**, 064422 (2005).

8:36AM H22.00004 Shubnikov-de Haas Effect measured on single crystals of $CeOs_4Sb_{12}$ and $NdOs_4Sb_{12}$ along the high symmetry directions , P.-C. HO, Physics/CSU-Fresno, J. SINGLETON, NHMFL/LANL, New Mexico, M.B. MAPLE, D.B. SHREKENHAMER, X. LEE, A. THALE, Physics/UCSD, T. YANAGISAWA, Hokkaido U, Japan — The filled skutterudite compounds $CeOs_4Sb_{12}$, $PrOs_4Sb_{12}$, and $NdOs_4Sb_{12}$ are respectively a 1 K antiferromagnetic (AFM) Kondo insulator, a 1.85 K unconventional superconductor, and a 1 K mean-field type ferromagnet (FM), suggesting that superconductivity in $PrOs_4Sb_{12}$ may result from proximity to AFM and FM quantum-critical points. Fermi-surface measurements of $NdOs_4Sb_{12}$ and $CeOs_4Sb_{12}$ could therefore give insights into the pairing mechanism. We have used a MHz skin-depth technique to observe Shubnikov-de Haas oscillations (SdHos) in single crystals of these materials at fields of up to 60 T. In $CeOs_4Sb_{12}$ for $\mathbf{H}$ // [001], a previously-unobserved semimetal-to-metal transition was detected at ≈ 25 T; above this, a series of SdHos with a frequency of 1700 T and $m_{\rm CR} \approx 3.6m_{\rm e}$ emerge. For $\mathbf{H}$ // [011] in $NdOs_4Sb_{12}$, a single series of SdHos, frequency ≈ 874 T, was found. These may correspond to the β band in $PrOs_4Sb_{12}$, but with a much smaller $m_{\rm CR} \approx 1.5m_{\rm e}$. Research at CSU-Fresno is supported by RC CCSA #7669 and the start-up fund; at NHMFL by DOE, NSF, and FL.; at UCSD by NSF#0802478 and US DOE DE FG02-04ER46105; at Hokkaido U by MEXT, Japan.

8:48AM H22.00005 The non-centrosymmetric heavy fermion ferromagnet $Sm_2Fe_{12}P_7$[1] , MARC JANOSCHEK, RYAN E. BAUMBACH, JAMES J. HAMLIN, IVY K. LUM, M. BRIAN MAPLE, University of California, San Diego — The investigation of quantum critical points (QCPs) in heavy fermion compounds (HF) has proven to be a useful tool in gaining insight into strongly correlated electron physics. However, the body of work on HF systems mainly focuses on antiferromagnetic QCPs. We report measurements of the electrical resistivity, magnetization and specific heat on single crystals of the non- centrosymmetric compound $Sm_2Fe_{12}P_7$, that exhibits ferromagnetic (FM) order below $T_{M,1}$ = 6.3 K. The ratio of the effective magnetic moment in the paramagnetic state, to the saturation magnetic moment in the ordered state indicates that the ordered state is associated with itinerant electrons. An enhanced value for the coefficient of the electronic speci?c heat $\gamma \sim 450$ mJ mol^{-1}K^{-1} is observed, that is accompanied by a large coefficient A of the T^2 term in the electrical resistivity, suggesting a HF ground state. Three consecutive magnetic phase transitions, indicative of competing magnetic energy scales, and the observation of a metamagnetic transition additionally suggest proximity to a QCP. Thus, we propose that $Sm_2Fe_{12}P_7$ is a possible candidate to study a FM QCP in a HF compound.

[1]Financial support was provided by AFOSR-MURI (FA9550-09-1-0603), US DOE (DE FG02-04ER46105), and NSF (0802478).

9:00AM H22.00006 Multiple regions of quantum criticality in YbAgGe , G.M. SCHMIEDESHOFF, Occidental College, S.L. BUD'KO, P.C. CANFIELD, Ames Laboratory, Iowa State University — YbAgGe is a stoichiometric heavy fermion antiferromagnet that exhibits field-induced quantum criticality. We present and discuss thermal expansion and magnetostriction measurements that reveal a new field-induced state. On the low-field side of this state we find evidence for a first-order phase transition and suggest that YbAgGe may be close to a quantum critical end point at 4.5 T. On the high-field side we find evidence for a second-order phase transition suppressed to a quantum critical point near 7.2 T. We will discuss these results in light of global phase diagrams proposed for Kondo lattice systems. Work at Occidental College was supported by the National Science Foundation under DMR-1006118. Work at Ames Laboratory was supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

9:12AM H22.00007 Quasiparticle duality in the Kondo-screened state of YbInCu4 , MARCO GUARISE, EPFL, Lausanne, JASON HANCOCK, JOHN SARRAO, Los Alamos, THORSTEN SCHMITT, PSI, Switzerland, MARCO GRIONI, EPFL, Lausanne — We present a study of the excitation spectra of YbInCu4. This system exhibits a first- order isoelectronic phase transition which separates regimes with very different T/T_K. Using infrared optics, we were first able to demonstrate the existence of a hybridization gap feature which is ubiquitous in heavy fermion systems. More recently, using the burgeoning technique of resonant inelastic X-ray scattering (RIXS) at the Yb M5 edge, we identify a feature at the same energy, strongly suggesting that components of this excitation have mixed itinerant and localized character. Prospects for the future studies using the RIXS technique in the context of heavy fermion materials will be discussed.

9:24AM H22.00008 High-resolution angle-resolved photoemission studies of $YbRh_2Si_2$ using 7 eV laser , S.-K. MO, Advanced Light Source, LBNL, W.S. LEE, F. SCHMITT, Y.L. CHEN, Stanford University and SLAC National Lab, D.H. LU, SLAC National Lab, C. CAPAN, D.J. KIM, Z. FISK, UC Irvine, C.-Q. ZHANG, Shandong University, China, Z. HUSSAIN, Advanced Light Source, LBNL, Z.-X. SHEN, Stanford University and SLAC National Lab — We present angle-resolved photoemission spectra of prototypical heavy fermion compound $YbRh_2Si_2$ measured with 7 eV ultraviolet laser. Much improved energy and momentum resolutions enable us to resolve the sharp weakly dispersing peaks at the lowest energy of single-electron spectra. This coherent state grows in intensity and weight as temperature decreases below a characteristic temperature. The characteristic temperature is not only different from the single-ion Kondo temperature of $YbRh_2Si_2$ derived from thermodynamic measurements, it is of the same scale as the energy and the lifetime of the coherent state.

9:36AM H22.00009 Zeeman-driven Lifshitz transition: A scenario for the Fermi-surface reconstruction in YbRh2Si2 , MATTHIAS VOJTA, Technische Universitaet Dresden, ANDREAS HACKL, California Institute of Technology — The heavy-fermion metal $YbRh_2Si_2$ displays a field-driven quantum phase transition where signatures of a Fermi-surface reconstruction have been identified, often interpreted as breakdown of the Kondo effect. We argue that instead many properties of the material can be consistently described assuming a Zeeman-driven Lifshitz transition of heavy-fermion bands. Using a suitable quasiparticle model, we find a smeared jump in the Hall constant and maxima in susceptibility and specific heat, very similar to experimental data. An intermediate non-Fermi liquid regime emerges due to the small effective Fermi energy near the transition. Further experiments to discriminate the different scenarios are proposed.

9:48AM H22.00010 Neutron magnetic form factor in strongly correlated materials , MARIA PEZZOLI, KRISTJAN HAULE, GABRIEL KOTLIAR, Serin Physics Laboratory, Rutgers University,Piscataway, NJ 08854, USA. — We introduce a formalism to compute the neutron magnetic form factor F(q) within a first-principles Density Functional Theory (DFT) + Dynamical Mean Field Theory (DMFT). We use our method to compute the form factor of PuCoGa5. We find that the local physics of this material is described by a mixed valence mechanism of the type observed in elemental Plutonium. This picture explains nicely the experimental neutron form factor of PuCoGa5 and it is consistent with the photo-emission spectra shape and the value of the specific heat linear coefficient.

10:00AM H22.00011 Formation of heavy electron bands by ordering in two-channel Kondo lattice , SHINTARO HOSHINO, Tohoku university, JUNYA OTSUKI, YOSHIO KURAMOTO — Itinerant and localized characters of electrons are one of the most fundamental problems in condensed matter physics. In typical Kondo lattice systems, the f electrons are localized in the high temperature region, and acquire the itinerancy by the interaction between f and conduction electrons with decreasing temperature. In the present work, however, we show that the localized character of f electrons changes into itinerant one at the transition point in two-channel Kondo lattice systems. We have analyzed the system using the dynamical mean-field theory combined with the continuous-time quantum Monte Carlo method. With one conduction electron per site, which corresponds to the quarter filling of each band, a channel order emerges in wide parameter region with metal-insulator transition. At the same time, the heavy electron bands are formed, which indicates the itinerant f-electron states. Since f electrons acquire the itinerancy only below the transition temperature, this behavior can be regarded as itinerant-localized transition of electronic states. We will discuss these behaviors through temperature dependence of the single-particle spectrum.

10:12AM H22.00012 Hard X-Ray Photoelectron Spectroscopic Analysis of single crystal UPd_3, UGe_2, and USb_2 , M. BEAUX, T. DURAKIEWICZ, J. JOYCE, E. BAUER, LANL, Los Alamos, NM 87545, L. MORESCHINI, Lawrence Berkeley National Laboratory, Berkeley, California, F. OFFI, CNISM and Dipartimento de Fisica, Universita Roma Tre, Via della Vasca Navale 84, 1-00146 Rome, Italy, M. GRIONI, IPN, EPFL,CH-1015 Lausanne, Switzerland, G. MONACO, ESRF, B.P. 220, F-38042 Grenoble, France, G. PANNACIONE, Laboratorio Nazionale TASC-INFM-CNR, Area Science Park, Basovizza S.S. 14Km 163.5, I-34012 Trieste, Italy — Hard X-ray Photoelectron Spectroscopy (HAXPES) with 7.6 keV photons has been performed on single crystals of UPd3, UGe2, and USb2 at the European Synchrotron Radiation Facility (ESRF). A potential correlation between the localization/itinerancy of the 5f electrons and the core levels of these materials is investigated. The greatly reduced surface sensitivity of HAXPES enabled observation of the bulk core levels in spite of some surface oxidation. An 800 meV splitting of the Sb 3d and 4d core levels was observed. The splitting of the Sb core levels is attributed to manifestations of two distinct binding modes within the USb2 single crystal as supported by consideration of interatomic distances and charge transfer calculations.

10:24AM H22.00013 Small Angle Neutron Scattering and the Vortex Lattice of UPt_3[1] , W.J. GANNON, W.P. HALPERIN, J.A. SAULS, J.P. DAVIS, Northwestern University, IL, USA, K. SCHLESINGER, M.R. ESKILDSEN, University of Notre Dame, IN, USA, J. GAVILANO, ETH Zurich and Paul Scherrer Institute, Switzerland — UPt_3 is among the most well studied of the unconventional superconductors. However, there are still many unanswered questions, two of which are: understanding chirality in the superconducting B-phase and understanding the nature of the B-C transition. Central to theories describing both of these areas are predictions for unusual vortex structures. Small angle neutron scattering (SANS) provides a unique way to explore the bulk vortex lattice (VL) and thus can be used to investigate the bulk superconducting state without electronic surface scattering which complicates results from other probes. Ongoing SANS experiments on high quality single crystals in a novel geometry seek to explore the the relationship between field history and the VL in UPt_3. Preliminary results show well defined diffraction patterns and narrow rocking curves at fields well into the C-phase and interesting behavior for a variety of field histories. These results will shed new light on chirality, the B-C transition, and VL (meta)stability.

[1]Support from DOE/BES awards DE-SC0005051 and DE-FG02-05ER46248.

10:36AM H22.00014 Unconventional Anomalous Hall Effect in UCu_5[1] , B.G. UELAND, C.F. MICLEA, I. MARTIN, E.D. BAUER, R. MOVSHOVICH, F. RONNING, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, Z. FISK, Department of Physics & Astronomy, University of California, Irvine, California 92697, USA, J.D. THOMPSON, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — Field-dependent resistivity, magnetization, and specific heat measurements have been carried out on the heavy fermion compound UCu_5. We find an unconventional anomalous Hall resistance below the lower temperature magnetic transition at $T_2 \sim 1$ K that is proportional to neither the magnetization nor the longitudinal resistivity. We discuss the origin of this resistance in terms of the itinerant carriers' interaction with the magnetically ordered U cations. Complementary measurements on $Lu_{1-x}U_xCu_5$, x = 0 to 0.15 show how non-magnetic dilution affects the Hall resistance and magnetic phase diagram. Interestingly, light Lu substitution for U appears to stabilize the low temperature magnetic phase.

[1]Work at Los Alamos National Laboratory was performed under the auspices of the U.S. Department of Energy, Office of Science and Los Alamos Laboratory Directed Research and Development. Z.F. acknowledges funding from NSF-DMR-0801253.

10:48AM H22.00015 Temperature Dependent Hybridization Gaps[1] , PETER RISEBOROUGH, Physics Department Temple University — A number of heavy-fermion/mixed-valent materials show hybridization gaps either at the Fermi-energy or close to the Fermi-energy. In the former case, a heavy-fermion semiconducting state ensues and in the later case, the system remains metallic at low temperatures. In either case, the electronic structure is extremely temperature-dependent. It has been observed that the gap closes and the heavy quasiparticle bands disappear at high temperatures. The magnitude of the gaps scale with effective quasiparticle masses. A phenomenological model is presented that exhibits a temperature-dependence which is consistent with the above behavior. The model is based on a periodic array of Anderson impurities in which the electron correlations are represented by the coupling to bosons with an Einstein spectra. The model can be solved via systematic approximation. The solution describes the temperature- dependence of coherent and incoherent structures in the electronic excitation spectra. The predicted hybridization gaps for the metallic case are compared with data from photoemission experiments on UPd_2Al_3.

[1]This work was supported by the US DOE Office of Basic Energy Science through DE-FG02-01ER45872.

Tuesday, March 22, 2011 8:00AM - 10:48AM –
Session H23 DCMP: Superconductivity: Mainly ARPES D165

8:00AM H23.00001 Doping dependence of the electron-phonon and electron-spin fluctuation interactions in Bi-2212 , ELBERT CHIA, DANIEL SPRINGER, SARITHA NAIR, XINAQUAN ZOU, SIEW ANN CHEONG, CHRISTOS PANAGOPOULOS, Nanyang Technological University, ANTOINETTE TAYLOR, Los Alamos National Laboratory, TSUYOSHI TAMEGAI, University of Tokyo, HIROSHI EISAKI, AIST, SHIGEYUKI ISHIDA, SHIN-ICHI UCHIDA, University of Tokyo, JIAN-XIN ZHU, Los Alamos National Laboratory — In the BCS theory of conventional superconductors, electrons form (Cooper) pairs via interactions with the underlying crystal lattice. In the cuprate superconductors, it is not clear whether Cooper pairing takes place via electrons interacting with phonons, spin fluctuations, or whether a bosonic mechanism is necessary at all. Though time-integrated optical measurements on the cuprates can give information on the coupling strength between electrons and an effective boson, it is difficult to tell whether one or more bosons are involved, or the nature of these bosons. We report measurements of time-resolved quasiparticle relaxation of $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystals (hole concentration p = 0.10-0.22). Our data indicate that *two* bosonic modes are associated with superconductivity: the electron-phonon coupling constant (λ_{e-ph}) peaks at optimal doping, while the electron-spin fluctuation coupling constant (λ_{e-sf}) decreases monotonically with doping.

8:12AM H23.00002 Time-Resolved ARPES Study of Non-Equilibrium Quasiparticle Dynamics in Cuprate Superconductors , CHRISTOPHER SMALLWOOD, University of California, Berkeley; Lawrence Berkeley National Laboratory, JEFF GRAF, CHRIS JOZWIAK, Lawrence Berkeley National Lab, HIROSHI EISAKI, University of Tokyo; CREST, Japan Science and Technology Agency; RIKEN (The Institute of Physical and Chemical Research), ROBERT KAINDL, Lawrence Berkeley National Lab, DUNG-HAI LEE, ALESSANDRA LANZARA, University of California, Berkeley; Lawrence Berkeley National Laboratory — We use Time- and Angle-Resolved Photoemission (TR-ARPES) to measure the relaxation dynamics of low energy excitations in the cuprate superconductor Bi-2212. We find an as-yet unreported temperature dependence in nodal quasiparticle spectral weight which is sensitive to the critical temperature. We also find possible evidence for non-thermal transient electronic behavior.

8:24AM H23.00003 Ultra High Resolution Pump Probe Angle Resolved Photoemission Experiments on High Temperature Superconductor Bi2Sr2CaCu2O8 , WENTAO ZHANG, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, CHRIS SMALLWOOD, Department of Physics, University of California, Berkeley, CA 94720, USA, CHRIS JOZWAIK, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, HIROSHI EISAKI, Nanoelectronics Research Institute (NeRI), National Institute of Advanced Industrial Science and Technology, Ibaraki 305-8568, Japan, ALESSANDRA LANZARA, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA — Ultra high resolution laser-based pump probe angle-resolved photoemission measurements have been carried out on underdoped Bi2Sr2CaCu2O8 high temperature superconductor. In this talk, we will report on the observation and analysis of quasiparticle relaxation in Bi2Sr2CaCu2O8.

8:36AM H23.00004 Bands, spin fluctuations and traces of Fermi surfaces in ARPES intensities on high-T_C cuprates , THOMAS JARLBORG, DPMC, University of Geneva, CH1211 Geneva 4, Switzerland — The band structures of pure and hole doped La_2CuO_4 with anti-ferro magnetic (AFM) spin-fluctuations are calculated and compared to spectral weights of ARPES. It is shown that the observation of coexisting Fermi surface (FS) arcs and closed FS pockets are consistent with antiferromagnetic spin fluctuations of varying wave lengths. The FS signal of the underlying non-magnetic material is mixed with echos of FS-breaks from domains with AFM spin waves. Large variations of strong spin fluctuations make the outer part of the FS break diffuse at low doping. This part of the FS is suppressed at high doping when spin fluctuations becomes weak. The resulting superimposed spectral weight has features both from FS arcs and closed pockets. This makes a connection between results of ARPES and neutron scattering, and it implies that spin-phonon coupling is an important mechanism for cuprate properties.

8:48AM H23.00005 Origin of magnetic resonance spectrum in cuprate high-temperature superconductors and related issues , A. BANSIL, Northeastern U, TANMOY DAS, Northeastern U and LANL, R.S. MARKIEWICZ, Northeastern U. — A distinct low energy magnetic mode has been observed in almost all the cuprate materials in a broad range of experiments including ARPES, Raman, optical, STM, RIXS, as well as neutron scattering. This mode is enhanced in the superconducting (SC) state and its energy scales universally as $\omega_{res} \propto 2\Delta$, suggesting that these modes play an important role in the mechanism of superconducting pairing. Here we study this resonance via first-principle susceptibility calculations in a Hubbard model with $d-$wave superconductivity [1]. The resulting excitation mode produces the universal $\omega_{res} \propto 2\Delta$ relation as well as the puzzling 'hour-glass' dispersion and the 45° rotation of the spin excitations with energy in a series of cuprates in accord with experiments [2]. Work supported by US DOE.

[1] Tanmoy Das, R.S. Markiewicz, and A. Bansil, Phys. Rev. B **81**, 174504 (2010).
[2] A. Bansil, *et al.* Journal of Physics and Chemistry of Solids (2010).

9:00AM H23.00006 Particle-hole asymmetric components of QPI in the pseudogap phase of underdoped Bi-2212 , C.K. KIM, Cornell, BNL, JHINHWAN LEE, KAIST, Cornell, K. FUJITA, Cornell, H. EISAKI, AIST, S. UCHIDA, Tokyo U, J.C. DAVIS, Cornell, BNL, St. Andrews, JINHO LEE, BNL — QPI visualized by SI-STM became an extremely useful tool in the study of complex electronic matter. Particle-hole(p-h) symmetric QPI observed in the superconducting cuprates revealed many interesting phenomena including the disappearance of the QPI signal around the reduced zone boundary[1], and the persisting QPI signal above the T_c[2]. Recently, the most dominating band of $Sr_3Ru_2O_7$ was identified above the metamagnetic nematic phase transition temperature by analyzing p-h asymmetric QPI [3]. Also p-h asymmetric QPI in the parent compound of the ferropnictide superconductor revealed a nematic like electronic structure[4]. Within the same rationale, it is of great interest to find the QPI signature of the band before the superconducting gap opens in the cuprates. Here we explore QPI with particle-hole asymmetric dispersion in the pseudogap phase of underdoped $Bi_2Sr_2CaCu_2O_8$; it appears to disperse continuously through E_F. Our measured value of the v_F of this dispersion is 0.2×10^6m/s which compares well with the reported value 1.7eVÅ from ARPES. We will discuss the possible origin of this QPI by examining its symmetry and dispersion near the zone boundary using theoretical models and currently available experimental data from other probes. [1] Y. Kohsaka et al., Nature(2008) [2] Jhinhwan Lee et al., Science(2009) [3] Jinho Lee et al., Nature Physics(2009) [4] T.-M. Chuang et al., Science(2010)

9:12AM H23.00007 Oxygen reduction effects on the electronic structures of electron doped cuprates: investigating the mechanism of the metal insulator transition , D.J. SONG, S.R. PARK, C.S. LEEM, CHUL KIM, Y.K. KIM, S.K. CHOI, W.S. JUNG, C. KIM, Yonsei university, H. EISAKI, AIST, D.H. LU, Z.-X. SHEN, Stanford university, S. ISHIDA, S. UCHIDA, University of Tokyo — In electron doped cuprates, oxygen reduction process not only induces superconductivity but also causes changes in many physical properties. In order to understand these oxygen reduction effects, we performed ARPES studies on as-grown and de-oxygenated superconducting electron doped cuprates, PLCCO, NCCO and SCCO. We observe Fermi surface topology change and pseudo gap filling due to weakening of AFM as reported in other studies. In addition, sharp quasi-particles (QP) appear out of broad incoherent features as the as-grown samples are de-oxygenated through the oxygen reduction process. We believe that this behavior of the QP peak closely related to the insulator to metal transition in the reduction process. We attribute the suppression of the QP states in as-grown sample to the Anderson localized electron states due to strong disorder and impurity scattering.

9:24AM H23.00008 Renormalization of f-levels away from the Fermi energy in electron excitation spectroscopies: Density functional results of $Nd_{2-x}Ce_xCuO_4$, B. BARBIELLINI, Northeastern U., T. JARLBORG, DPMC, University of Geneva (Switzerland), H. LIN, R.S. MARKIEWICZ, A. BANSIL, Northeastern U. — Relaxation energies for photemission, when an occupied electronic state is excited, and for inverse photoemission, when an empty state is filled, are calculated within the density functional theory with application to $Nd_{2-x}Ce_xCuO_4$ (NCCO). The associated relaxation energies are obtained by computing differences in total energies between the ground state and an excited state in which one hole or electron is added into the system. The relaxation energies of f-electrons are found to be of the order of several eV's, indicating that f-bands will appear substantially away from the Fermi energy (E_F) in their spectroscopic images, even if these bands lie close to the E_F in the ground state of NCCO. Our analysis explains why it would be difficult to observe f electrons at the E_F even in the absence of strong electronic correlations. Work supported by the US DOE.

9:36AM H23.00009 Differential heat capacity studies of $Nd_{2-x}Ce_xCuO_4$[1] , JOHN COOPER, JAMES STOREY, EDWARD CAVANNA, JOHN LORAM, Cavendish Laboratory, University of Cambridge, CB3 0HE, U.K — The electronic heat capacity of several *hole*-doped cuprate systems has been determined accurately over a wide temperature range using a unique differential calorimeter. It gives important thermodynamic information about the electronic excitations and the pseudogap [1] that is difficult to obtain in other ways, so it is clearly of interest to extend these studies to some *electron*-doped materials. Here we report progress in measuring the specific heat capacity of a series of polycrystalline $Nd_{2-x}Ce_xCuO_4$ samples with x varying from 0.14 to 0.18 in steps of 0.01, between 2K and 100K, in magnetic fields from 0 – 13T and complementary magnetic and transport data. The aims of this work are to look for possible signatures of the pseudogap and to compare our results with recent quantum oscillation studies [2].

[1] For example, J. W. Loram *et al.*, J. Phys. Chem. Solids **62**, 59 (2001).
[2] T. Helm *et al.*, Phys. Rev. Lett. **103**, 157002 (2009).

[1]This work is supported by the Engineering and Physical Sciences Research Council (UK).

9:48AM H23.00010 Consequences of two-dimensionality for the quantum oscillations in underdoped YBCO , NEIL HARRISON, Los Alamos National Labs, SUCHITRA SEBASTIAN, Cavendish Lab, Cambridge, MOAZ ALTARAWNEH, LANL, RX. LIANG, D.A. BONN, W.N. HARDY, UBC, Canada, GIL LONZARICH, Cavendish Lab, Cambridge — We report new high resolution measurements on underdoped YBCO over an unprecedented magnetic field range with a high signal- to-noise ratio. The reduced-dimensionality of the Fermi surface is found to strongly influence the quantum oscillations and result in unusual properties. Careful analysis of these unconventional properties is found to severely constrain the Fermi surface topology.

10:00AM H23.00011 Lifshitz transitions in the underdoped cuprates with spin-density wave order[1] , JIE LIN, Materials Science Division, Argonne National Laboratory — It has recently been proposed that a neck-disrupting Lifshitz transition can explain the disappearance of quantum oscillations and diverging cyclotron mass observed in underdoped YBCO. We found that both pocket-disappearing and neck-disrupting types of Lifshitz transitions can be realized in two-dimensional spin-density wave models for underdoped cuprates. Close to Lifshitz transitions, the impurity relaxation rate acquires strong energy-dependence. The thermoelectric power is strongly enhanced, and behaves differently for the two types of transitions.

[1]Work supported by the U.S. DOE, Office of Science, under Contract No. DE-AC02-06CH11357

10:12AM H23.00012 ABSTRACT WITHDRAWN –

10:24AM H23.00013 Observation of Electronic Structures on Alkali-earth Metal Intercalated Superconducting GICs , WONSHIK KYUNG, C.S. LEEM, CHUL KIM, Y.K. KIM, G.R. HAN, C. KIM, Yonsei University, J.S. KIM, Y.W. KIM, Pohang University of Science and Technology, YONSEI UNIVERSITY TEAM, POHANG UNIVERSITY OF SCIENCE AND TECHNOLOGY COLLABORATION — We synthesized alkali-metal intercalated GICs(Ca, Ba, Sr). To compare electronic structure of these GICs, we performed high resolution angle-resolved photoemission spectroscopy (ARPES) on it. Through quantitative analysis of band structure, we can see alkali metal dependent band structure.

10:36AM H23.00014 Evidence of nodes in the non-centrosymmetric superconductor Y_2C_3 , J. CHEN, Dept. Physics, Zhejiang Univ., H.Q. YUAN, Dept. Physics, Zhejiang Univ., M.B. SALAMON, Dept. Physics, U. Texas at Dallas, S. AKUTAGAWA, J. AKIMITSU, Dept. Physics, Aoyama Gakuin U. — In a non-centrosymmetric superconductor, antisymmetric spin-orbit coupling (ASOC) can admix spin-singlet and spin-triplet pairing states, leading to accidental nodes in the energy gap [1]. Y_2C_3 is such a superconductor with a T_c of 18K. Early NMR and μSR results [2] indicated a gap structure incompatible with either BCS s-wave or typical d-wave behavior. To further elucidate its superconducting properties, we have measured the temperature dependence of the magnetic penetration depth using a tunneling-diode oscillator technique. While the high temperature penetration depth, and therefore its corresponding superfluid density, can be well described by a two-gap BCS model, as discussed in Ref. [2], the low temperature penetration depth follows a linear temperature dependence, indicating possible existence of nodes in the energy gap. Together with the large upper critical field observed in Y_2C_3 [3], the existence of nodes, we argue, might be attributed to the ASOC as a result of absent inversion symmetry even though other possibilities cannot be excluded. [1] H. Q. Yuan et al, Phys. Rev. Lett. **97**, 017006 (2006). [2] A. Harada et al, J. Phys. Soc. Jpn. **76**, 023704(2007); S. Kuroiwa et al, Phys. Rev. Lett. **100**, 097002 (2008). [3] H. Q. Yuan et al, J. Phys. Chem. Solids (in press).

Tuesday, March 22, 2011 8:00AM - 10:36AM –

Session H24 DCOMP: Focus Session: What is Computational Physics? I D167

8:00AM H24.00001 Computational Physics' Greatest Hits , AMY BUG, Swarthmore College — The digital computer, has worked its way so effectively into our profession that now, roughly 65 years after its invention, it is virtually impossible to find a field of experimental or theoretical physics unaided by computational innovation. It is tough to think of another device about which one can make that claim. In the session "What is computational physics?" speakers will distinguish computation within the field of computational physics from this ubiquitous importance across all subfields of physics. This talk will recap the invited session "Great Advances...Past, Present and Future" in which five dramatic areas of discovery (five of our "greatest hits") are chronicled: The physics of many-boson systems via Path Integral Monte Carlo, the thermodynamic behavior of a huge number of diverse systems via Monte Carlo Methods, the discovery of new pharmaceutical agents via molecular dynamics, predictive simulations of global climate change via detailed, cross-disciplinary earth system models, and an understanding of the formation of the first structures in our universe via galaxy formation simulations. The talk will also identify "greatest hits" in our field from the teaching and research perspectives of other members of DCOMP, including its Executive Committee.

8:36AM H24.00002 Nicholas Metropolis Award Talk for Outstanding Doctoral Thesis Work in Computational Physics: Computational biophysics and multiscale modeling of blood cells and blood flow in health and disease , DMITRY FEDOSOV, Forschungszentrum Juelich GmbH — Computational biophysics is a large and rapidly growing area of computational physics. In this talk, we will focus on a number of biophysical problems related to blood cells and blood flow in health and disease. Blood flow plays a fundamental role in a wide range of physiological processes and pathologies in the organism. To understand and, if necessary, manipulate the course of these processes it is essential to investigate blood flow under realistic conditions including deformability of blood cells, their interactions, and behavior in the complex microvascular network. Using a multiscale cell model we are able to accurately capture red blood cell mechanics, rheology, and dynamics in agreement with a number of single cell experiments. Further, this validated model yields accurate predictions of the blood rheological properties, cell migration, cell-free layer, and hemodynamic resistance in microvessels. In addition, we investigate blood related changes in malaria, which include a considerable stiffening of red blood cells and their cytoadherence to endothelium. For these biophysical problems computational modeling is able to provide new physical insights and capabilities for quantitative predictions of blood flow in health and disease.

9:12AM H24.00003 Computational Physics Across the Disciplines , VINCENT CRESPI, PAUL LAMMERT, TYLER ENGSTROM, BEN OWEN, Penn State University — In this informal talk, I will present two case studies of the unexpected convergence of computational techniques across disciplines. First, the marriage of neutron star astrophysics and the materials theory of the mechanical and thermal response of crystalline solids. Although the lower reaches of a neutron star host exotic nuclear physics, the upper few meters of the crust exist in a regime that is surprisingly amenable to standard molecular dynamics simulation, albeit in a physical regime of density order of magnitude of orders of magnitude different from those familiar to most condensed matter folk. Computational results on shear strength, thermal conductivity, and other properties here are very relevant to possible gravitational wave signals from these sources. The second example connects not two disciplines of computational physics, but experimental and computational physics, and *not* from the traditional direction of computational progressively approaching experiment. Instead, experiment is approaching computation: regular lattices of single-domain magnetic islands whose magnetic microstates can be exhaustively enumerated by magnetic force microscopy. There resulting images of island magnetization patterns look essentially like the results of Monte Carlo simulations of Ising systems... statistical physics with the microstate revealed.

9:24AM H24.00004 Role of Electronic Structure Calculations in Understanding Superconductors[1] , DAVID SINGH, Oak Ridge National Lab — Superconductivity remains one of the most challenging and exciting areas in condensed matter physics. It is a field that often sees surprises. These come in the form of new superconducting materials with unprecedented properties that need explanation. Here we briefly discuss the role that computational electronic structure studies have played in understanding some of these new systems over the years. The materials discussed are high temperature cuprates, borocarbides, Sr_2RuO_4, MgB_2, and the iron-based superconductors. Computation has played a key role in understanding properties of these materials and in some but not all cases pointing directly to the mechanism of superconductivity.

[1]This work was supported by the Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Technology Division

9:36AM H24.00005 What is computational physics? An embarrassment of riches for teaching computational physics , LARRY ENGELHARDT, Francis Marion University — The first decade of the 21^{st} century has provided a wealth of exceptional resources for teaching computational physics, including numerous textbooks, libraries of computer codes (visual as well as numerical), and high-level interfaces for accessing these libraries. We are now faced with the very real challenge of choosing which of these resources to incorporate into the finite number of courses available in a given curriculum. This choice depends on several factors: How much time can be allocated to teaching computational methods and at what stage in the curriculum? What are the goals? (Learning physics better? Learning to individually implement numerical solutions for small-scale problems? Being prepared to work in research labs studying large-scale problems?) Are commercial packages an appropriate option for your student population? There are no right and wrong answers to these questions, and I will present more questions than answers! However, in recent years I have taught three undergraduate computational physics courses per year, and I will discuss some of the decisions that have been made regarding those courses.

9:48AM H24.00006 Computational Physics? Some perspectives and responses of the undergraduate physics community[1] , NORMAN CHONACKY, Yale University — Any of the many answers possible to the evocative question "What is ..." will likely be heavily shaded by the experience of the respondent. This is partly due to absence of a canon of practice in this still immature, hence dynamic and exciting, method of physics. The diversity of responses is even more apparent in the area of physics education, and more disruptive because an undergraduate educational canon uniformly accepted across institutions for decades already exists. I will present evidence of this educational community's lagging response to the challenge of the current dynamic and diverse practice of computational physics in research. I will also summarize current measures that attempt respond to this lag, discuss a researched-based approach for moving beyond these early measures, and suggest how DCOMP might help. I hope this will generate criticisms and concurrences from the floor.

[1]Research support for material in this talk was from: IEEE-Computer Society; Shodor Foundation; Teragrid Project.

10:00AM H24.00007 High-performance scientific computing in the cloud[1] , KEVIN JORISSEN, FERNANDO VILA, JOHN REHR, University of Washington — Cloud computing has the potential to open up high-performance computational science to a much broader class of researchers, owing to its ability to provide on-demand, virtualized computational resources. However, before such approaches can become commonplace, user-friendly tools must be developed that hide the unfamiliar cloud environment and streamline the management of cloud resources for many scientific applications. We have recently shown that high-performance cloud computing is feasible for parallelized x-ray spectroscopy calculations.[2] We now present benchmark results for a wider selection of scientific applications focusing on electronic structure and spectroscopic simulation software in condensed matter physics. These applications are driven by an improved portable interface that can manage virtual clusters and run various applications in the cloud. We also describe a next generation of cluster tools, aimed at improved performance and a more robust cluster deployment.

[1]Supported by NSF grant OCI-1048052.
[2]J.J. Rehr et al., CiSE, **12**, 34 (2010)

10:12AM H24.00008 Characterizing Large-Scale Computational Physics , TIMOTHY WILLIAMS, Argonne National Laboratory — Large-scale computational physics calculations typically share some of a number of basic characteristics:

- Brute-force approaches: Atomistic molecular dynamics, particle-in-cell plasma physics, particle-mesh cosmological simulations, DNS of turbulence, lattice QCD, Monte Carlo, ...
- Wide range of relevant scales: Angstroms to millimeters in molecular dynamics, ion/electron cyclotron period to seconds or minutes in plasmas, galaxy to observable universe in cosmology, high Reynolds number turbulence, ...
- Obvious need for yet larger scale: higher resolution, larger simulation domain, more particles, ...
- Code is named, parallel, community, long-lived (but evolving).

This talk views the computational physics landscape from the perspective a physicist who has worked at three DOE large-scale computing centers: the Argonne Leadership Computing Facility, the (former) Advanced Computing Laboratory, and NERSC. The "usual suspects" at the large-scale end of computational physics are remarkably persistent, even in the face of an ever-increasing definition of large-scale.

10:24AM H24.00009 Discussion of DCOMP Activities[1] , RICHARD SCALETTAR, University of California, Davis — The APS Division of Computational Physics, founded in 1986, explores the use of computers in physics research and education as well as the role of physics in the development of computer technology. Its goals are to promote research and development in computational physics, enhance the prestige and professional standing of its members, encourage scholarly publication, and promote international cooperation in these activities. This talk will mainly invite an open discussion of these objectives and how best to achieve them.

[1]Research supported by the DOE SCIDAC program, DOE-DE-FC0206ER25793, and under ARO Award W911NF0710576 with funds from the DARPA OLE Program.

Tuesday, March 22, 2011 8:00AM - 10:48AM –
Session H25 DCMP: Superconductivity: Tunneling Spectroscopy D166

8:00AM H25.00001 Pairing Glue in High Tc Cuprates from Tunneling Spectroscopy , JOHN ZASADZINSKI, OMID AHMADI, LIAM COFFEY, Illinois Institute of Technology, LUTFI OZYUZER, Izmir Institute of Technolgy, NOBUAKI MIYAKAWA, Tokyo University of Science — Break junction tunneling spectroscopy data in Bi2212 over a wide range of doping are fit using a d-wave Eliashberg model. Self consistency is achieved as the electron-boson spectral function, α^2F(ω), that fits the tunneling conductance dip feature also leads to the correct superconducting gap. The anomalous negative dI/dV observed in break junctions on optimal doped Bi2212 is also reproduced in the analysis. The diagonal and off-diagonal self energies, $\Sigma(\omega)$ and $\phi(\omega)$, respectively are generated in the analysis and they show trends with doping which are in agreement with numerical simulations of the Hubbard model. The peak in α^2F(ω) is consistent with the resonance mode in the spin fluctuation spectrum. Tunneling data of other cuprates are also discussed.

8:12AM H25.00002 How Topological Defects Couple the Smectic and Nematic Electronic Structure of the Cuprate Pseudogap States , K. FUJITA, Cornell Univ., A. MESAROS, Universiteit Leiden, H. EISAKI, AIST, Japan, S. UCHIDA, Univ. of Tokyo, J. C. DAVIS, Cornell Univ., S. SACHDEV, Harvard Univ., J. ZAANEN, Universiteit Leiden, M. LAWLER, Binghamton Univ., EUN-AH KIM, Cornell Univ. — We study the recently discovered coexisting smectic and nematic broken symmetries in the pseudogap-energy electronic structure of underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$. By visualizing their spatial components separately, we discover 2π topological defects throughout the phase-fluctuating smectic states. Imaging the locations of large numbers of these topological defects simultaneously with the fluctuations of the electronic nematicity about its average, reveals strong empirical evidence for a coupling between them. We also found the same phenomenology in a single layer compound of $Bi_2Sr_{1.6}La_{0.4}CuO_{6+\delta}$. From these observations, we propose a Ginzburg-Landau free energy describing the quantum nematic/smectic coupling and demonstrate how it can explain the coexistence of these states and correctly predict their interplay at the atomic scale. This theoretical understanding of the coupling between the quantum nematic and smectic broken symmetries can lead to unraveling the complexities of the phase diagram of cuprate high-T_c superconductors[1]. [1]A. Mesaros, K. Fujita, H. Eisaki, S. Uchida, J. C. Davis, S. Sachdev, J. Zaanen, M. J. Lawler, and Eun-Ah Kim, *Submitted* (2010).

8:24AM H25.00003 Universal properties of disordered electron nematics from surface probes , BENJAMIN PHILLABAUM, ERICA CARLSON, Purdue University, KARIN DAHMEN — When the electronic degrees of freedom break the rotational symmetry of the host crystal, i.e. from C_4 to C_2, the resulting state is an electronic Ising nematic. However the combination of reduced dimensionality and material disorder can forbid the formation of a long- range-ordered electron nematic, especially in strongly layered materials. Nevertheless, large domains are still possible. In this talk we will present results from a new kind of analysis for Scanning Tunneling Microscopy (STM) experiments as well as other surface probes. We map the locally broken C_4 to C_2 rotational symmetry of the electronic degrees of freedom to an Ising-type order parameter,use the local order parameter configuration to shed light on the universality class controlling the local pattern formation in cuprate superconductors.

8:36AM H25.00004 Vacuum-aging effect on electronic structure of $YBa_2Cu_3O_{6+x}$ thin film: a STM/STS study , Y.H. LIU, J. XIONG, D. YAROTSKI, Q. JIA, A.J. TAYLOR, MPA-CINT, MS K771, Los Alamos National Laboratory, NM 87545 — It is well known that oxygen plays a key role in the occurrence of superconductivity in high-temperature cuprate superconductors. Variation of oxygen content changes carrier concentration and directly affects electronic structure and superconducting properties of cuprate superconductors. Majority of previous studies relied on the intake process of oxygen to change the oxygen content in samples, while the reverse process, oxygen depletion, was rarely investigated. Nevertheless, the escape of oxygen from the surface of cuprate sample that was kept at room temperature under ultrahigh vacuum for extended period of time might lead to significant degradation of its superconducting properties due to the decrease of the carrier concentration. Here, we report this so-called vacuum-aging effect in $YBa_2Cu_3O_{6+x}$ thin films grown by laser-MBE technique. In particular, we use variable-temperature scanning tunneling microscopy/spectroscopy to follow the evolution of superconductivity and pseudogap states in this material as a function of aging time and tip position on the surface.

8:48AM H25.00005 Influence of the tunneling property on the noise thermometry using a metal-insulator-metal tunnel junction , JUNG HWAN PARK, MUSHTAQ REHMAN, Korea Research Institute of Standards and Science, ZHEONG G. KHIM, Seoul National University, SANG-WAN RYU, Chonnam National University, WOON SONG, YONUK CHONG, Korea Research Institute of Standards and Science — We are developing a noise thermometry setup based on precision RF measurement, where temperature can be inferred from the noise of a tunnel junction as a function of the bias voltage. We measure the electrical noise of an Al-AlOx-Al tunnel junction around 1 GHz with a bandwidth of a few hundred MHz. In this presentation, as an analysis on the source of error in thermometry, we studied the influence of the junction quality and the inelastic process on the temperature measurement. We compared the noise of an as-fabricated tunnel junction with that of a degraded tunnel junction after thermal cycling. Except for the junction degradation, all measurement environments were kept exactly same. We observed an apparently higher noise value near the zero-bias, which leads to an overestimation of temperature. We present a simple model to describe how the inelastic process in a tunnel junction affects the temperature measurement.

9:00AM H25.00006 ABSTRACT WITHDRAWN –

9:12AM H25.00007 Mapping the Pseudogap by Fourier Transform Scanning Tunneling Spectroscopy in $Bi_2Sr_2CaCu_2O_{8+x}$[1] , E.W. HUDSON, MIT, E MAIN, A.E. PIVONKA, I. ZELJKOVIC, Harvard, G. GU, Brookhaven, J.E. HOFFMAN, Harvard — The relationship between pseudogap and superconductivity in cuprate superconductors remains an important open question. To shed light on this issue, we have used Fourier-transform scanning tunneling microscopy to map quasiparticle interference (QPI) patterns as well as the "checkerboard," a weak charge modulation associated with the pseudogap, as a function of doping and temperature in $Bi_2Sr_2CaCu_2O_{8+x}$ (Bi-2212). We can extract the doping dependence of the pseudogap transition temperature T* within the superconducting dome. Our results strongly suggest that the pseudogap is a competing order.

[1]We acknowledge support from AFOSR PECASE grant FA9550-06-1-0531, AFOSR DURIP grant FA9550-06-1-0359, NSF Career grant DMR-0847433 and NSF grant DMR-0904400

9:24AM H25.00008 Phenomenological model for extracting local energy scales across dopings and temperatures in cuprates[1] , KYLE MCELROY, EDUARDO CALLEJA, JIXIA DAI, University of Colorado Boulder, GENDA GU, Brookhaven National Laboratory, JACOB ALLDREDGE, National Institute of Standards and Technology Boulder — One of the key questions that remains unanswered in the cuprate high temperature superconductors is the nature of the pesudogap phase that exists above the superconducting transition temperature in underdoped materials. In order to differentiate the different proposed origins of this phase, a detailed phenomenology of the different energy scales that characterize it and the superconducting phase is required. In addition, many of these materials (BSCCO-2212 in particular) have shown striking inhomogeneity that further complicates observations of these scales. Spectroscopic imaging scanning tunneling microscopy has the unique ability to resolve density of states features with the needed spatial resolution for seeing through this inhomogeneity. We will present a new phenomenological model for extracting three different energy scales that are present with atomic resolution across several dopings. In addition, preliminary data on the temperature dependence of these scales will be shown. Lastly, how these different scales relate to the different phases present in the underdoped cuprates will be discussed.

[1]Alfred P. Sloan Foundation

9:36AM H25.00009 Understanding the Measurement of the K-Space Gap Using Spectroscopic Imaging Scanning Tunneling Microscopy[1] , EDUARDO CALLEJA, JIXIA DAI, University of Colorado, GENDA GU, Brookhaven National Laboratory, KYLE MCELROY, University of Colorado — Two of the many tools used to probe the High Tc cuprates are Angle Resolved Photo Emission (ARPES) and Spectroscopic Imaging Scanning Tunneling Microscopy (SI-STM). While the two probes have had many qualitative agreements recently there has been a movement in the field to strive for quantitative agreement in order to better understand the phase diagram of the cuprates. When looking for quantitative agreement we are met with striking disagreements such as, the measurement of the super conducting gap by both probes and the observation of Fermi arcs. We have generated a preliminary simulation based on a superconducting tight binding model where we can tune different parameters in order to begin exploring some of these issues. With our STM just beginning to take data our simulation is allowing us to understand the type of data we need to shed some light on these issues.

[1]Alfred P. Sloan Foundation

9:48AM H25.00010 a-axis NIS tunnel junctions using LaSrCuO4[1] , MAO ZHENG, Department of Physics, University of Illinois, Urbana, IL, YIZE LI, JAMES ECKSTEIN — Planar tunneling in NIS structures with crystalline order reveals the density of states largely focused in the tunneling direction. Earlier experiments with a-axis YBCO showed an unexpected strongly broken particle hole symmetry in the CuO bond direction. Here we report on work to make similar structures with a-axis LaSrCuO4.

[1]This work is supported by the US Department of Energy

10:00AM H25.00011 Determining the pseudogap Dirac point in the underdoped cuprate superconductors using FT-STS and AC-ARPES , E.J. NICOL, K.A.G. FISHER, University of Guelph, J.P. CARBOTTE, McMaster University — Prominent in the underdoped cuprate superconductors is the existence of a pseudogap in the excitation spectrum which opens above T_c but below a temperature T^*. Whether this gap is the same as the superconducting energy gap or is a manifestation of a competing order independent of the superconductivity remains an open and central question. If there are two distinct gaps of d-wave symmetry, they each will exhibit a Dirac point at a different energy and momentum in the band structure. We demonstrate how to find the pseudogap Dirac point by using quasiparticle interference (QPI) measurements from Fourier transform scanning tunneling spectroscopy (FT-STS) or by extrapolating information from the autocorrelation function of angle-resolved photoemission spectroscopy (AC-ARPES) to positive energies. Current examination of photoemission data supports our proposal and suggests that a Dirac point exists at positive energy relative to the Fermi level.

10:12AM H25.00012 Spatial Variations in the Fermi Surface of Bi-2212[1] , ELIZABETH MAIN, A.E. PIVONKA, I. ZELJKOVIC, Harvard, G. GU, Brookhaven, E.W. HUDSON, MIT, J.E. HOFFMAN, Harvard — In cuprate superconductors, scanning tunneling microscopy can be used to see variations in the Fermi surface on a nanometer length scale caused by doping inhomogeneity. Prior STM studies show that the local wavelength of the checkerboard, a weak charge modulation ascribed to antinodal Fermi surface nesting, varies with the size of the pseudogap in $Bi_2Sr_2CuO_{6+\delta}$ (Bi-2201) [1]. Here we report similar STM measurements in Bi-2212. We therefore confirm the local relationship between pseudogap energy and charge ordering wavevector in a second high-Tc superconductor.

[1] W. D. Wise, et al. Nature Physics 5, 213 (2009).

[1]We acknowledge support from AFOSR PECASE grant FA9550-06-1-0531, AFOSR DURIP grant FA9550-06-1-0359, NSF Career grant DMR-0847433 and NSF grant DMR-0904400.

10:24AM H25.00013 Vortex-core structure in d-wave superconductors with weak triplet pairing attraction , MIKAEL FOGELSTRÖM, Chalmers University of Technology, ANNICA BLACK-SCHAFFER, NORDITA — The quasiparticle states found in the vortex core of an d-wave high-T_c cuprate superconductor may be probed by STM experiments. Results of such experiments have revealed typical spectra that are quite different from what is seen in conventional low-T_c superconductors. In particular the Caroli-deGennes-Matricon state at $E \sim 0$ in the core center is not seen. Instead, in a high-T_c vortex core, quasiparticle states are found at energies that are at a sizable fraction of the gap energy. One explanation for this could be that a finite amplitude of a competing orderparameter stabilizes in the vortex-core center. We explore the possibility of nucleating a vortex-core state that locally breaks inversion symmetry. The vortex-core orderparameter is of mixed parity, in our case a (d + ip)-wave, and the quasiparticle spectra in the core center lacks the $E = 0$ states. We compare our results with available experimental data.

10:36AM H25.00014 Possible mechanism of enhanced pairing correlation near dopant oxygen in cuprate , MICHIYASU MORI, Japan Atomic Energy Agency, GINIYAT KHALIULLIN, Max-Planck-Institut fur Festkorperforschung, TAKAMI TOHYAMA, Kyoto University, SADAMICHI MAEKAWA, Japan Atomic Energy Agency — Recent experiments on Bi-based cuprate superconductors have revealed an unexpected enhancement of the pairing correlations near the interstitial dopant oxygens. We propose a mechanism by which the dopant oxygens strongly enhance the interaction J locally [1]. We notice that there is a strong covalency between the dopant oxygen and closely located apical oxygens, forming a molecular orbital complex. By considering virtual p-d and d-d charge transitions within the Cu-O-Cu bond that lead to the spin exchange J, we will show that the corresponding excitation energies are screened by the polarization of molecular orbitals hence enhancing J. The effect is greatly amplified due to cooperative response of the spatially extended oxygens complex. We will also show, by an exact diagonalization of the t-J model, that local enhancement of J leads to the spatial variations in density of electronic states observed in STM experiments. Our findings suggest an interesting possibility of quantum-chemistry control of the key interaction J in cuprates.

[1] G. Khaliullin, M. Mori, T. Tohyama, and S. Maekawa, arXiv:1008.0435

Tuesday, March 22, 2011 8:00AM - 11:00AM –

Session H26 DMP DCOMP: Focus Session: Iron Based Superconductors – Anisotropic Spin Dynamics D162/164

8:00AM H26.00001 Impact of the Spin Density Wave Order on the Superconducting Gap of $Ba(Fe_{1-x}Co_x)_2As_2$, LUDIVINE CHAUVIERE, YANN GALLAIS, MAXIMILIEN CAZAYOUS, MARIE-AUDE MEASSON, ALAIN SACUTO, Laboratoire Materiaux et Phenomenes Quantiques UMR 7162 CNRS Universite Paris Diderot, Paris, France, DOROTHEE COLSON, ANNE FORGET, CEA Saclay IRAMIS, SPEC CNRS URA 2464, Gif-sur-Yvette, France, SQUAP TEAM, SPEC COLLABORATION — We report a doping dependent electronic Raman scattering measurements on iron-pnictide superconductor $Ba(Fe_{1-x}Co_x)_2As_2$ single crystals. The B_{2g} Raman spectrum at optimal doping is consistent with a strongly anisotropic gap on the electron pocket. Upon entering the coexistence region between superconducting (SC) and spin-density-wave (SDW) orders, the effective pairing energy scale is strongly reduced. Our results are interpreted in terms of a competition between SC and SDW orders for electronic states at the Fermi level. Our findings advocate for a strong connection between the SC and SDW gaps anisotropies which are both linked to interband interactions.

8:12AM H26.00002 Frustrated square lattice Heisenberg model and magnetism in Iron Telluride , IGOR ZALIZNYAK, ZHIJUN XU, GENDA GU, JOHN TRANQUADA, Brookhaven National Laboratory, MATTHEW STONE, Oak Ridge National Laboratory — We have measured spin excitations in iron telluride Fe1.1Te, the parent material of (1,1) family of iron-based superconductors. It has been recognized that J1-J2-J3 frustrated Heisenberg model on a square lattice might be relevant for the unusual magnetism and, perhaps, the superconductivity in cuprates [1,2]. Recent neutron scattering measurements show that similar frustrated model might also provide reasonable account for magnetic excitations in iron pnictide materials. We find that it also describes general features of spin excitations in FeTe parent compound observed in our recent neutron measurements, as well as in those by other groups. Results imply proximity of magnetic system to the limit of extreme frustration. Selection of spin ground state under such conditions could be driven by weak extrinsic interactions, such as lattice distortion, or strain [3]. Consequently, different nonuniversal types of magnetic order could arise, both commensurate and incommensurate. These are not necessarily intrinsic to an ideal J1-J2-J3 model, but might result from lifting of its near degeneracy by weak extrinsic perturbations.

[1] A. V. Chubukov, Phys. Rev. B 48, 5588 (1992). [2] P. A. Lindgard, Phys. Rev. Lett. 95, 217001 (2005). [3] I. A. Zaliznyak, Phys. Rev. B 68, 134451 (2003); ibid. 69, 092404 (2004).

8:24AM H26.00003 Superconductivity and Magnetism in the Checkerboard Models for Iron-based Superconductors , CHEN FANG, Purdue University, XIAOLI LU, YONGJIN JIANG, Zhejiang Normal University, WEI-FENG TSAI, Tokyo University, JIANGPING HU, Purdue University — We study three different checkerboard models for iron-based superconductors and obtain their phase diagrams in the solvable limit of weakly coupled checkerboards. We demonstrate that the strongest superconducting pairing is in the A_{1g}-S wave channel and the development of the superconductivity (SC) is correlated with the emergence of the next nearest neighbor antiferromagnetism (AFM). Moreover, this study suggests that the superconductivity and magnetism are orbital-selective. In the three-band model, the AFM is more robust in the d_{xy} orbital and the superconductivity is easier to be generated in the d_{xz} and d_{yz} orbitals. Comparisons between our theoretical results and current experimental measurements are discussed.

8:36AM H26.00004 Anisotropy of the spin dynamics in hole and electron-doped 122 , PENGCHENG DAI, University of Tennessee/ORNL — This abstract not available.

9:12AM H26.00005 Magnetic properties in the Mott-insulating iron oxychalcogenides $La_2O_2Fe_2OSe_2$[1] , JIAN-XIN ZHU, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, RONG YU, QIMIAO SI, Department of Physics & Astronomy, Rice University, Houston, TX 77005 — The role of electron correlation and magnetism in high-temperature superconductivity of the iron pnictides has been a topic of discussion. It has also motivated interest to compare related compounds with the iron pnictides and chalcogenides. Recently both electronic structure calculations and experimental measurements have indicated that the iron oxychalcogenides $La_2O_2Fe_2OSe_2$, which contains an Fe square lattice with an enlarged unit cell, has a larger U/t and is a Mott insulator [1]. We focus here on the understanding of the magnetism of this system. Within the density functional theory, we consider the magnetic phase diagram. Using an effective frustrating spin-exchange model in a doubled checker-board lattice, we study the magnetic excitation spectrum. Our theoretical results are compared with the emerging elastic and inelastic neutron scattering data in this compound.

[1] J.-X. Zhu, R. Yu *et. al*, Phys. Rev. Lett. **104**, 216405 (2010).

[1]This work was supported by the NNSA of the U.S. DOE at LANL under Contract No. DE-AC52-06NA25396 (J.X.Z), the NSF Grant No. DMR-0706625, the Robert A. Welch Foundation Grant No. C-1411, and the W. M. Keck Foundation (R.Y. and Q.S.).

9:24AM H26.00006 Consistent model of magnetism in ferropnictides , ALEKSANDER WYSOCKI, KIRILL BELASHCHENKO, Department of Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln, VLADIMIR ANTROPOV, Ames Laboratory — The character of magnetic interactions and spin fluctuations in ferropnictides has until now resisted understanding within any conventional model of magnetism. We show that the most puzzling features can be naturally reconciled within a rather simple effective spin model with biquadratic interaction, which is consistent with electronic structure calculations. While preserving the symmetry of the lattice, this model spin Hamiltonian stabilizes the collinear stripe ground state and generates an anisotropic spin wave spectrum. A natural reinterpretation of the measured spin wave spectra in ferropnictides is presented based on this model. Classical Monte Carlo simulations with experimentally motivated parameters produce reasonable Neel temperatures for 122 compounds. The model predicts that the phase transition to the paramagnetic phase changes from second to first order as the magnitude of the biquadratic term is increased. This property agrees with the observed behavior of the 122 compounds under doping. A clear signature of the separation of the nematic and antiferromagnetic phase transitions is also found. Preprint: arXiv:1011.1715.

9:36AM H26.00007 Spin-resolved electron-phonon coupling in FeSe[1] , TIMUR BAZHIROV, JESSE NOFFSINGER, MARVIN L. COHEN, University of California Berkeley — FeSe is one of the simplest iron-based superconductors. There are previous studies indicating that including the iron magnetic moment ordering has a significant effect on electron-phonon interactions and thus might be important for superconductivity. To explore the role of spin-dependent phonon induced pairing of the electrons, we apply first principle techniques based on the pseudopotential density functional approach and the local spin density approximation to calculate the electron-phonon coupling properties of FeSe. Our results indicate that introducing magnetic moments leads to a significant increase in coupling at least for certain phonon modes. At the gamma point in the Brillouin zone the increase is two-fold. Both phonon renormalization and electron-phonon matrix elements increases are present.

[1]This work was supported by National Science Foundation Grant No. DMR10-1006184, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at Lawrence Berkeley National Laboratory's NERSC facility

9:48AM H26.00008 Spin-phonon coupling and superconductivity in iron pnictides , TANER YILDIRIM, UPENN & NIST, XUHUI LUO, UIC & NIST, SERDAR OGUT, UIC — Early electron-phonon (el-ph) coupling calculations for iron pnictide system based on standard non-spin-polarized perturbation theory indicate that conventional el-ph coupling cannot explain the observed high Tc in these systems. However, the experimental phonon spectrum indicates features which are not produced in the standard linear response non-magnetic phonon calculations. The magnetic phonon calculations clearly indicate that the observed phonon-DOS at room temperature is much closer to the magnetic phonon-DOS rather than non-magnetic DOS and Fe-magnetism must present in the iron-pnictide systems all the time [1-2]. Thus we need to calculate the magnetic el-phonon coupling with the Fe-spins included before we can rule out any type of phonon-mediated mechanism. In order to carry out such complex self-consistent magnetic el-ph coupling calculations we are developing a finite-displacement method in which both the phonon energies and the corresponding el-ph coupling constant are easily calculated. Implications of our results on the mechanism of superconductivity in iron pnictides will be discussed. Finally, we will compare our calculations with the available phonon energy and line-width measurements.

[1] T. Yildirim, Phys. Rev. Lett. 102, 037003 (2009).
[2] T. Yildirim, Physica C 469, 425-441 (2009).

10:00AM H26.00009 Gap structure of the iron-pnictide superconductor LiFeAs via low-temperature thermal conductivity , J.-PH. REID, S. RENÉ DE COTRET, LOUIS TAILLEFER, University of Sherbrooke, Sherbrooke, Canada, M.A. TANATAR, H. KIM, K. CHO, R. PROZOROV, Ames Laboratory, Ames, Iowa, Y.J. SONG, Y.S. KWON, Sungkyunkwan University, Gyeonggi-Do, Korea — The thermal conductivity of the stoichiometric iron-pnictide superconductor LiFeAs was measured at temperatures down to $T \sim 50$ mK in magnetic fields up to $H = 17$ T on high-quality single crystals with $T_c \simeq 18$ K. The absence of any residual linear term at $T \to 0$ shows that there are no nodal quasiparticles. The slow increase of thermal conductivity with magnetic field shows that the gap is large everywhere on the Fermi surface. The same behaviour is observed for both in- plane and out-of-plane directions. We conclude that the superconducting gap in LiFeAs is basically isotropic. This is similar to what has been found in the iron-pnictide superconductors $Ba_{1-x}K_xFe_2As_2$ [1] and $Ba(Fe_{1-x}Co_x)_2As_2$ [2] at optimal doping (maximal T_c).

[1] X.-G. Luo *et al.*, Phys. Rev. B **80**, 140503 (2009).
[2] J.-Ph. Reid *et al.*, Phys. Rev. B **82**, 064501 (2010).

10:12AM H26.00010 NMR Study of the SDW ordering and the Spin Fluctuations on NaFeAs single crytals[1] , WEIQIANG YU, L. MA, S. ZHANG, J. ZHANG, T.-L. XIA, G.F. CHEN, Department of Physics, Renmin University of China, Beijing 100872, China, DAO-XIN YAO, School of Physics and Engineering, Sun Yat-sen University, Guangzhou 510275, China — In iron pnictides, the nature of the spin density wave (SDW) ordering is still not clear. Recently, increasing attention has been drawn to the correlation between the SDW transition and the high-temperature tetragonal to the low-temperature orthorhombic structure transition. In NaFeAs, the magnetic moment is small and both transitions are well separated, and therefore NaFeAs could be a good candidate to study the interplay of different degrees of freedom microscopically. In this talk, we report our ^{23}Na and ^{75}As NMR observations on NaFeAs single crystals. We found that 1) the spin fluctuations are largely enhanced below the structure transition; 2) the SDW transition temperature and the magnetic moment increase significantly with pressure; and 3) the NMR linewidth and the temperature/field dependence of the spin- lattice relaxation rate show signatures of an incommensurate SDW ordering in a limited temperature range just below the SDW transition. Based on these results, we discuss the coupling between the magnetism and the lattice/band structure in NaFeAs.

[1]Supported by NSFC and National Basic Research Program of China.

10:24AM H26.00011 Spin excitation in LiFeAs[1] , MENG WANG, HUIQIAN LUO, XIANCHENG WANG, Institute of Physics Chinese Academy of Sciences, YANG ZHAO, JEFFREY LYNN, NIST Center for Neutron Research, CHANGQING JIN, Institute of Physics Chinese Academy of Sciences, PENGCHENG DAI, University of Tennessee, PENGCHENG DAI TEAM, CHANGQING JIN COLLABORATION, JEFFREY LYNN COLLABORATION — We used inelastic neutron scattering to study the spin excitations in LiFeAs. Clear spin excitations were found but there was no spin resonance. Surprisingly, very big spin gap exists in this material.

[1]Institute of Physics Chinese Academy of Sciences

10:36AM H26.00012 Neutron Diffraction Studies of PrFe(1-x)Ru(x)AsO[1] , YUEN YIU, Univ of Tenn, OVIDIU GARLEA, ASHFIA HUQ, Oak Ridge Natl Lab, MICHAEL MCGUIRE, Oak Ridge National Laboratory, DAVID MANDRUS, Univ of Tenn, Oak Ridge Natl Lab, STEPHEN NAGLER, Oak Ridge Natl Lab — We report neutron powder diffraction (NPD) studies of Ru doped PrFe(1- x)Ru(x)AsO. The parent compound PrFeAsO undergoes a structural transition as well as magnetic transitions involving Fe and Pr moments upon cooling. Previous measurements (M. A. McGuire et al, Jrnl of Solid State Chem, 182- 8, 2326-2331) showed that Ru doping suppresses the above transitions. However, unlike most 1111's, this does not lead to superconductivity. To investigate the origin of this odd behavior we performed NPD measurements as a function of temperature for values of x up to 0.75. The results showed that although the structural and magnetic transitions are suppressed, the c axis displayed apparent negative thermal expansion (NTE) for all values of x. Such NTE has been seen in the parent compound (S. A. J. Kimber et al, PRB 78-140503), but to our knowledge there are no reports of NTE in superconducting samples. This suggests that the mechanism producing the NTE could also be responsible for the absence of superconductivity. We also report data on the magnetic transitions for lightly doped samples with x up to 0.1.

[1]Supported by the USDOE BES SUF and MSE Division.

10:48AM H26.00013 Interactions between rare earth and iron magnetism in *RE*FeAsO single crystals[1] , A. KREYSSIG[2,3], [2]Ames Laboratory; [3]Dep. of Physics and Astronomy, Iowa State University, Ames, M.G. KIM[2,3], W. TIAN[2], W. RATCLIFF II[4], [4]NIST, NCNR, Gaithersburg , J.-W. KIM[5], [5]APS, ANL, Argonne , S. NANDI[2,3], J.-Q. YAN[2], B. JENSEN[2], K.W. DENNIS[2], R.W. MCCALLUM[2,6], [6]Dep. of Materials Science and Engineering, Iowa State University, Ames , T.A. LOGRASSO[2], J.W. LYNN[4], J.L. ZARESTKY[2], R.J. MCQUEENEY[2,3], A.I. GOLDMAN[2,3] — In iron-based pnictides high-temperature superconductors, magnetic fluctuations and magneto-elastic effects are believed to be important for the superconducting electron pairing mechanism. To gain insight into the interplay between the different ordering phenomena and the underlying couplings we studied the tetragonal-to-orthorhombic distortion and the magnetic order by x-ray and neutron diffraction on *RE*FeAsO single crystals. The onset of rare earth (*RE* = Nd, Pr) magnetic order is coupled to changes in the iron magnetic structure without affecting the lattice distortion. High-resolution neutron and x-ray resonant magnetic scattering measurements down to 0.4 K revealed complex magnetic structures with multiple propagation vectors at low temperatures.

[1]The work at the Ames Laboratory was supported by US DOE, Office of Basic Energy Sciences, contract DE-AC02-07CH11358.

Tuesday, March 22, 2011 8:00AM - 11:00AM –
Session H27 GQI: Focus Session: Semiconductor Qubits- Silicon Spin Qubits C155

8:00AM H27.00001 Considerations for spin-based quantum computing in the solid-state , CHARLES TAHAN, RUSKO RUSKOV, ONEY SOYKAL, Laboratory for Physical Sciences — We give an update on recent work towards practical quantum computing using gated spins in semiconductors, especially in silicon.

8:12AM H27.00002 Fast initialization of a silicon spin qubit via an excited orbital state , C.B. SIMMONS, J.R. PRANCE, B.J. VAN BAEL, TECK SENG KOH, ZHAN SHI, D.E. SAVAGE, M.G. LAGALLY, R. JOYNT, MARK FRIESEN, S.N. COPPERSMITH, M.A. ERIKSSON, University of Wisconsin-Madison — We present data showing the initialization and measurement of individual electron spins in a silicon quantum dot. Spectroscopy of the electronic excited states of the dot reveals a relatively low-lying excited orbital state that is much more strongly coupled to the reservoir than the ground orbital state. As a function of an applied magnetic field, Zeeman splitting is observed for both the ground and the excited orbital states. By tuning a gate voltage, electron spins can be preferentially loaded into the quantum dot via any of these spin-split orbital states. Loading at either of the excited orbital states is measured to be over an order of magnitude faster than loading at directly into the orbital ground state. We use single-shot readout to measure the spin state of the loaded electrons. We observe two clear peaks in the fraction of spin-up electrons that are loaded, and these peaks correlate with loading through the spin-up ground or excited orbitals.

8:24AM H27.00003 Measurement of the electron spin relaxation time in a silicon quantum dot using single-shot readout , J.R. PRANCE, C.B. SIMMONS, B.J. VAN BAEL, TECK SENG KOH, ZHAN SHI, D.E. SAVAGE, M.G. LAGALLY, R. JOYNT, MARK FRIESEN, S.N. COPPERSMITH, M.A. ERIKSSON, University of Wisconsin-Madison — Electron spins in Si/SiGe quantum dots are promising candidates as qubits for quantum information processing, because spins in silicon couple weakly to the host material. We present a measurement of the spin lifetime for electrons in a silicon quantum dot. The spin state of individual electrons is measured using single-shot charge readout and spin-to-charge conversion: only spin-up electrons will tunnel off the quantum dot. Charge sensing is performed with an integrated quantum point contact that detects single electron tunnel events as steps in current. We determine the relaxation time by measuring the fraction of measurements that contain spin-up tunneling events as a function of the time that the electron spins are held on the quantum dot. We observe a clear decay in this spin-up fraction versus time, and an exponential fit yields $T_1 \sim 2.8$ seconds at a magnetic field of 1.85 T.

8:36AM H27.00004 Measurement of the Spin Relaxation Lifetime (T_1) in a One-Electron Strained-Si Accumulation-Mode Quantum Dot , EDWARD CROKE, MATTHEW BORSELLI, ANDREY KISELEV, PETER DEELMAN, IVAN MILOSAVLJEVIC, IVAN ALVARADO-RODRIGUEZ, RICHARD ROSS, ADELE SCHMITZ, MARK GYURE, ANDREW HUNTER, HRL Laboratories, LLC — We report measurements of the spin-relaxation lifetime (T_1) as a function of magnetic field in a strained-Si, accumulation-mode quantum dot. An integrated quantum-point contact (QPC) charge sensor was used to detect changes in dot occupancy as a function of bias applied to a single gate electrode. The addition spectra we obtained are consistent with theoretical predictions starting at N=0. The conductance of the charge sensor was measured by applying an AC voltage across the QPC and a 3 kΩ resistor. Lifetime measurements were conducted using a three-pulse technique consisting of a load, read, and flush sequence. T_1 was measured by observing the decay of the spin bump amplitude as a function of the load pulse length. We measured decay times ranging from approximately 75 msec at 2T to 12 msec at 3T, consistent with previous reports and theoretical predictions. Sponsored by United States Department of Defense. Approved for Public Release, Distribution Unlimited.

8:48AM H27.00005 Undoped Si/SiGe Depletion-Mode Few-Electron Double Quantum Dots , MATTHEW BORSELLI, HRL Laboratories LLC, BIQIN HUANG, RICHARD ROSS, EDWARD CROKE, KEVIN HOLABIRD, THOMAS HAZARD, CHRISTOPHER WATSON, ANDREY KISELEV, PETER DEELMAN, IVAN ALVARADO-RODRIGUEZ, ADELE SCHMITZ, MARKO SOKOLICH, MARK GYURE, ANDREW HUNTER — We have successfully formed a double quantum dot in the sSi/SiGe material system without need for intentional dopants. In our design, a two-dimensional electron gas is formed in a strained silicon well by forward biasing a global gate. Lateral definition of quantum dots is established with reverse-biased gates with $\sim$40 nm critical dimensions. Low-temperature capacitance and Hall measurements confirm electrons are confined in the Si-well with mobilities $>10^4$ cm^2/V-s. Further characterization identifies practical gate bias limits for this design and will be compared to simulation. Several double dot devices have been brought into the few-electron Coulomb blockade regime as measured by through-dot transport. Honeycomb diagrams and nonlinear through-dot transport measurements are used to quantify dot capacitances and addition energies of several meV. Sponsored by United States Department of Defense. Approved for Public Release, Distribution Unlimited.

9:00AM H27.00006 Transport, Charge Sensing, and Quantum Control in Si/SiGe Double Quantum Dots[1] , KE WANG, PANU KOPPINEN, YULIYA DOVZHENKO, JASON PETTA, Department of Physics, Princeton University, Princeton, NJ 08544 — Si/SiGe quantum dots hold great promise as ultra-coherent qubits [1]. In comparison with the GaAs system, Si has a weaker hyperfine interaction due to the zero nuclear spin of ^{28}Si and smaller spin-orbit coupling due to its lighter atomic weight [2]. However, the fabrication of highly controllable Si/SiGe quantum dots is complicated by valley degeneracy, the larger effective electron mass, and the difficulty of obtaining high quality samples [3]. Here we develop a robust fabrication process for depletion mode Si/SiGe quantum dots, demonstrating high quality ohmic contacts and low-leakage Pd top gates. We report DC transport measurements as well as charge sensing in single and double quantum dots. The quantum dot gate electrode pattern allows a relatively high level of control over the confinement potential, tunneling rates, and electron occupation.

[1] C. B. Simmons *et al.*, arXiv:1010.5828v1 (2010).
[2] R. Hanson *et al.*, Rev. Mod. Phys. **79**, 1217 (2007).
[3] F. Schäffler, Semicond. Sci. Tech. **12**, 1515 (1997).

[1]Funded by the Sloan and Packard Foundations, NSF, and DARPA QuEST. We thank Jag Shah for logistical support.

9:12AM H27.00007 Double quantum dot with tunable coupling in an enhancement-mode silicon metal-oxide semiconductor device with lateral geometry , L.A. TRACY, R.W. YOUNG, G.A. TEN EYCK, K. ENG, K.D. CHILDS, J.R. WENDT, R.K. GRUBBS, J. STEVENS, M.P. LILLY, M.S. CARROLL, Sandia National Labs, E.P. NORDBERG, Sandia National Labs; University of Wisconsin-Madison, C. BORRAS PINILLA, Universidad Industrial de Santander-Colombia, H.L. STALFORD, Sandia National Laboratories; University of Oklahoma-Norman, M.A. ERIKSSON, University of Winsconsin-Madison — We present transport measurements of a tunable silicon metal- oxide-semiconductor double quantum dot device with lateral geometry. Experimentally extracted gate-to-dot capacitances show that the device is largely symmetric under the gate voltages applied. Intriguingly, these gate voltages themselves are not symmetric. Comparison with numerical simulations indicates that the applied gate voltages serve to offset an intrinsic asymmetry in the physical device. We also show a transition from a large single dot to two well isolated coupled dots, where the central gate of the device is used to controllably tune the interdot coupling.
This work was supported by the LDRD program at Sandia National Laboratories, a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary Lockheed-Martin Company, for the U. S. DOE NNSA under Contract No. DE-AC04-94AL85000

9:24AM H27.00008 The effect of donors on lateral gated quantum-devices in Si/SiGe heterostructures[1] , XI LIN, JINGSHI HU, A. LAI, MIT, Z. ZHANG, UCLA, K. MACLEAN, MIT, Y.H. XIE, UCLA, M.A. KASTNER, MIT — Much activity has focused on the development of quantum dots in Si/SiGe because of its potentially very long decoherence times (T2). However, to fabricate well-controlled quantum dots in Si/SiGe heterostructures, one must overcome complications that do not arise in GaAs/AlGaAs heterostructures. We demonstrate that switching charge noise and donor-layer conduction can lead to instability and cross-coupling among the tunnel barriers, thus making it difficult to achieve highly stable and tunable quantum devices in a Si/SiGe heterostructure. In particular, we have used an integrated charge-sensing quantum point contact to investigate the charge motion that originates from the excess donors, and present a systematic capacitance measurement to show how the donor layer affects device function in devices with large ($\sim$100 μm^2) gates as well as nanometer-size ones.

[1]This work has been supported by the Nanoscale Science and Engineering Center program of NSF (PHY-0117795), NSF (DMR-0701386).

9:36AM H27.00009 Pauli Spin Blockade and Lifetime-Enhanced Transport in a Si/SiGe double quantum dot[1] , TECK SENG KOH, C.B. SIMMONS, NAKUL SHAJI, MADHU THALAKULAM, L.J. KLEIN, HUA QIN, H. LUO, D.E. SAVAGE, M.G. LAGALLY, University of Wisconsin-Madison, A.J. RIMBERG, Dartmouth College, ROBERT JOYNT, ROBERT BLICK, MARK FRIESEN, S.N. COPPERSMITH, M.A. ERIKSSON, University of Wisconsin-Madison — We analyze electron transport data through a Si/SiGe double quantum dot in terms of spin blockade and lifetime-enhanced transport (LET), which is transport through excited states that is enabled by long spin relaxation times. We present a series of low-bias voltage measurements showing the sudden appearance of a strong tail of current that we argue is an unambiguous signature of LET appearing when the bias voltage becomes greater than the singlet-triplet splitting for the (2,0) electron state. We present eight independent data sets, in both forward and reverse bias regimes, and show that excellent fits to all data sets were obtained using one consistent set of parameters. We also obtain quantitative estimates for the tunneling rates and currents in the reverse bias regime using the Lindblad formalism. [Ref: arXiv:1008.5398v1]

[1]This work was supported in part by ARO and LPS (W911NF-08-1-0482), by NSF (DMR-08325634, DMR- 0805045), and by DOE (DE-FG02-03ER46028).

9:48AM H27.00010 Fabrication of Few-Electron Carbon Nanotube Single and Double Quantum Dots , HUGH CHURCHILL, PATRICK HERRING, RUBY LAI, CHARLES MARCUS, Harvard University — We discuss fabrication methods for carbon nanotube quantum dot devices designed to satisfy the requirements of spin qubit applications. These requirements include low disorder for reliable access to the few-electron regime, detection of charge states, and rapid manipulation with multiple gates. Nanotube growth occurs at or near the end of the fabrication process, a scheme that has been shown previously to produce clean devices for transport studies. In our devices the nanotubes are grown over pre-patterned gates or the nanotubes are located and gates are placed on top. A new atomic layer deposition process was developed to coat the nanotubes in a high-k dielectric for effective gating and suppression of electron interactions. We find in these devices that disorder on the length scale of the quantum dot is made small enough for routine occupancy with few charges, but disorder with sufficiently short range to couple valleys remains an uncontrolled parameter that is important for qubit applications of nanotubes. We acknowledge support from NSF-MWN, IBM, and Harvard University.

10:00AM H27.00011 Undoped Heterostructure Materials for SiGe Quantum Devices , R.S. ROSS, M.G. BORSELLI, B. HUANG, K.S. HOLABIRD, T.M. HAZARD, A.A. KISELEV, P.W. DEELMAN, I. ALVARADO-RODRIGUEZ, A.E. SCHMITZ, M. SOKOLICH, A.T. HUNTER, M.F. GYURE, HRL Laboratories LLC, 3011 Malibu Canyon Road, Malibu CA 90265 — Quantum well heterostructures, widely used for the fabrication of quantum dots and related devices, typically make use of modulation doping. Removal of the dopants, by use of globally "field-gated" and/or back-gated heterostructure designs, eliminates the dominant sources of scattering, charge noise and instability in devices intended for low-temperature operation. In this talk we present recent progress in designing and fabricating undoped quantum well heterostructures in sSi/SiGe. A combination of simulation based modeling and experimental work has enabled us to successfully engineer materials for stable and quiet quantum dot operation. Specific topics to be presented include the important role of substrate and buffer layer background doping, concurrent MOS accumulation, leakage to front and back gates via barrier tunneling, and the expected range of electric fields that determine valley mixing in quantum dots. Sponsored by United States Department of Defense. Approved for Public Release, Distribution Unlimited.

10:12AM H27.00012 Heterostructure surface effects on Si/SiGe 2DEGs , XIAN WU, C.B. SIMMONS, J.R. PRANCE, D.E. SAVAGE, M.G. LAGALLY, M.A. ERIKSSON, University of Wisconsin-Madison — We present the results of Hall and Shubnikov-de Haas measurements of the two-dimensional electron gas (2DEG) in Si/SiGe heterostructures at 2 K. We demonstrate that the condition of the surface has significant effects on the carrier density and mobility of electrons in the quantum well. Results from multiple samples show that the carrier density and mobility decrease with the amount of time that the samples are exposed to air. Surface treatment via a forming gas anneal or by dipping the samples in HF restores the carrier density and mobility of the degraded samples, and storing the samples in vacuum slows the rate of degradation. We believe that the reduction in carrier density of the 2DEG is a result of interface traps that form in the surface native oxide. Forming gas anneal passivates the interface traps, and HF strips the oxide. Illuminating the degraded samples at 2 K also improves the carrier density and mobility, possibly by activating electrons out of trap states. Deposition of AL2O3 on the surface using ALD caused a severe reduction in carrier density, which we believe is the result of a high trap density.

10:24AM H27.00013 Density and Depth of Natural Quantum Dots in Silicon MOS Structures , R.M. JOCK, S. SHANKAR[1], A.M. TYRYSHKIN, J.-H. HE, S.A. LYON, Princeton University, K. ENG[2], K. CHILDS, L. TRACY, M. LILLY, M. CARROLL, Sandia National Laboritories — Electron spins in MOS structures have shown promise as qubits for quantum information processing. Typically, characteristics such as mobility, mid-gap interface states and oxide fixed charge are considered figures of merit for the Si/SiO_2 interface, however, other properties may be important. Recently, we have shown that, by biasing the gate above threshold and then reducing V_G to 0V, we freeze electrons into natural quantum dots, where 2D electrons are confined by interface disorder. The depth of these dots is determined by the temperature and can be extracted using a Schottky-Hall-Read model. Additionally, we measure the density of confined electron states from the magnitude of the ESR signal. These measurements offer us a means to characterize the interface disorder in these MOS structures. Experiments have been performed on devices from different labs. Preliminary results from industrial quality devices fabricated at Sandia National Laboratories indicate a shallower dot depth, though a similar mobility. The shallower confinement suggests a higher quality for single-electron quantum devices.

[1]Now at Yale
[2]Now at HRL

10:36AM H27.00014 Real time electron counting through wavelet edge detection[1] , BJORN VAN BAEL, JONATHAN PRANCE, CHRISTIE SIMMONS, TECK SENG KOH, ZHAN SHI, DON SAVAGE, MAX LAGALLY, ROBERT JOYNT, MARK FRIESEN, SUSAN COPPERSMITH, MARK ERIKSSON, University of Wisconsin-Madison — We have recently demonstrated single-shot measurements of individual electron spins in a Si/SiGe quantum dot. These experiments were analyzed using a wavelet-based technique that allows detection of charging events in real time. An alternative method, based on level thresholding, is not well suited for real time detection, due to drifting background currents in the charge sensor. In contrast, the wavelet technique relies on edge detection and is hence robust against drifting currents levels. In this talk, we describe our wavelet algorithm and its applications for charge sensing. We benchmark the performance of the algorithm under realistic signal noise conditions.

[1]This work was supported by ARO, LPS, NSF and DARPA.

10:48AM H27.00015 Triangulating the source of tunneling resonances in a point contact with nanometer scale sensitivity , N.C. BISHOP, Sandia National Labs, C. BORAS PINILLA, Universidad Industrial de Santander-Colombia, H.L. STALFORD, University of Oklahoma, R.W. YOUNG, G.A. TEN EYCK, J.R. WENDT, K. ENG, M.P. LILLY, M.S. CARROLL, Sandia National Labs — We observe resonant tunneling in split gate point contacts defined in a double gate enhancement mode Si-MOS device structure. We determine the capacitances from the resonant feature to each of the conducting gates and the source/drain two dimensional electron gas regions. In our device, these capacitances provide information about the resonance location in three dimensions. Semi-classical electrostatic simulations of capacitance, already used to map quantum dot size and position [Stalford et al., IEEE Nanotechnology], identify a combination of location and confinement potential size that satisfy our experimental observations. The sensitivity of simulation to position and size allow us to triangulate possible locations of the resonant level with nanometer resolution. We discuss our results and how they may apply to resonant tunneling through a single donor. This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

Tuesday, March 22, 2011 8:00AM - 11:00AM –

Session H28 DMP: Focus Session: Carbon Nanotubes and Related Materials: Devices I C156

8:00AM H28.00001 Individual SWCNT based ionic field effect transistor[1] , PEI PANG, Department of Physics, Biodesign Institute, Arizona State University, JIN HE, Biodesign Institute, Arizona State University, JAE HYUN PARK, PREDRAG KRSTIC, Physics Division, Oak Ridge National Laboratory, STUART LINDSAY, Department of Physics, Biodesign Institute, Department of Chemistry and Biochemistry, Arizona State University — Here we report that the ionic current through a single-walled carbon nanotube (SWCNT) can be effectively gated by a perpendicular electrical field from a top gate electrode, working as ionic field effect transistor. Both our experiment and simulation confirms that the electroosmotic current (EOF) is the main component in the ionic current through the SWCNT and is responsible for the gating effect. We also studied the gating efficiency as a function of solution concentration and pH and demonstrated that the device can work effectively in the physiological relevant condition. This work opens the door to use CNT based nanofluidics for ion and molecule manipulation.

[1]This work was supported by the DNA Sequencing Technology Program of the National Human Genome Research Institute (1RC2HG005625-01, 1R21HG004770-01), Arizona Technology Enterprises and the Biodesign Institute.

8:12AM H28.00002 Chemically-Driven Two Level Fluctuations in Single-Walled Carbon Nanotubes (SWCNTs) with Defects , DANNY WAN, STEVEN R. HUNT, BRAD L. CORSO, ISSA S. MOODY, GREGORY A. WEISS, PHILIP G. COLLINS, Departments of Physics and Astronomy, Chemistry, Molecular Biology and Biochemistry, University of California, Irvine, CA 92697 — When a SWCNT conductor contains a defect, its electronic fluctuations are sensitive indicators of the surrounding chemical environment and of the chemical state of the defect itself. We demonstrate this effect by fabricating single SWCNT devices and then engineering their defect condition through the method of electrochemical point-functionalization. By characterizing the same SWCNT before and after the introduction of a point defect, we clearly establish the defect's contribution to the overall device noise. Carboxylate defects are particularly interesting because they have a deprotonated state that is sensitive to pH, electrolyte, and electrochemical potential. Large amplitude, two level fluctuations are observed from carboxylate sites when probed under conditions near the dissociation constant pKa, and the occupation statistics can be reversibly tuned by either pH or potential. We interpret the fluctuation in terms of the controlled protonation and deprotonation of the defect site, and describe a simple electrostatic gating model that supports this conclusion.

8:24AM H28.00003 Gas detection mechanism for single-walled carbon nanotube networks[1] , ANTHONY BOYD, ISHA DUBE, Georgtown University Washington, DC 20057, GEORGY FEDOROV, RRC Kurchatov Institute, Moscow, Russia 123182, MAKARAND PARANJAPE, PAOLA BARBARA, Georgtown University Washington, DC 20057, GEORGETOWN/RRC KURCHATOV COLLABORATION[2] — We study field-effect transistors fabricated with carbon nanotube (CNT) networks to determine whether the gas sensing mechanism is due to molecules adsorbed on the nanotubes, or changes at the interface between the nanotubes and the contacts. Our previous work showed that in devices made with isolated CNT, the response to nitrogen dioxide was mainly due to the contact interfaces [1]. Here, we focus on CNT networks and use SU-8 layers patterned with e-beam lithography to passivate the contact interfaces, while leaving the network exposed. We look to investigate possible differences in sensing mechanism for devices made with isolated tubes versus networks.

[1] J. Zhang, A. Boyd, A. Tselev, M. Paranjape, and P. Barbara, *Mechanism of NO_2 detection in carbon nanotube field effect transistor chemical sensors*, Applied Physics Letters **88,** 123112-123115 (2006)

[1]Work funded by NSF, DMR 1008242
[2]Material World Network

8:36AM H28.00004 Effects of adsorbed gases on the conductance of individual carbon nanotubes[1] , DAVID COBDEN, HAO-CHUN LEE, ERIK FREDRICKSON, University of Washington, RICHARD ROY, University of Puget Sound, OSCAR VILCHES, University of Washington — We investigate the effects of adsorbed monolayers of Ar, Kr and other gases on individual suspended single-walled carbon nanotubes. The down-shifts of the vibrational resonances of a nanotube can be used to determine the monolayer density[2] while the electrical conductance is measured simultaneously, at temperatures as low as 4.3 K. In the case of Ar, by studying density isotherms in the range 38 to 65 K, we see behavior resembling that of the well known two-dimensional vapor, liquid and solid phases on exfoliated graphite, although the correspondence is not exact and is device dependent. In addition, we find that the conductance changes significantly and non-monotonically with the density, and there are indications that it is sensitive to ordering in the monolayer.

[1]Work supported by NSF DMR-0907690 and PHY-0754333 (REU)(Roy)
[2]Z. Wang et al, Science 327, 552 (2010)

8:48AM H28.00005 Anomalous Current-Voltage Characteristics in Suspended Carbon Nanotubes in Various Gas Environments , MOH AMER, University of Southern California, ADAM BUSHMAKER, The Aerospace Corporation, STEVE CRONIN, University of Southern California — Electrically-heated suspended, carbon nanotubes (CNTs) exhibiting negative differential conductance in the high bias regime experience a sudden drop in current (or "kink") in various gaseous environments. We study the effect of different gas molecules on these $I-V$characteristics while simultaneously monitoring the changes in the nanotube vibrational structure under high bias voltages using Raman spectroscopy. When the nanotube is electrically biased at the kink, the G band Raman mode is observed to downshift, as is typical of electrically heated devices. However, the G band frequency at the kink (ω_G^{kink}) lies in the narrow range between 1575 and 1579cm^{-1} for all samples measured, regardless of gas environment. The voltage at which the kink occurs depends on the type of the gas environment with the following dependence: $V_{kink}^{Ar} < V_{kink}^{He} < V_{kink}^{CO_2}$. The magnitude of the kink, however, has the following ordering: $\Delta I_{kink}^{Ar} < \Delta I_{kink}^{CO_2} < \Delta I_{kink}^{He}$. This ordering was observed consistently in all samples measured. Several possible mechanisms underlying this phenomenon are discussed within the context of these findings.

9:00AM H28.00006 Heat Dissipation from Suspended Carbon Nanotubes to their Surrounding Gas Environment , I. KAI HSU, MICHAEL T. PETTES, MEHMET AYKOL, LI SHI, STEPHEN CRONIN — The assistance of gas molecules to dissipate heat in 5-μm-long, electrical heated suspended carbon nanotubes (CNTs) is observed by comparing the Gband Raman phonon temperature profiles measured in different gas environments and in vacuum. The measurement results show that 50-60% of the heat generated in the CNT is carried away by its surrounding gas molecules. By analyzing the temperature profiles investigated in different gases, the thermal boundary conductance (TBC) between the gas molecules and the CNT can also be extracted. We find the TBC to be higher in carbon dioxide than in nitrogen, argon and helium.[1] Moreover, we report another optical method to explore the heat spreading behavior on a longer suspended CNTs in air, in which one laser is used as a heat source while another laser is used as a local temperature probe. A fin-shape thermal transport model is applied to fit the exponentially decaying temperature profiles measured away from the heat source. These results yield a heat decay length and TBC for air to be around 6.5 μm and 3×10^5 W/m^2 •K, respectively.

[1]I Kai Hsu *et al. Journal of Applied Physics* **2010,** 108, (084307).

9:12AM H28.00007 Electroluminescence from a single nanotube-molecule-nanotube junction , RALPH KRUPKE, Karlsruhe Institut für Technologie — The reliable fabrication of metallic singlewall carbon nanotube (mSWNT) electrode pairs with sub-10 nm spacing allows us to contact organic molecules (M) via dielectrophoresis and to form mSWNT-M-mSWNT junctions. For this purpose we used specific designed molecules which have an appropriate length to bridge the SWNT electrode gap, and a sufficient polarizability to allow the molecule deposition between the SWNT electrodes via DC-dielectrophoresis. The molecules comprise a fluorescent chromophore subunit. During transport measurements several mSWNT-M-mSWNT junctions showed light emission at voltages > 4 V. The electroluminescence spectrum from the junction is very similar to the photoluminescence signal of the molecules on HOPG-surfaces. This result together with control experiments indicates that light is emitted from the chromophore core of the mSWNT contacted molecule [1]. If time allows I will also report on a related work about phonon-assisted electroluminescence from biased metallic single wall carbon nanotubes (SWNT), multi wall carbon nanotube (MWNT) and few layer graphene (FLG) devices [2].

[1] C.W. Marquardt, S. Grunder, A. Blaszczyk, S. Dehm, F. Hennrich, H. v. Löhneysen, M. Mayor, R. Krupke, Nature Nanotechnology 2010; DOI: 10.1038/NNANO.2010.230
[2] S. Essig et al., Nano Letters 10, 1589 (2010)

9:48AM H28.00008 Thermal Emission of Suspended Carbon Nanotube , ZUWEI LIU, ADAM BUSHMAKER, MEHMET AYKOL, STEVE CRONIN, USC TOPRAMAN TEAM — We study the thermal emission spectra of individual suspended carbon nanotube induced by electrical heating. Semiconducting and metallic devices exhibit different spectra, based on their distinctive bandstructures. These spectra are compared with the ideal blackbody emission spectrum. In the response region of our detector, i.e. visible to near infrared, the thermal emission spectra of semiconducting devices agree well with Planck's law, while the spectra of metallic devices show an additional peak around 1.65 eV. For semiconducting devices, the temperature of the nanotube was fitted to Planck's law, and was compared with the temperature fitted from the G band downshift as well as the Stokes:anti-Stokes intensity ratio. For devices showing thermal non-equilibrium, the electron temperature agrees well with G+ downshift, but deviates from G- downshift. Finally, for metallic devices, partially polarized IR emission was observed, and possible mechanisms are discussed.

10:00AM H28.00009 Electric field dependence of photoluminescence from individual single-walled carbon nanotubes[1] , S. YASUKOCHI, T. MURAI, T. SHIMADA, S. CHIASHI, S. MARUYAMA, Y.K. KATO, The University of Tokyo — Using suspended single-walled carbon nanotubes, we investigate electric field effects on photoluminescence. Trenches are fabricated on SiO_2/Si substrates, and Pt is deposited for electrical contacts. Carbon nanotubes are grown by patterned chemical vapor deposition. These devices operate as back-gate field effect transistors, allowing application of electric fields on as-grown ultraclean nanotubes. Individual suspended carbon nanotubes are identified by taking photoluminescence images using a home-built laser-scanning confocal microscope. After determining the chirality by photoluminescence excitation spectra, we measure gate voltage dependence of photoluminescence. We observe quenching of photoluminescence intensity and shifts of emission wavelength as gate voltages are applied.

[1]This work is supported by KAKENHI, Mizuho Foundation for the Promotion of Sciences, Research Foundation for Opto-Science and Technology, TEPCO Research Foundation, SCAT, SCOPE, and Photon Frontier Network Program of MEXT, Japan.

10:12AM H28.00010 Simultaneous Rayleigh and Raman spectroscopy on suspended single-walled carbon nanotubes under electrostatic gating , YUHEI MIYAUCHI, ZHENGYI ZHANG, MITSUHIDE TAKEKOSHI, VIKRAM DESHPANDE, Columbia University, New York, NY 10027, STÉPHANE BERCIAUD, Université de Strasbourg, PHILIP KIM, JAMES HONE, TONY HEINZ, Columbia University, New York, NY 10027 — The optical properties of single-walled carbon nanotubes (SWNTs) under electrostatic gating are of great interest for fundamental understanding of one-dimensional physics and for their application as optoelectronics devices. Here, we report how the electronic transitions are modified by gating conditions through direct measurements of Rayleigh (elastic) light scattering from individual suspended SWNTs [1]. With increasing gate voltage, we observed both a broadening and shift of the excitonic resonances in the Rayleigh scattering spectra. The influence of carrier doping on the optical resonances and, as gauged through simultaneous Raman measurements, on vibrational transitions will be discussed.

[1] M. Y. Sfeir et al., Science 306, 1540 (2004).

10:24AM H28.00011 Photoconductivity measurements of single-walled carbon nanotube field effect transistors[1] , T. MURAI, S. YASUKOCHI, S. MORITSUBO, T. SHIMADA, S. CHIASHI, Y. MURAKAMI[2], S. MARUYAMA, Y.K. KATO, The University of Tokyo — Photoconductivity measurements are performed on carbon nanotube field effect transistors. Carbon nanotubes are grown on SiO_2/Si substrate by patterned chemical vapor deposition using ethanol as carbon source. Next, electron beam lithography, metal deposition, and liftoff processes are performed to form source and drain electrodes. The Si substrate is used as a back-gate in these devices. Wavelength tunable Ti:sapphire laser is focused onto the sample with an objective lens, and the laser spot is scanned with a steering mirror. A lock-in amplifier is used to detect the photoconductivity signal of carbon nanotube field effect transistors.

[1]This work is supported by Research Foundation for Opto-Science and Technology, NSG Foundation, SCAT, SCOPE, and Photon Frontier Network Program of MEXT, Japan.
[2]current affiliation: Tokyo Institute of Technology

10:36AM H28.00012 Role of defects in optical phonon decay, softening and 1/f noise resonance in carbon nanotubes , MOONSUB SHIM, University of Illinois — Scattering and relaxation of optical phonons are especially important processes in carbon nanotubes. Strong phonon softening near the Dirac point in metallic nanotubes occurs by coupling of carrier excitation to optical phonon transitions. Current saturation and negative differential conductance in the high bias regime in nanotube devices are attributed optical phonon absorption and emission. Cooling of hot carriers occurs mostly via optical phonons which eventually decay anharmonically into acoustic phonons. Whether intentional or unavoidable, defects will strongly influence these fundamentally important processes. In this talk, how defects affect optical phonon scattering will be discussed. In particular, defect-dependent optical phonon lifetime and resonant 1/f noise associated with phonon softening via the Kohn anomaly will be discussed.

10:48AM H28.00013 Micro-scale "air-gap" circuitry with conducting carbon nanotube-copper composite , CHANDRAMOULI SUBRAMANIAM, Technology Research Association for Single Wall Carbon Nanotubes, Central 5, 1-1-1 Higashi, Tsukuba, Ibaraki, 305-8565, Japan, TAKEO YAMADA, DON N. FUTABA, KENJI HATA, Super-growth CNT Team, Nanotube Research Centre, National Institute of Advanced Industrial Science and Technology, Central 5, 1-1-1 Higashi, Tsukuba, — The ability of water-assisted CVD to produce aligned close-packed single wall carbon nanotubes(CNT) with superior thermal and mechanical properties make them ideal materials for use in microelectronics. However, their poor electrical conductivity has been a major obstacle in realizing this. To overcome this, we report the synthesis of conducting CNT-copper composite (conductivity σ=10^5 Scm^{-1}) through a novel organic phase electrodeposition. The conductivity enhancement (10^3 times over CNT) is due to the high, uniform filling of Cu in the aligned CNT matrix. Micro-scale, three-dimensional lithographic engineering of CNT-Cu, involving fully suspended CNT-Cu beams, is achieved for microelectronic applications. Multi-tier CNT-Cu circuits are also fabricated, with the constituent lines separated by air (replaceable with vacuum). This "vacuum-separation" exists in the horizontal and vertical directions providing unique multi-tier "air-gap" circuits. This realization of dielectric-less, air-gap circuits with CNT-Cu is thought to be a breakthrough for developing faster and efficient microelectronic devices.

Tuesday, March 22, 2011 8:00AM - 11:00AM –

Session H29 GQI: Focus Session: Quantum Information for Quantum Foundations - Axiomatics and Toy Models C148

8:00AM H29.00001 Toward a conceptual foundation of Quantum Information Processing , GIULIO CHIRIBELLA, Perimeter Institute for Theoretical Physics — Quantum Information Science has brought to light an enormous amount of new protocols showing that the structure of quantum theory dramatically impacts the way in which information can be processed. It also made clear that the rules of information processing are dictated by physics and that different physical theories entail different models of information processing. Quantum Information poses an exciting challenge to foundational research: the challenge is to reduce the multiplicity of quantum protocols to a small number of basic physical principles and to answer questions like "What are the physical roots of the power of quantum information?" A satisfactory answer to these questions calls for the solution of a long-standing problem: deriving quantum theory from physical principles, as opposed to the abstract mathematical principles of the Hilbert space formulation. In this talk I will show that quantum theory can be derived from few principles about information processing. The central principle of the derivation will be the purification principle, stating that ignorance about a part (subsystem) is always compatible with maximal knowledge of the whole (compound system). A large number of quantum information features, including e.g. teleportation and no-cloning, are direct consequences of the purification principle, which appears a strong candidate for the conceptual foundation of Quantum Information Processing. Moreover, the derivation of quantum theory from purely informational principles provides a rigorous justification of the diffuse claim that quantum theory is ultimately a theory of information.

8:36AM H29.00002 Physics as Information , GIACOMO MAURO D'ARIANO, Università di Pavia — The experience from Quantum Information has lead theorists to look at Quantum Theory and the whole Physics from a different angle. A new information-theoretic paradigm is emerging, long time ago prophesied by John Archivald Wheeler with his popular coinage "It from bit." Theoretical groups are now addressing the problem of deriving Quantum Theory from informational principles, and similar lines are investigated e.g. in new approaches to Quantum Gravity. In my talk I will review some recent advances on these lines. The general idea synthesizing the new paradigm is that there is only Quantum Theory (without quantization rules), and the whole Physics—including space-time and relativity–is emergent from the quantum-information processing. And, since Quantum Theory itself is made with purely informational principles, the whole Physics must be reformulated in information-theoretical terms. The review is divided into four parts: a) Very short review of the informational axiomatization of Quantum Theory; b) How space-time and relativistic covariance emerge from the quantum computation; c) What is the information-theoretical meaning of inertial mass and Planck constant, and how the Dirac field emerges; d) Observable consequences of the new theory. I will then conclude with some possible future research lines.

8:48AM H29.00003 A derivation of quantum theory from physical requirements , MARKUS MUELLER, Perimeter Institute for Theoretical Physics, Waterloo (ON), Canada, LLUIS MASANES, ICFO-Institut de Ciencies Fotoniques, Barcelona, Spain — Quantum theory is usually formulated by postulating the mathematical structure and representation of states, transformations, and measurements. The general physical consequences that follow (like violation of Bell-type inequalities, the possibility of performing state tomography with local measurements, or factorization of integers in polynomial time) come as theorems which use the postulates as premises. In this work, this procedure is reversed: we impose five simple physical requirements, and this suffices to single out quantum theory and derive its mathematical formalism uniquely. This is more similar to the usual formulation of special relativity, where two simple physical requirements —the principles of relativity and light speed invariance— are used to derive the mathematical structure of Minkowski space-time and its transformations.

9:00AM H29.00004 Homogeneous Self-Dual Cones and the Structure of Quantum Theory , ALEXANDER WILCE, Susquehanna University — This talk reviews recent and on-going work with Howard Barnum on the origins of the Jordan-algebraic structure of finite-dimensional quantum theory. I begin by surveying various principles — e.g., that every state of a bipartite system arise as the marginal of a "steering" bipartite state – - that force the cone of (un-normalized) states of a finite-dimensional probabilistic system to be homogenous and *weakly* self-dual, that is, isomorphic to its dual cone. Where this weak self-duality can be implemented by an inner product, the cone is *strongly* self dual. In this case, classical results of Koecher and Vinberg show that it is isomorphic to the cone of squares in a formally real Jordan algebra. If this is the case, then (using a theorem of H. Hanche-Olsen) one can show that the only locally-tomographic theory containing at least one qubit is finite-dimensional Complex QM. I conclude with a brief discussion of how one might motivate strong self-duality.

9:12AM H29.00005 Quaternions and the Quantum[1] , MATTHEW GRAYDON, University of Waterloo and Perimeter Institute for Theoretical Physics — Birkhoff and von Neumann pointed out that quantum probability calculi could be formulated over rings admitting involutory anti-automorphisms [1]. We discuss a model for generalized quantum measurements and quantum states based on quaternionic matrix algebras. We show that the usual Born rule for calculating probabilities for outcomes of quantum measurements can be carried over into quaternionic quantum theories within a Jordan-algebraic framework. We exploit a group isomorphism between Sp(1) and SU(2) to show that single-system unitary dynamics and generalized measurements in a quaternionic quantum theory can be simulated by corresponding processes in usual quantum mechanics. We resurvey the divide between quaternionic and complex quantum theories given this quadit-qudit correspondence. Reference: [1] G. Birkhoff and J. Von Neumann, "The logic of quantum mechanics", Ann. Math., 37, 823-843 (1936).

[1]This work was supported in part by the U. S. Office of Naval Research (Grant No. N00014-09-1-0247).

9:24AM H29.00006 Quantum theory cannot be extended , ROGER COLBECK, Perimeter Institute, Canada, RENATO RENNER, ETH Zurich, Switzerland — Predictions made by quantum theory are generally not deterministic: the theory tells us only how to calculate the probabilities with which measurement outcomes occur. This indeterminism is one of the key differences from classical mechanics and one can ask whether this is the best any theory can offer, or whether observable quantities could be better predicted by some higher theory. In a famous work, Bell considered extensions of quantum theory in the form of local hidden variables and showed that these cannot determine the outcomes of measurements on maximally entangled particles. Here, we go beyond the case of such classical extensions and ask whether any improved predictions can be achieved by any extension of quantum theory. We answer this question in the negative. More precisely, under the assumption that measurement settings can be chosen freely, there cannot exist any extension of quantum theory that provides us with any additional information about the outcomes of future measurements.

9:36AM H29.00007 Eliminating remnants of classical mechanics and the birth of the Schrödinger equation , WOLFGANG P. SCHLEICH, Institute of Quantum Physics, Ulm University, DANIEL GREENBERGER, City College, City University of New York, DONALD H. KOBE, Department of Physics, University of North Texas — We show that the Schrödinger equation emerges from the Hamilton-Jacobi equation for a specific choice of the amplitude R of a wave $\psi \equiv R\exp[IS/\hbar]$ where S is the classical action. This choice eliminates in the wave equation for ψ all remnants of classical mechanics associated with S but at the same time builds via the wave equation for R a bridge to classical mechanics and to the de Broglie pilot wave theory.

9:48AM H29.00008 Modal Quantum Theory , MICHAEL WESTMORELAND, Denison University, BENJAMIN SCHUMACHER, Kenyon College — We present a class of toy model theories similar in structure to ordinary quantum mechanics. Some of these models are based on finite fields instead of complex amplitudes. The interpretation of such theories involves only the "modal" concepts of possibility and necessity rather than quantitative probability measures. Despite its very simple structure, our toy model nevertheless includes many of the key phenomena of actual quantum systems: interference, complementarity, entanglement, nonlocality, and the impossibility of cloning. These results are detailed in arXiv:1010.2929 and arXiv:1010.5452.

10:00AM H29.00009 Time-asymmetry and causal structure , BOB COECKE, RAYMOND LAL, Oxford University — We consider devices with two inputs and two outputs, Alice and Bob each having access to one input and one output. To such a device we associate time-reverses by exchanging the roles of the inputs and the outputs. We find that there are devices which admit a local hidden variable representation, but for which time- reverses enable perfect signaling between Alice and Bob. That is, a "perfect channel in one time direction" becomes a "non-channel in the other direction." Also, for PR boxes time-reverses enable signaling between Alice and Bob, but never as a perfect channel. This result has several consequences. Firstly, it establishes that the arrow of time can be read from signaling structure: signaling means backward in time. It undermines the representation of causal structures as partial orders or similar 'time-symmetric structures', as is often assumed in search of a theory of quantum gravity. They also provide new insights into the structure of the polytope of generalized probabilistic correlations, hence on theories more general than quantum theory. Finally, it contributes to the growing area of research into quantum information processing in relativistic spacetimes. Ref: arXiv:1010.4572

10:12AM H29.00010 Topos formulation of History Quantum Theory , CECILIA FLORI, Perimeter Institute — In this talk I will describe a topos formulation of consistent histories obtained using the topos reformulation of standard quantum mechanics put forward by Doering and Isham. Such a reformulation leads to a novel type of logic with which to represent propositions. In the first part of the talk I will introduce the topos reformulation of quantum mechanics. I will then explain how such a reformulation can be extended so as to include temporally-ordered collection of propositions as opposed to single time propositions. Finally I will show how such an extension will lead to the possibility of assigning truth values to temporal propositions.

10:24AM H29.00011 Causal Tapestries , WILLIAM SULIS, McMaster University — Causal sets provide one of many approaches to the problem of quantum gravity. Causal tapestries generalize the concept of a causal set, extending the range of putative dynamics from sequential growth to include iterative and non deterministic methods, and the range of embedding manifolds to include those with curvature. Like causal sets, causal tapestries are manifestly Lorentz invariant in spite of possessing a form of "transient now". It is shown that the order relations of the local causal structures must possess an order theoretic (Dushnik & Miller) dimension not exceeding the topological dimension of the embedding manifold and the finite free dimension is bounded by the number of elementary processes generating the causal relations.

10:36AM H29.00012 ABSTRACT WITHDRAWN –

10:48AM H29.00013 The quantal algebra and abstract equations of motion , SAMIR LIPOVACA — Classical and quantum mechanics common characteristics reveal core physics features that are hidden by the details related to the realizations of those theories in phase and Hilbert space respectively. The quantal algebra combines classical and quantum mechanics into an abstract structurally unified structure. It is based on two observations which can be made about classical and quantum mechanics. The first observation is that classical and quantum mechanics use two products: one symmetric and one anti-symmetric. The second observation is that classical and quantum mechanics obey the so-called composability principle: any two physical systems can interact with each other. The local structure of spacetime is contained in the quantal algebra without having been postulated. We will generalize classical and quantum mechanics equations of motion to abstract equations of motion in which the anti-symmetric product of the quantal algebra plays a central role. We will express the defining identities of the quantal algebra in terms of the abstract derivation. In this form it is easy to see that the first defining identity (the Jacobi identity) captures the essence of the Bianchi identity in general relativity which is one set of gravitational field equations for the curvature tensor.

Tuesday, March 22, 2011 8:00AM - 10:00AM –

Session H30 DCMP: Graphene: Synthesis and Characterization C147/154

8:00AM H30.00001 Electrical breakdown of graphene and few-layer graphene structures , ABHISHEK SUNDARARAJAN, STEPHEN JOHNSON, D. PATRICK HUNLEY, ROEL FLORES, University of Kentucky, A.T CHARLIE JOHNSON, University of Pennsylvania, DOUGLAS STRACHAN, University of Kentucky — The electrical breakdown of graphene and few-layer graphene (FLG) structures are investigated. To better understand the dynamics of these nano-scale thermal effects, we investigate graphene and FLG nanowires of various dimensions and find that significant joule heating occurs inducing the structures to evolve. A distinct change in the behavior during electrical stressing indicates that different mechanisms occur at the various stages of evolution. The results are compared to detailed thermal modeling of our structures and could have implications on the development of high current carrying nanoscale graphene devices. Supported in part by NSF Award No. DMR-0805136, the Kentucky NSF EPSCoR program, the University of Kentucky Center for Advanced Materials, and the University of Kentucky Center for Nanoscale Science and Engineering.

8:12AM H30.00002 Designing all-graphene nano-junctions by covalent functionalization , CATERINA COCCHI, ALICE RUINI, S3 CNR-Nano & University of Modena, IT, DEBORAH PREZZI, S3 CNR-Nano, IT, MARILIA J. CALDAS, University of Sao Paulo, BR, ELISA MOLINARI, S3 CNR-Nano & University of Modena, IT — We study the effect of covalent edge functionalization, with organic functional groups, on the opto-electronic properties of graphene nano-flakes and nano-junctions. We work within the frame of Hartree-Fock-based semi-empirical methods [1,2]. Our study shows that functionalization can be designed to tune electron affinities and ionization potentials of graphene flakes. The stability of the proposed mechanism is analyzed with respect to the functional groups, the functionalization rate and the width of graphene nanostructures. We show that this effect can be exploited to realize type-II all-graphene nano-junctions. Different frontier orbital alignments can be engineered varying the functionalization, leading to specific optical properties: The conditions to obtain charge transfer excitations are investigated.

[1] Dewar, et al., J. Am. Chem. Soc. 107, 3902 (1985)
[2] Ridley and Zerner, Theoret. Chim. Acta 32, 111 (1973)

8:24AM H30.00003 Schottky diode via dielectrophoretic assembly of reduced graphene oxide sheets between dissimilar metal contacts , MUHAMMAD R. ISLAM, DAEHA JOUNG, SAIFUL KHONDAKER, Nanoscience Technology Center, Department of Physics, University of Central Florida, Orlando, Florida 32826 — Reduced graphene oxide (RGO) has attracted significant attention due to its ability to produced graphene nanostructures in large quantities. It has been also considered as a promising building block for future generation of electronic and optoelectronic devices. Here we demonstrate fabrication of RGO Schottky diodes with high yield via dielectrophoretic (DEP) assembly between two dissimilar metal contacts. Titanium (Ti) was used to make a Schottky contact, while palladium (Pd) was used to make an Ohmic contact. From the current - voltage characteristics, we obtain rectifying behavior with a rectification ratio of up to 600. The ideality factor was high (4.9) due to the presence of a large number of defects. The forward biased threshold voltage was 1 V while the reverse bias breakdown voltage was - 3.1 V which improved further upon mild annealing at 200° C and can be attributed to an increase of work function of RGO due to annealing.

8:36AM H30.00004 Graphitic carbon molecular beam epitaxy on dielectric substrates[1] , ULRICH WURSTBAUER, RUI HE, ALBERT RIGOSI, Dept. of Physics, Columbia University, THEANNE SCHIROS, Energy Frontier Research Center, Columbia University, ANNETTE PLAUT, School of Physics, Exeter University, LOREN N. PFEIFFER, Princeton University, PHILIP KIM, ABHAY PASUPATHY, ARON PINCZUK, Dept. of Physics, Columbia University, JORGE M. GARCIA, Dept. of Physics, Columbia University, Instituto de Microelectrónica de Madrid, IMM-CNM, CSIC — We report on growth of thin large area graphitic layers on dielectric substrate materials by means of molecular beam epitaxy (MBE) under UHV conditions. This solid source MBE technique offers highly controllable conditions without the need of gas precursors or metal surfaces. Our initial experiments on dielectric substrates such as mica, SiO_2 and BN clearly demonstrates the potential of this new growth technique. NEXAFS studies show that the binding mechanism in our sheets is dominated by sp^2 bonds and the Raman spectra confirm their graphitic nature. We will also describe STM measurements of the topography and local electronic structure of these films.

[1]Work supported by ONR (N000140610138 and Graphene Muri), NSF (CHE-0117752 and CHE-0641523), NYSTAR, CSIC-PIF (200950I154), Spanish CAM (Q&C Light (S2009ESP-1503), Numancia 2 (S2009/ENE-1477)), Spanish MICINN (NANINPHO-QD, TEC2008-06756-C03-01).

8:48AM H30.00005 Stability of epitaxial graphene on pristine Si(111) , BRANDEN KAPPES, TERESA DAVIES, Colorado School of Mines, SUKKY JUN, University of Wyoming, ADRI VAN DUIN, Penn State University, CRISTIAN CIOBANU, Colorado School of Mines — Incorporation of carbon nanostructures with silicon-based nanoelectronics will involve the direct integration of graphene with silicon chips, but so far graphene has not been grown on pristine silicon surfaces. Because usual synthesis routes would likely lead to the formation of silicon carbide, we calculate the binding energy of graphene transferred onto the Si(111) surface and also analyze its stability at various temperatures. Our calculations based on (commensurate) moiré superstructures with periodic boundary conditions show a strong graphene–substrate binding, about 1.5 eV/carbon atom, over a wide range of in-plane orientations of the graphene layer. Molecular dynamics simulations based on bond-order and reactive force field interatomic potentials suggest that the graphene binds to the substrate where carbon is rehybridized sp^3, and that this rehybridized graphene structure does not lead to the decomposition of graphene into silicon carbide even at temperatures as high as 80% of the substrate melting temperature.

9:00AM H30.00006 Synthesis and characterization of graphene patterned with Fe_3O_4 nanoparticles , SAYAN CHANDRA, K. STOJAK, D. FERIZOVIC, M. MUNOZ, M.H. PHAN, H. SRIKANTH, University of South Florida — Graphene has emerged as a very exciting material with its outstanding physical, chemical, and mechanical properties. Due to the presence of excess free electrons on a graphene surface, the possibility of graphene-mediated long-range interactions between magnetic nanoparticles would open up new avenues of research and device development. Our studies aimed to deposit $\sim$9 nm Fe_3O_4 NPs on graphene layers to understand the role of the metallic interface in mediating the magnetic interactions between the particles. We successfully grew the high-quality graphene on Ni films using CVD and used the Langmuir-Blodgett technique to pattern different layers of the Fe_3O_4 nanoparticles on the graphene sheets. The samples were well structurally characterized by XRD, TEM, AFM, and Raman spectroscopy. Interestingly we have observed strong variation in the magnetic properties such as magnetic anisotropy of the NPs pattered graphene samples when compared to just the NPs. These results point to the important role of the metallic interface in mediating the magnetic interactions between the Fe_3O_4 nanoparticles.

9:12AM H30.00007 Scaled-Up Synthesis and Characterization of High-Purity Graphene , PATRICIA JOHNSON, MARK GRIEP, KRISTOPHER BEHLER, ROSE PESCE-RODREQUEZ, SHASHI KARNA, WENDY SARNEY, Army Research Laboratory, KATE DUNCAN, CERDEC — Graphene, a two-dimensional, single-atom sheet of carbon atoms, discovered in 2004, has emerged as a new class of novel nano-scale material due to its unique chemical and physical properties, and potential applications in a wide range of civilian and military technologies. However, a major challenge in its technological application is a lack of chemical/physical method(s) to produce/synthesize high-purity graphene in viable quantity. Another challenge in the technological application of graphene is a lack of detailed understanding of its structure-property relationship. In order to address these issues, we have developed a chemical exfoliation method that yields high-purity graphene in bulk quantity. The method is scalable to produce large quantities of high purity graphene. In this paper, we present the results of our synthetic approach and structure-property characterization of graphene.

9:24AM H30.00008 Two-Dimensional Molecular Crystals of Phosphonic Acids on Graphene , MARIANA PRADO, BERNARDO NEVES, REGIANE NASCIMENTO, LUCIANO MOURA, MATHEUS MATOS, MARIO MAZZONI, LUIZ CANCADO, HELIO CHACHAM, Universidade Federal de Minas Gerais — The synthesis and characterization of two-dimensional (2D) molecular crystals comprised of long and linear phosphonic acids atop graphene is reported. Using scanning probe microscopy in combination with first-principles calculations, we show that these true 2D crystals are oriented along graphene armchair direction only, thereby enabling an easy determination of graphene flake orientation. We have also compared the doping level of graphene flakes via Raman spectroscopy. The presence of the molecular crystal atop graphene induces a well-defined shift in the Fermi level, corresponding to hole doping, which is in agreement with our ab initio calculations.

9:36AM H30.00009 Carbon chains grown perpendicularly on graphene: Nanobrush , CAN ATACA, Department of Physics, Bilkent University, Ankara, Turkey, 06800, SALIM CIRACI, Department of Physics, Bilkent University, Ankara, Turkey, 06800; UNAM-Material Science and Nanotechnology, Bilkent University, Ankara, Turkey, 06800. — We predict a peculiar growth process, where carbon adatoms adsorbed to graphene readily diffuse above room temperature and form linear chains. These chains grow longer on graphene through insertion of carbon atoms one at a time from the bottom end. Through this growth process two allotropic forms of carbon, namely graphene and polyyne are combined to make several novel nanostructures. Brush like graphene sheets with protruding polyynes can achieve chemical activity and attain new functionalities.

9:48AM H30.00010 Size Control of Nanographene Directly Grown On Glass , JAEWU CHOI, Kyung Hee University — We directly deposited very thin carbon film was on glass by thermal chemical deposition at 750 °C without using any catalyst. The directly deposited carbon film consists of nanographene with an in-plane crystal size of $\sim$ 15 nm. The in-plane crystal size of nanographene increased up to 23 nm by annealing of the post-deposited nickel film on the nanographene film at 300 °C to 500 °C. This study suggests that nanographene can be directly deposited on glass at low temperature and that the crystalline size can be controlled.

Tuesday, March 22, 2011 8:00AM - 10:48AM –

Session H31 DMP GSCCM DCOMP: Focus Session: Materials at High Pressure I: Molecular and Simple Materials C145

8:00AM H31.00001 Structural investigation and shock Hugoniot calculations of methane under high temperatures and pressures , BENJAMIN SHERMAN, California State University, Northridge, BURKHARD MILITZER, HUGH WILSON, University of California, Berkeley, DAYANTHIE WEERARATNE, California State University, Northridge — The behavior of methane under pressures and temperatures spanning 0.02-7.75 Mbar and 300-30,000 K was studied using density functional molecular dynamics. The structural properties of fluid and crystalline methane were analyzed with simulations at various (P,T) conditions. These simulations were also used to calculate the shock Hugoniot curves of methane for a range of initial densities between 0.4-0.57 g/cc. These curves allow us to make predictions of state and phase that correspond to future methane shock experiments.

8:12AM H31.00002 Proton Exchange Reactions in Deuterium Water Mixtures[1] , GUSTAV BORSTAD, Institute for Shock Physics, Dept. of Physics, Washington State University, Pullman, WA 99164, CHOONG-SHIK YOO, Institute for Shock Physics, Dept. of Chemistry, Washington State University, Pullman, WA 99164 — Binary mixtures of water and hydrogen under pressure are of interest both as fundamental systems in physics and chemistry and due to their applicability to fuel cells. Their behaviors at extreme pressures and temperatures are also of significance to understanding the interaction of chemical species in the interiors of giant gas planets and other planetary objects. In this talk, we will present high-pressure Raman data of deuterium water mixtures, which provides both kinetic information regarding the proton exchange reactions and the structure of deuterium in the mixtures.

[1]The work has been supported by NSF (DMR-0854618) and DOE-NNSA (# DE-F603-97SF21388).

8:24AM H31.00003 Zero-Temperature Structures of Atomic Metallic Hydrogen , JEFFREY MCMAHON, DAVID CEPERLEY, Department of Physics, University of Illinois, Urbana-Champaign, IL 61801 — Since the first prediction of an atomic metallic phase of hydrogen by Wigner and Huntington over 75 years ago, there have been many theoretical efforts aimed at determining the crystal structures of the zero-temperature phases. We present results from ab initio random structure searching with density functional theory performed to determine the ground state structures from 500 GPa to 5 TPa. We estimate that molecular hydrogen dissociates into a monatomic body-centered tetragonal structure near 500 GPa ($r_s = 1.225$), which then remains stable to 2.5 TPa ($r_s = 0.969$). At higher pressures, hydrogen stabilizes in an $...ABCABC...$ planar structure that is remarkably similar to the ground state of lithium, which compresses to the face-centered cubic lattice beyond 5 TPa ($r_s < 0.86$). Our results provide a complete ab initio description of the atomic metallic crystal structures of hydrogen, resolving one of the most fundamental and long outstanding issues concerning the structures of the elements.

8:36AM H31.00004 Phase Diagram of Carbon Dioxide at High Pressure and Temperatures: Implications to the Deep Carbon Cycle[1] , CHOONG-SHIK YOO, Dept of Chemistry and Institute for Shock Physics, Washington State University, Pullman, WA 99164, AMARTYA SENGUPTA, Institute for Shock Physics, Washington State University, Pullman, WA 99164 — Carbon dioxide is an important terrestrial volatile often considered to exist in the deep interior of the Earth. The phase diagram of carbon dioxide is critical to validate such hypothesis. In this study, we will present the phase diagram of carbon dioxide including the most recent finding of coesite-like carbon dioxide, a missing analog to SiO_2, address several controversies in terms of phase metastabilities and thermal path dependent transitions, and discuss about the implication to the deep carbon cycle.

[1]The work has been supported by NSF (DMR-0854618) and DARPA (W911NF-10-1-0081).

8:48AM H31.00005 Structural and optical properties of liquid CO_2 up to 1 terapascal[1] , BRIAN BOATES, Lawrence Livermore National Laboratory & Dalhousie University, SEBASTIEN HAMEL, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, STANIMIR BONEV, Lawrence Livermore National Laboratory & Dalhousie University — The properties of liquid CO_2 have been studied through first-principles molecular dynamics simulations in the pressure-temperature range of 0-1 TPa and 200-100,000 K. The resulting equation of state data is used to predict shock Hugoniots for several initial conditions. Comparison with available experimental data up to 70 GPa is excellent. We find a gradual phase transition characterized by the destabilization of CO_2 molecules and the formation of other molecular compounds. The liquid phase diagram is divided into several regimes based on a thorough analysis on changes in bonding, structural properties, and chemical composition. Calculations of optical properties such as conductivity and reflectivity will also be discussed.

[1]Work supported by NSERC, LLNL, the Killam Trusts, and Acenet. Prepared by LLNL under Contract DE-AC52-07NA27344.

9:00AM H31.00006 Density Functional Theory (DFT) simulations of CO2 under shock compression and design of liquid CO2 experiments on Z[1] , T. R. MATTSSON, L. SHULENBURGER, S. ROOT, Sandia National Laboratories, Albuquerque, NM., K. R. COCHRANE, Ktech Corporation, Albuquerque, NM. — Quantitative knowledge of the thermo-physical properties of CO2 at high pressure is required to confidently model the structure of gas-giants like Neptune and Uranus and the deep carbon cycle of the earth. DFT based molecular dynamics has been established as a method capable of yielding high fidelity results for many materials, including shocked gases, at high pressure and temperature. We predict the principal Hugoniot for liquid CO2 up to 500GPa. Our simulations also show that the plateau in shock pressure identified by Nellis and co-workers [1] is the result of dissociation. At low temperatures we validate the DFT results by comparing with diffusion Monte Carlo calculations. This allows for a more accurate determination of the initial conditions for the shock experiments. We also describe the design of upcoming flyer-plate experiments on the Z-machine aimed at providing high-precision shock compression data for CO2 between 150 and 600 GPa. [1] W. Nellis, et. al. , J. Chem. Phys. **95**, 5268 (1991).

[1]Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corp. for the US Dept. of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

9:12AM H31.00007 Novel phases of simple substances at megabar pressures , MIKHAIL EREMETS, Max Planck Institute for Chemistry — Under megabar pressures solids can be strongly compressed: volume of solid hydrogen decreases in $\sim$20 times, even diamond is 1.5 fold compressed at achievable pressures of $>$300 GPa. This dramatically changes interatomic distances in materials eventually leading to metallization in a number of presenting substances. Metals under compression supposedly remain in metallic state. But at high densities the core electrons come in to play and the electronic structure significantly departs from the simple metal as it was demonstrated for lithium. We present an ultimate case: sodium - simple metal - becomes transparent at pressures of $\approx$200 GPa transforming into ionic- electride-like state. We will present also our recent studies on nitrogen and nitrogen-rich materials: ammonia, azides and others, and progress on studies at pressures $\sim$400 GPa.

9:48AM H31.00008 Diamond as a high pressure gauge up to 2.7 MBar , NATALIA DUBROVINSKAIA, LEONID DUBROVINSKY, RAZVAN CARACAS, MICHAEL HANFLAND — Diamond anvil cell (DAC) technique has become a very important method of probing materials behaviour under pressure in various fields of research ranging from physics to biology and geoscienses. Optical methods of pressure determining in DAC experiments are based on fluorescent markers or calibrated pressure dependence of the Raman shift of suitable materials. Diamond has been since long recognised as a good pressure marker in experiments conducted in a diamond anvil cell. It is stable at ultra-high pressures that allows one to use the pressure dependence of the Raman frequency of the LTO optical phonon of diamond as a pressure gauge. A pressure gauge is a key issue of any high pressure experiment in a diamond anvil cell. Here we present a method of *in situ* synthesis of microcrystals of diamond that can be further used as a pressure standard in course of the same DAC experiment. Calibration curve of the Raman shift *vs* pressure is extended up to 270 GPa and experimental results are compared with those of *ab initio* calculations.

10:00AM H31.00009 High-pressure and high temperature deformation studies of polycrystalline diamond , XIAOHUI YU — With Vicker's hardness 120 GPa, shear modulus 535 GPa, diamond is the hardest material known to mankind. However, because diamond is difficult to deform, little is known with regard to its constitutive properties such as yield strength. In this work, we present results obtained at NSLS using deformation-DIA on polycrystalline diamond at different P-T conditions. As expected, even at total strains up to 20%, we did not observe the yield point of diamond at room temperature and a confining pressure of 4 GPa. However, for deformation at 1000 and 1200 °C, we observed an plastic flow of diamond at total strains of 10% and 5%, respectively, indicating that diamond weakens rapidly when temperature is over 1000 °C. We further derived the micro stress of diamond from peak width analysis, and found that the micro and macro stresses show similar variations with total strain at both room temperature and 1000 °C. However, at 1200 °C, the micro stress remains constant in entire deformation, indicating that stress is uniformly distributed within diamond particles at 1200 °C. We also carried out SEM studies on the recovered samples to investigate the miscrostructures, and find that the grain size of diamond decreases substantially during the deformation, from the initial microns to sub-microns for the room temperature deformation, however, almost doesn't change for the 1200 °C.

10:12AM H31.00010 New primary pressure calibrants for high pressure and temperature scale: SiC-3C and cBN are possible candidates , KIRILL ZHURAVLEV, ALEXANDER GONCHAROV, Carnegie Institution of Washington, VITALI PRAKAPENKA, University of Chicago — Since the invention of a diamond-anvil cell, various high-pressure scales for in situ pressure measurements have been realized. Ruby-based pressure scale (Mao et al., 1986) is the best known and high-pressure scientific community has been using it for over two decades. However, it has limited use at elevated temperatures, due to the weakening and broadening of the ruby fluorescence line. The recent developments in the field of high temperature, high pressure physics and geophysics require some alternative pressure scale, capable of measuring pressures at temperatures up to 3000 K. Cubic boron nitride (cBN) was recently proposed as the possible pressure calibrant. It has been suggested that the simultaneous use of x-ray diffraction to measure density and Brillouin spectroscopy to obtain elastic properties of the crystal can be used to construct the pressure scale independent of any other pressure standards. However, the acoustic velocities of cBN are very close to those of diamond and, therefore, are hard to resolve in experiment in diamond-anvil cell. Another possible primary pressure calibrant is cubic silicon carbide (SiC-3C). We performed single crystal x-ray diffraction and Brillouin spectroscopy up to 1 Mbar in pressure at room temperature in the diamond-anvil cell and show that cBN and SiC-3C, indeed, can be used in constructing reliable and accurate high-pressure, high-temperature scale.

10:24AM H31.00011 Formation and superconductivity of hydrides under pressure[1] , DUCK YOUNG KIM, TCM group, Cavendish laboratory, University of Cambridge, UK, RALPH H. SCHEICHER, Uppsala University, Sweden, CHRIS J. PICKARD, University College London, UK, RICHARD J. NEEDS, TCM group, Cavendish laboratory, University of Cambridge, UK, RAJEEV AHUJA, Uppsala University, Sweden — Hydrogen is the lightest and smallest element in the periodic table. Despite its simplest electronic structure, enormous complexity can arise when hydrogen participates in the formation of solids. Pressure as a controllable parameter can provide an excellent platform to investigate novel physics of hydrides because it can induce structural transformation and even changes in stoichiometry accompanied with phenomena such as metallization and superconductivity. In this presentation, we will briefly overview contemporary high-pressure research on hydrides and show our most recent results on predicting crystal structures of metal hydrides under pressure using ab initio random structure searching. Our findings allow for a better understanding of pressure-induced metallization/superconductivity in hydrides which can help to shed light on recent observations of pressure-induced metallization and superconductivity in hydrogen-rich materials.

[1]Wenner-Gren Foundations and VR in Sweden, The Royal Society in UK

10:36AM H31.00012 Mechanical properties of icosahedral boron carbide explained from first principles , ROMAN RAUCOULES[1], NATHALIE VAST, EMMANUEL BETRANHANDY, JELENA SJAKSTE, LSI - Ecole Polytechnique — An exhaustive DFT study of the structural defects of icosahedral B_4C and of their behavior under high pressure has been performed. Among the possible atomic structures, the lowest value of the formation energy has been found for the *polar* model B_4C^P, which consists of one distorted icosahedron and of one CBC chain. This result, together with the inspection of the vibrational and NMR spectra, has proved that B_4C^P is the proper structural model for B_4C.[1,2] Consequently, B_4C^P has been used as a matrix to isolate the defects. The native defects have been identified and shown to be energetically stable at high pressure. Most vacancy locations in B_4C^P are found to be energetically unstable and only a boron vacancy in the CBC chain is stable. A cluster of this vacancy is shown to induce a dynamical instability of the icosahedra when the pressure is increased. The dynamical failure of shocked B_4C [3] is attributed to the increase in the concentration of these unstable vacancies under plastic deformation. 1. R. Lazzari, N.Vast, J.M. Besson, S. Baroni and A. Dal Corso, Phys. Rev. Lett. 83 (1999) 3230. 2. F. Mauri, N. Vast and C.J. Pickard, Phys. Rev. Lett. 87 (2001) 085506. 3. T. Vogler, W. Reinhart and L. Chhabildas, J. Appl. Phys. 95 (2004) 4173.

[1]Membership pending

Tuesday, March 22, 2011 8:00AM - 11:00AM –

Session H32 DMP: Focus Session: Photonic Crystals, Metamaterials and Other Optical Systems C144

8:00AM H32.00001 Disordered Hyperuniform Photonic Band Gap Materials , MARIAN FLORESCU, Department of Physics, Princeton University, WEINING MAN, Department of Physics and Astronomy, San Francisco State University, PAUL CHAIKIN, Department of Physics, New York University, SALVATORE TORQUATO, Department of Chemistry, Princeton University, PAUL J. STEINHARDT, Department of Physics, Princeton University — Until recently, the only materials known to have complete photonic band gaps were photonic crystals, periodic structures, and it was generally assumed that long-range periodic order was instrumental in the band gap formation. We have shown that there exists a more general class of systems, called hyperuniform photonic structures, which exhibit large and complete photonic band gaps. This classification includes not only crystalline structures, but also non-crystalline materials, ranging from quasicrystals with crystallographically-forbidden rotational symmetries to isotropic, translationally-disordered structures. Remarkably, we find that the photonic band gaps in hyperuniform disordered structures are not only comparable to those found in photonic crystals, but also display a high degree of isotropy. These new materials possess unique photonic and physical properties that provide important advantages for applications. Our results show that hyperuniform disordered structures enable the realization of optical cavities with ultimate isotropic confinement of the electromagnetic radiation, lossless waveguides with arbitrary bending angles and flexible optical insulator platforms.

8:12AM H32.00002 Experimental observation of photonic bandgaps in two dimensional hyperuniform disordered materials , SEYED HASHEMIZAD, WEINING MAN, San Francisco State University, MARIAN FLORESCU, Princeton University, POLIN YADAK, KAZUE MATSUYAMA, San Francisco State University, SALVATORE TORQUATO, PAUL STEINHARDT, Princeton University, PAUL CHAIKIN, New York University — We report the first experimental demonstration of photonic bandgaps (PBGs) in 2D hyperuniform disordered materials and show that is possible to obtain isotropic, disordered, photonic materials of arbitrary size with complete PBGs. There are only limited numbers of allowed rotational symmetries in periodic or quasiperiodic structures. Periodicity and Bragg scattering lead to different stop gap center frequencies in different directions, since periodicities change in different directions. Hyperuniformity together with short range geometric order and uniform local topology are enough to give raise to an isotropic PBG. Hyperuniform systems have a variance in mass or particle number which varies with distance, r, from an arbitrary point less rapidly than the d dimensional volume. We present a new class of photonic materials posessing PBGs that have a number of advantages, including: isotropy, robustness against disorder (they are already disordered), flexibility (can fit arbitrary regions of space in which one may have trouble putting a periodic system), and possibly lower minimum dielectric contrast.

8:24AM H32.00003 Photonic density of states of 2D quasicrystals from level set equations and decorated quasiperiodic tiling patterns , LIN JIA, ION BITA, EDWIN THOMAS, DMSE Massachusetts Institute of Technology — The TE and TM photonic band gaps (PBG) of 8mm, 10mm, and 12mm rotationally symmetric 2D quasicrystals (QCs) were numerically investigated for families of morphologies generated from level set equations and from quasiperiodic tiling patterns decorated with cylindrical rods, respectively. We discovered a 12mm QC with 56.5% TE PBG, which is the largest reported TE PBG for aperiodic crystals to date. Further, we find that the TM PBG of 2D QC is highly related to the shape of the structural features comprised by the QC morphology. Two physical models are presented to explain the decrease of the center frequency of PBG as dielectric filling ratio increases.

8:36AM H32.00004 Measurement of photonic band diagram in non-crystalline photonic band gap (PBG) materials , WEINING MAN, ERIC WILLIAMSON, SEYED HASHEMIZAD, POLIN YADAK, San Francisco State Univ., Dept. of Physics & Astronomy, MARIAN FLORESCU, Princeton University, Physics Dept. — Non-crystalline PBG materials have received increasing attention recently and sizeable PBGs have been reported in quasi-crystalline structures or even in disordered structures. Band calculations for periodic structures produce accurate dispersion relations in them and refraction properties at their surfaces. However, band calculations for non-periodic structures employ large super-cells of N $>$100 building blocks, and provide little useful information other than the PBG frequency and width. Since band is folded into N bands, within the first Brillouin zone of the supper-cell. Using stereolithography, we construct various quasi-crystalline or disordered PBG materials and perform transmission measurements. The dispersion relations of EM wave (band diagrams) are reconstructed from the measured phase data. Our experiments not only verify the existence of sizeable PBGs in these structures, but also provide detailed information of the effective band diagrams, dispersion relation, group velocity vector, and their angular dependence. Slow light phenomena are also observed in these structures near gap frequencies. This study presents a powerful tool to investigate photonic properties of non-crystalline structures and provides important dispersion information, which is otherwise impossible to obtain.

8:48AM H32.00005 MWIR tunable polarmetric scatterometery applied to a fishnet structure , STEPHEN NAUYOKS, MICHAEL MARCINIAK, Air Force Institute of Technology — Understanding how light is scattered by a material, such as a metamaterial, which is engineered to have specific optical properties is necessary for a better understanding of the design parameters and for refining designs. Because of their high irradiance and small spot size, lasers are an ideal light source for these scatter measurements. However, lasers are highly monochromatic and it can be very difficult to manufacture metamaterials to resonate at such specific wavelengths. By modifying a Schmitt Measurement System's Complete Angle Scatter Instrument (CASI) with the addition of 6 external cavity Quantum Cascade Lasers by Daylight Solutions we were able to have a tunable laser light source from 4.35 to 9.71 μm with a small exclusion from 6.54 to 7.40 μm. The CASI system was further modified with the addition of a dual rotating retarder which allows the full Mueller matrix to be calculated for both specular scatter and off specular scatter. This makes the system unique to commercially available systems like Woollam's IR-VASE which can only measure the Mueller matrix elements for the specular reflection. This unique system was used to measure a fishnet structure at both resonate and off resonate frequencies. The fishnet sample was also measured using an IR-VASE system to compare specular results.

9:00AM H32.00006 Electromagnetism in multicoaxial negative-index metamaterial cables , BAHRAM DJAFARI-ROUHANI, University of Science & Technology of Lille1, France, MANVIR KUSHWAHA, Rice University — By using an elegant Green [or response] function theory, which does not require matching of the messy boundary conditions, we investigate the surface plasmon excitations in the multicoaxial cylindrical cables made up of negative-index metamaterials. The multicoaxial cables with *dispersive* metamaterial components exhibit rather richer (and complex) plasmon spectrum with each interface supporting two modes: one TM and the other TE for (the integer order of the Bessel function) $m \neq 0$. The cables with *nondispersive* metamaterial components bear a different tale: they do not support simultaneously both TM and TE modes over the whole range of propagation vector. The computed local and total density of states enable us to substantiate spatial positions of the modes in the spectrum. Such quasi-one dimensional systems as studied here should prove to be the milestones of the emerging optoelectronics and telecommunications systems.

9:12AM H32.00007 Universal shift of the Brewster angle in stratified random media , KWAGN JIN LEE, KIHONG KIM, Division of Energy Systems Research, Ajou University, Suwon, 443-749, Korea — We study theoretically the propagation and the Anderson localization of p-polarized electromagnetic waves incident obliquely on randomly stratified dielectric media with weak uncorrelated Gaussian disorder. Using the invariant imbedding method, we calculate the localization length and the disorder-averaged transmittance in a numerically precise manner. We find that the localization length takes an extremely large maximum value at some critical incident angle, which we call the generalized Brewster angle. The disorder-averaged transmittance also takes a maximum very close to one at the same incident angle. Even in the presence of an arbitrarily weak disorder, the generalized Brewster angle is found to be substantially larger than the ordinary Brewster angle in uniform media. It is a rapidly increasing function of the average dielectric permittivity and approaches 90 degrees when the average relative dielectric permittivity is slightly larger than two. We find that the dependence of the generalized Brewster angle on the average dielectric permittivity is universal in the sense that it is independent of the strength of disorder and the wave frequency. We also make a surprising observation that when the p wave is incident from an optically denser region, the localization length and the average transmittance become larger for stronger disorder in a wide range of incident angle.

9:24AM H32.00008 Unidirectional suppresion of Bragg reflection in grated PT-symmetric media , ZIN LIN, Wesleyan University, HAMIDREZA RAMEZANI, TSAMPIKOS KOTTOS, TONI EICHELKRAUT, DEMETRIS CHRISTODOULIDES, University of Central Florida, COMPLEX QUANTUM DYNAMICS AND MESOSCOPIC PHENOMENA GROUP, WESLEYAN UNIVERSITY TEAM, COLLEGE OF OPTICS AND PHOTONICS-CREOL,UNIVERSITY OF CENTRAL FLORIDA TEAM — We study the scattering properties of light through optical fibers with grating that involves gain/loss modulation that respect Parity-Time (PT) symmetry. We derive analytical expressions for transmission and reflection coefficients both in the presence and absence of Kerr non-linearity. At the spontaneous PT-symmetric point we have found that Bragg reflection is suppressed once the light is injected from the left, while it is amplified (with respect to the passive medium) if the fiber is illuminated from the right. Our results are robust for a large interval of the detuning parameter away from the Bragg wavelength.

9:36AM H32.00009 Application of Iterative Time-Reversal for Electromagnetic Wave Focusing in a Wave Chaotic System[1] , BINIYAM TADDESE, THOMAS ANTONSEN, EDWARD OTT, STEVEN ANLAGE, University of Maryland — Time-reversal mirrors exploit the time-reversal invariance of the wave equation to achieve spatial and temporal focusing, and they have been shown to be very effective sensors of perturbations to wave chaotic systems. The sensing technique is based on a classical analogue of the Loschmidt echo [1]. However, dissipation results in an imperfect focusing, hence we created a sensing technique employing exponential amplification to overcome this limitation [1,2]. We now apply the technique of iterative time-reversal, which had been demonstrated in a dissipative acoustic system, to an electromagnetic time-reversal mirror, and experimentally demonstrate improved temporal focusing. We also use a numerical model of a network of transmission lines to demonstrate improved focusing by the iterative technique for various degrees and statistical distributions of loss in the system. The application of the iterative technique to improve the performance and practicality of our sensor is explored.

[1] B. T. Taddese, et al., Appl. Phys. Lett. 95, 114103 (2009).
[2] B. T. Taddese, et al., J. Appl. Phys. 108, (2010) in press; arXiv:1008.2409.

[1]This work is supported by an ONR MURI Grant No. N000140710734, AFOSR Grant No. FA95501010106, and the Maryland CNAM.

9:48AM H32.00010 Optimizing energy transfer efficiency in highly branched nanoplasmonic waveguides , DMITRI VORONINE, ANDREW TRAVERSO, KAI WANG, ZHENHUAN YI, ALEXEI SOKOLOV, Institute for Quantum Science and Engineering, Texas A&M University, College Station TX — Energy transfer in highly branched nanoplasmonic particle waveguides is simulated and optimized by varying the waveguide branching geometry and composition. The periodically branched nanostructures provide a new route towards efficient nanoscale light concentration and local field enhancement. On the one hand, they mimick the analogous randomly branched plasmonic nanostructures which have been previously used for surface-enhanced optical spectroscopy such as SERS. On the other hand, the design is inspired by branched molecular aggregates used for energy funneling. The proposed nanostructures may find applications in sensing, light harvesting and nanophotonics.

10:00AM H32.00011 A Novel Nanoscale Coaxial Optical Microscope by Converging Array of Subwavelength Waveguides , FAN YE, GREGORY MCMAHON, KYLE MARRA, KRZYSZTOF KEMPA, MICHAEL J. NAUGHTON, Boston College — A novel nanoscale coaxial optical microscope (NCOM) is proposed by constructing a converging array of coaxial subwavelength optical waveguides (nanocoax). This new design has potential for deep subdiffraction limit resolution, essentially independent of wavelength of the light source. The coaxial structure also has the capability of modal confinement, which can be utilized to extract phase information in the imaging plane. The transmittance and energy dissipation properties of a single nanocoax are obtained, in the visible light range, by numerical simulation. Optical properties of a converging nanocoax array are also investigated numerically. Finally, progress toward an experimental realization of this novel NCOM is discussed.

10:12AM H32.00012 Trap rainbow in a self-similar coaxial optical waveguide[1] , RU-WEN PENG, QING HU, FENG GAO, RUI-LI ZHANG, MU WANG, National Laboratory of Solid State Microstructures — We report in this work that the light waves with different frequencies can be selectively guided and spatially separated in a self-similar dielectric waveguide, where a hollow core is surrounded by a coaxial Thue-Morse multilayer. Due to the self-similar furcation feature in the photonic band structure, the transmission multibands are achieved. More interestingly, this dielectric waveguide supports cladding modes, which are spatially separated and confined along the waveguide. Consequently, a rainbow can be trapped (spatial confined but not stopped) in the Thue-Morse waveguide. The finding can be applied to designing miniaturized compact photonic devices, such as spectroscopy on a chip. Reference: Qing Hu, Jin-Zhu Zhao, Ru-Wen Peng, Feng Gao, Rui-Li Zhang, and Mu Wang, Appl. Phys. Lett. (2010) 96, 161101.

[1]Supported by NSF and MOST in China.

10:24AM H32.00013 Optical Transmission through Archimedeam Spiral Nanotrenches in Ti Film , FENG WANG, Kent State University, XUEJIN WEN, Ohio State University, KAI SUN, University of Michigan, WU LU, Ohio State University, QIHUO WEI, Kent State University — We study the optical transmission of circularly polarized light through nanoscale Archimedean spiral trenches in Ti film through experiments and numerical simulations; the focus of these studies is on the effect of radial repetition of the spiral nanotrenches. Experimental measurements show that the left and right circularly polarized light exhibit different transmission through the spiral nanotrenches, and the transmission difference decays when the number of the radial periods of the spiral trenches is increased. Numerical simulations reproduce this interesting phenomenon. The underlying physical mechanism of the radial period dependence is attributed to the absorption difference at the center of the spirals.

10:36AM H32.00014 Bio inspired replication and mimicry of optical structure from nature , BEOM-JIN YOON, MATIJA CRNE[1], JUNG OK PARK, MOHAN SRINIVASARAO, CHRISTOPER J. SUMMERS, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA, 30332 — The optical response from some insects and animals is not from dye or pigment but from their complex structure. The so-called structural color involves interference, diffraction, scattering and photonic crystal effect in various combinations. Structures associated with the structural color have been invasively attended because they have been considered as essentials of optical and photonic devices. The diffraction grating was replicated from beetles by the atomic layer deposition (ALD), and the optical response of resulting structures was characterized. We also present our result on mimicry of the structure of Papilio butterfly. To mimic the structure in the butterfly, we created the basic cup-like structure from polymer films having ordered array of holes, and coated it with an alternating multilayer of the materials. The optical properties of the mimicked structures are also investigated.

[1](Current affiliation: Proctor and Gamble, Germany)

10:48AM H32.00015 Carrier recombination lifetime in InGaN/GaN multiquantum well LED , ANTARYAMI MOHANTA, DER-JUN JANG, Department of Physics, National Sun Yat-sen University, Kaohsiung 80424, Taiwan, R.O.C., TAI-FA YOUNG, Department of Mechanical and Electromechanical Engineering, National Sun Yat-sen University, Kaohsiung 80424, Taiwan, R. O. C. — Carrier dynamics in InGaN/GaN multiquantum well LED with 5% In content in InGaN wells is studied by time-resolved photoluminescence (TRPL) using time-correlated single photon counting detection system. The excitation energy is 3.06 eV, frequency-doubled output of a Ti: sapphire laser operating at 808 nm (1.53 eV) with 100 fs pulse width and a repetition rate of 80 MHz. TRPL spectra are fitted biexponentially to obtain decay times. The fast decay process is carrier relaxation and slow decay is the carrier recombination process. The fast relaxation decay time shows insignificant variation with the photon energies and pump fluences. On the other hand carrier recombination time increases with increase of photon energies attaining maximum near photoluminescence peak energy and then decreases again on further increase of photon energies. The carrier recombination life time shows increasing behavior with increase of pump fluences and is obtained as long as $\sim$ 7 ns at pump fluence of 0.21 μJ/cm^2 at room temperature. As the temperature decreases, the carrier recombination life time increases indicating the dominating nature of radiative decay process at low temperatures.

Tuesday, March 22, 2011 8:00AM - 11:00AM –

Session H33 DMP DCOMP: Focus Session: Dielectric, Ferroelectric, and Piezoelectric Oxides: Multiferroics & Magnetoelectrics I C143/149

8:00AM H33.00001 Changing Dielectrics into Multiferroics—Alchemy Enabled by Strain , DARRELL SCHLOM, Cornell University — Ferroelectric ferromagnets are exceedingly rare, fundamentally interesting multiferroic materials. The properties of what few compounds simultaneously exhibit these phenomena pale in comparison to useful ferroelectrics or ferromagnets: their spontaneous polarizations (P_s) or magnetizations (M_s) are smaller by a factor of 1000 or more. The same holds for (magnetic or electric) field-induced multiferroics. Recently, however, Fennie and Rabe proposed a new route to ferroelectric ferromagnets[1]—transforming magnetically ordered insulators that are neither ferroelectric nor ferromagnetic, of which there are many, into ferroelectric ferromagnets using a single control parameter: strain. The system targeted, $EuTiO_3$, was predicted to simultaneously exhibit strong ferromagnetism ($M_s \sim 7\ \mu_B$/Eu) and strong ferroelectricity ($P_s \sim 10\ \mu$C/cm^2) under large biaxial compressive strain. These values are orders of magnitude higher than any known ferroelectric ferromagnet and rival the best materials that are solely ferroelectric or ferromagnetic. Hindered by the absence of an appropriate substrate to provide the desired compression, we show[3] both experimentally and theoretically the emergence of a multiferroic state under biaxial *tension* with the unexpected benefit that even lower misfits are required, thereby enabling higher quality crystalline films. The resulting genesis of a strong ferromagnetic ferroelectric points the way to high temperature manifestations of this spin-phonon coupling mechanism.[2] Our work[3] demonstrates that a single experimental parameter, strain, simultaneously controls multiple order parameters and is a viable alternative tuning parameter to composition for creating multiferroics.

[1]C.J. Fennie and K.M. Rabe, *Phys. Rev. Lett.* **97** (2006) 267602.

[2]J.H. Lee and K.M. Rabe, *Phys. Rev. Lett.* **104** (2010) 207204.

[3]J.H. Lee, L. Fang, E. Vlahos, X. Ke, Y.W. Jung, L. Fitting Kourkoutis, J-W. Kim, P.J. Ryan, T. Heeg, M. Roeckerath, V. Goian, M. Bernhagen, R. Uecker, P.C. Hammel, K.M. Rabe, S. Kamba, J. Schubert, J.W. Freeland, D.A. Muller, C.J. Fennie, P. Schiffer, V. Gopalan, E. Johnston-Halperin, and D.G. Schlom, *Nature* **466** (2010) 954-958.

8:36AM H33.00002 Magnetoelectric coupling in the strain-induced multiferroic $BiMnO_3$, PATRICK MICKEL, HYOUNGJEEN JEEN, AMLAN BISWAS, ARTHUR HEBARD, University of Florida — $BiMnO_3$ is a rare single phase, multiferroic compound which displays both ferromagnetic and ferroelectric properties. We have grown thin films of $BiMnO_3$on $SrTiO_3$ (100) substrates using pulsed laser deposition that display the presence of both order parameters. The ferroelectricity is found to be highly tunable, modulated by both magnetic fields (decreasing by more than 10%) and external strain (increasing by more than 50%). Time dependent ferroelectric measurements in addition to dielectric characterizations reveal $BiMnO_3$ is a relaxor ferroelectric. The polar-nano-regions (PNRs) responsible for relaxor ferroelectricity are shown to reside at the island edges where strain is inherently high. Understanding the PNR properties is shown to be essential for understanding the magnetoelectric and strain couplings.

8:48AM H33.00003 Magnetoelectric coupling in layered perovskites from first principles , TURAN BIROL, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — The rational design of a multiferroic with a large polarization and a strong coupling between the polarization and the magnetization remains a challenge. Recognizing the limitations of bulk materials, we attempt to design a strongly coupled multiferroic by focusing on artificial layered materials. In particular, strained Sr-Ti-O layered perovskites have recently been shown to have ferroelectric lattice instabilities that can be controlled by altering the effective dimensionality of the layered system. We use a combination of density-functional theory and group theoretical methods to investigate the interplay of magnetization with ferroelectricity when a layer of magnetic transition metal ions are introduced into this highly tunable dielectric superlattice.

9:00AM H33.00004 Electrical field control of interface magnetic anisotropy[1] , LEI XU, SHUFENG ZHANG, University of Arizona — The interface magnetic anisotropy of ferromagnetic metals comes from the spin-orbit interaction. By explicitly taking into account the interaction between the symmetry-broken interface potential and the spin-dependent electric dipoles of the Bloch states, we find that the interface spin-orbit coupling can be modeled by the Rashba spin-orbit Hamiltonian (RSOH). Due to the presence of the RSOH, the spin up and down states of the ferromagnet are spin mixed at the interface. Among other consequences, the RSOH induces a perpendicular surface magnetic anisotropy whose magnitude is comparable to the observed values in transition metals. When an external electric field is applied across the interface, the induced screening potential modifies the RSOH and thus the perpendicular anisotropy can be manipulated. Our calculated results are in agreement with the experiments [1].

[1] Endo et al., Appl. Phys. Lett. 96, 212503 (2010); T. Nozaki et al, Appl. Phys. Lett. 96, 022506 (2010).

[1]This work is partially supported by DOE (DE-FG02-06ER46307) and NSF (DMR-0704182).

9:12AM H33.00005 First Principles Studies of Electronic structure and Lattice Dynamics of Multiferroic $GaFeO_3$, AMRITENDU ROY, Indian Institute of Technology, Kanpur, RAJENDRA PRASAD, SUSHIL AULUCK, ASHISH GARG, ndian Institute of Technology, Kanpur — $GaFeO_3$ (GFO) is a room temperature piezoelectric material with antiferromagnetic ordering in the ground state. However, experimental observation reports ferrimagetic behavior below the magnetic transition temperature, attributed to the site disorder of Fe and Ga sites. This transition occurs at temperatures close to room temperature, depending upon the Fe content of the material. Previous structural characterization studies indicate that the room temperature crystal structure ($Pc2_1n$) is retained at least until 4 K. While there are a few experimental studies on this compound, there is no well established understanding of its electronic structure and lattice dynamics which can give insight into the piezoelectric and magnetic properties of the material. From this perspective, we started our calculations with the experimental lattice parameters of stoichiometric GFO assuming no partial occupancies of the constituent ions. The calculations are carried out using local spin density approximation (LSDA+U). Electronic structure and Born effective charges were calculated based on the ground state structure. First principles density functional theory based calculations using small displacement method was adopted to calculate the phonon dispersion relations for the material. On the basis of the dispersion relations modes were assigned.

9:24AM H33.00006 Ferroelectricity-ferromagnetism coexistence and electromagnons in multi-band electron systems , TAKAHIRO MIKAMI, TAKASHI OKA, HIDEO AOKI, Department of Physics, University of Tokyo — While it has been established that noncoliner spin textures can realize multiferroics through magnetoelectric effect, here we look into another senario. Namely, in multi-band systems that comprise odd- and even-parity orbits, homogeneous ferromagnetism and ferroelectricity can coexist as proposed by Batista. In multi-orbital systems Hund's exchange coupling is obviously expected to play an important role, but this has yet to be studied in the above scenario. We have here determined the finite-temperature phase diagram for the quarter-filled two-band Hubbard model in the strong coupling limit. A ferroelectric-ferromagnetic phase appears in multi-band insulator phases, where Hund's coupling, neglected in previous researches, is indeed found to be important for the multiferroic phase. We have further explored low-lying excitation spectrum in the multiferroic phase, since collective excitations should be an interesting experimental probe in the multiferroics. Similar to previous studies for the SU(4) Kugel-Khomskii model, magnon-pseudomagnon bound states appear as electromagnetic excitations due to a cross correlation in the homogeneous multiferroic phase.

9:36AM H33.00007 Electromagnon in $TbMnO_3$ under magnetic field by Raman scattering , PAULINE ROVILLAIN, MAXIMILIEN CAZAYOUS, YANN GALLAIS, ALAIN SACUTO, MARIE-AUDE MEASSON, Laboratoire Materiaux et Phenomenes Quantiques - Paris 7, HIDEAKI SAKATA, Department of physics University of Science Tokyo, LABORATOIRE MATERIAUX ET PHENOMENES QUANTIQUES - PARIS 7 TEAM, DEPARTMENT OF PHYSICS UNIVERSITY OF SCIENCE TOKYO COLLABORATION — Magnetoelectric excitations in the multiferroic $TbMnO_3$ have been investigated by Raman spectroscopy. Our observations reveal electromagnons excitations at 30 cm^{-1} and at 60 cm^{-1} with electric polarization of light parallel to the a axis [1]. When a magnetic field is applied along the c axis, no flop of the spiral plane or polarization is observed but $TbMnO_3$ becomes paraelectric and a simple antiferromagnetic phase is developed. We show that the dipole character of the electromagnons disappears whereas their magnon compound appears immediately when the spins spiral is destabilized with a magnetic field along the c axis. The magnon dispersion curve associated with the electromagnons is preserved before the construction of the magnon dispersion of the simple antiferromagnetic phase at higher magnetic field. The effect of the phase transition on the phonon modes shows that the Mn-O distance is the key that controls the polar character of the electromagnons.

[1] P. Rovillain et al., PRB 81, 054428 (2010)

9:48AM H33.00008 Dielectric and Resistive Response in Multiferroic Superlattices , SANDRA DUSSAN, ASHOK KUMAR, RAM S. KATIYAR, University of Puerto Rico — Building superlattices (SLs) with alternate layers of ultra thin films of ferroelectric and ferromagnetic materials is one of the ways to engineer magnetoelectric multiferroic materials. Alternate thin layers of ferroelectric $PbZr_{0.52}Ti_{0.48}O_3$ (PZT) and ferromagnetic $La_{0.67}Sr_{0.33}MnO_3$ (LSMO) materials were grown on $LaAlO_3$ (001) substrates using Pulsed laser deposition technique. X-ray diffraction patterns displayed the typical satellite peaks confirming SLs formation. The surface topography indicates homogeneous films with average surface roughness of $\sim$ 1.5 nm. Well saturated polarization and high dielectric tunability were observed at room temperature. Piezo-force microscopy (PFM) measurements revealed switching of polarization under the external DC bias field. The zero field cooled (ZFC) and field cooled (FC) magnetic measurements revealed the ferromagnetic behavior of SLs, and it undergoes phase transition at lower temperature compared to the bulk and thin films of pure LSMO. To gain further understanding of the electrical properties of the SLs, impedance spectroscopy, dielectric permittivity and ac conductivity were investigated. We observed dynamic magneto-resistive and magneto-dielectric effects around the LSMO metal-insulator and ferromagnetic phase transition temperature

10:00AM H33.00009 Enhanced resonant magnetoelectric coupling in frequency-tunable composite multiferroic bimorph structures , PETER FINKEL, NUWC, SAM LOFLAND, Rowan Unoversity, ED GARRITY, ACR Scientific Inc, DWIGHT VIEHLAND, Virginia Tech — We report on a giant tunable enhanced resonant magnetoelectric (ME) coupling in multiferroic magnetostrictive/piezoelectric composite based on Fe-Ni/PVDF and Metglas/PZT-fiber bimorph structures. The approach was shown to provide more than a tenfold gain in the ME coefficient, and a magnetic/electric field assisted stress-reconfigurable resonance frequency tuning, up to 100%. The studies were performed by laser Doppler spectroscopy. We also show that this principle of a continuously tuned resonance that might be used to enhance sensitivity and to reject noise for ME magnetic sensors.

10:12AM H33.00010 Interface magnetoelectric effect in ferroelectric/antiperovskite heterostructures , PAVEL LUKASHEV, KIRILL BELASHCHENKO, EVGENY TSYMBAL, University of Nebraska - Lincoln, RENAT F. SABIRIANOV, University of Nebraska at Omaha — We present results of the first principles calculations of the magnetoelectric effect in thin film layered heterostructures of typical ferroelectric (FE), such as PbTiO3, with Mn-based antiperovskite (AP), such as Mn3GaN. Mn-based antiperovskite materials are interesting due to a non-trivial magnetic order and a linear magnetic response to applied strain that makes them piezomagnetic. The symmetry breaking produces a net magnetization at the FE/AP heterostructure interfaces. This magnetization can be controlled by reversing the polarization of the FE layer. Our calculations show that for the positive FE polarization the induced net magnetization is 3.8 μ_B at the PbO/GaMn and 0.6 μ_B at the TiO2/Mn2N interface, while the corresponding values are 1.6 μ_B and 1.2 μ_B for the negative FE polarization and 2.2 μ_B and 0.4 μ_B for the zero FE polarization. Thus, the FE/AP interface magnetization exhibits a strong dependence on the direction of the FE polarization, with difference as large as by a factor of 2. The presented novel approach to electrically control the magnetic properties of thin-film layered ferroelectric/piezomagnetic heterostructures may be interesting for practical applications. Therefore, we hope that our results will stimulate experimental work on the FM/AP thin-film layered heterostructures.

10:24AM H33.00011 Electric field tuning of magnetic domains in permalloy thin films using elastic coupling with ferroelectric PZT bilayers[1] , ANBUSATHAIAH VARATHARAJAN, ARUN LUYKX, LUZ SANCHEZ, University of Maryland, R. POLCAWICH, Army Research Lab, ICHIRO TAKEUCHI, University of Maryland — We are investigating electric field controlled magnetic domain motion in permalloy films deposited on $Pb(Zr_xTi_{(1-x)})$ O_3 (PZT) bilayers. Previously, we have shown that bilayered heterostructures consisting of a tetragonal $PbZr_{0.3}Ti_{0.7}O_3$ film (70 nm) deposited on a rhombohedral $PbZr_{0.7}Ti_{0.3}O_3$ (70 nm) display large ferroelastic domains in the top tetragonal PZT layer (Adv. Mat. 21, 3497, 2009). The reversible non-volatile twin boundary motion in this layer can serve as a basis for inducing controlled strain on magnetic thin films deposited on top. We find that permalloy films (50 nm) sputtered on top of the ferroelastic layer exhibit out-of-plane magnetization whose domains can be imaged by magnetic force microscopy (MFM). Voltage pulses are applied between patterned pads of the permalloy film and the bottom electrode underneath the PZT bilayer. This results in different twin configurations in the tetragonal PZT layer, which in turn leads to changes in magnetic domains in the permalloy film as monitored by MFM.

[1]Work at Maryland was supported by UMD-NSF-MRSEC.

10:36AM H33.00012 Magnetism of Fe nanostructure on ultrathin $BaTiO_3$ film , X. CHEN, University of Nebraska-Lincoln, J. KIM, S. YANG, J.S KIM, G. ROJAS, R. SKOMSKI, M. BODE, A. BHATTACHARYA, T. SANTOS, N. GUISINGER, H. LU, A. GRUVERMAN, C. BINEK, V. SESSI, J. HONOLKA, A. ENDERS — A study of Fe nanostructure on $BaTiO_3$ (BTO) thin films with variable temperature scanning tunneling microscopy (STM) and X-Ray Magnetic Circular Dichroism (XMCD) under ultrahigh vacuum is presented. Fe/BTO is a prototype system for the study of magneto-electric effects but it is experimentally challenging to achieve high quality metal-oxide interfaces. Our approach is to use atomically flat, unreconstructed and stoichiometric BTO films of 13 unit cell thickness on $SrTO_3$, and to deposit Fe impurity atoms and small clusters with molecular beam epitaxy at T = 8 K and compact nanometer clusters by buffer layer assisted growth for comparison. The magnetism of both systems was studied by XMCD at the Fe L3/2 absorption edges. The key observation is that even isolated Fe atoms on the BTO have a sizeable magnetic moment, which quickly increases with increasing coverage. This, together with a detailed analysis of the L 3/2 line shape, is evidence that intermixing and oxidation at the Fe/BTO interface is strongly suppressed. The interface quality achieved can thus potentially be exploited to experimentally observe a magneto-electric interface effect predicted by Tsymbal et al. [Phys. Rev. Lett. 97, 047201 (2006)].

10:48AM H33.00013 Voltage Manipulation of Magnetic Anisotropy in MgO/Ferromagnet/Ag system , JARED WONG, ADRIAN SWARTZ, WEI HAN, ROLAND KAWAKAMI, University of California, Riverside — Recently, the development of new types of memory storage and processing devices has led to great interest in voltage-induced manipulation of magnetic properties in ferromagnetic metals (FM). We investigate the voltage-induced changes in the magnetic properties of a FM in an Indium Tin Oxide (ITO)/Poly(methyl methacrylate) (PMMA)/MgO/FM/Ag system. Samples are fabricated through molecular beam epitaxy (MBE) synthesis and PMMA resist is used as a dielectric layer. ITO is used for the top transparent conductive electrode and magnetic properties are examined through magneto-optic Kerr effect (MOKE) measurements. We report our results and observations of voltage-induced manipulation of the magnetic anisotropy in ITO/PMMA/MgO/FM/Ag system.

Tuesday, March 22, 2011 8:00AM - 11:00AM –

Session H34 DMP: Focus Session: Atomic, Molecular, and Memristive Junctions C141

8:00AM H34.00001 Memory effects in nanoscale systems , MASSIMILIANO DI VENTRA, University of California, San Diego — Memory emerges quite naturally in systems of nanoscale dimensions: the change of state of electrons and ions is not instantaneous if probed at specific time scales, and it generally depends on the past dynamics. This means that the resistive, capacitive and/or inductive properties of these systems generally show interesting time-dependent (memory) features when subject to time-dependent perturbations. In other words, nanoscale systems behave as a combination of (or simply as) memristors, memcapacitors or meminductors, namely circuit elements whose resistance, capacitance and inductance, respectively, depend on the past states through which the system has evolved. After an introduction to the theory and properties of memristors, memcapacitors and meminductors, I will discuss several memory phenomena in nanostructures associated to charge, ion and spin dynamics and their far-reaching applications ranging from information storage to computation to biologically-inspired systems. Work supported in part by NSF, NIH, and DOE.

8:36AM H34.00002 Multiple switching modes and multiple level states in memristive devices , FENG MIAO, J. JOSHUA YANG, JULIEN BORGHETTI, JOHN PAUL STRACHAN, M.-X. ZHANG, ILAN GOLDFARB, GILBERTO MEDEIROS-RIBEIRO, R. STANLEY WILLIAMS, Hewlett-Packard Laboratories, Palo Alto, California — As one of the most promising technologies for next generation non-volatile memory, metal oxide based memristive devices have demonstrated great advantages on scalability, operating speed and power consumption. Here we report the observation of multiple switching modes and multiple level states in different memristive systems. The multiple switching modes can be obtained by limiting the current during electroforming, and related transport behaviors, including ionic and electronic motions, are characterized. Such observation can be rationalized by a model of two effective switching layers adjacent to the bottom and top electrodes. Multiple level states, corresponding to different composition of the conducting channel, will also be discussed in the context of multiple-level storage for high density, non-volatile memory applications.

8:48AM H34.00003 Stochastic memory: getting memory out of noise[1] , ALEXANDER STOTLAND, MASSIMILIANO DI VENTRA, Department of Physics, University of California–San Diego, La Jolla, California 92093-0319 — Memory circuit elements, namely memristors, memcapacitors and meminductors [1], can store information without the need of a power source. These systems are generally defined in terms of deterministic equations of motion for the state variables that are responsible for memory. However, in real systems noise sources can never be eliminated completely. One would then expect noise to be detrimental for memory. Here, we show that under specific conditions on the noise intensity memory can actually be enhanced. We illustrate this phenomenon using a physical model of a memristor in which the addition of white noise into the state variable equation improves the memory and helps the operation of the system. We discuss under which conditions this effect can be realized experimentally, discuss its implications on existing memory systems discussed in the literature, and also analyze the effects of colored noise.

[1] M. Di Ventra, Y.V. Pershin, L.O. Chua, Circuit elements with memory: memristors, memcapacitors and meminductors, Proc. IEEE 97, 1717 (2009).

[1]Work supported in part by NSF.

9:00AM H34.00004 Nano-Ionic in Molecular Nanojunctions[1] , LAM YU, MATTHEW ROBERSON, University of Memphis — Metal filament growth can be induced on the surfaces of electrochemically active metals such as silver and copper by an external electric potential. We study the voltage-driven formation and dissolution of nanoscale silver filaments in silver/molecular-layer/gold junctions. In this system, an applied electric voltage causes oxidation at the silver surface and the resulting silver cations from the reaction are transported away from the silver surface toward the gold surface. The silver cations are reduced at the gold surface and from the accumulation of the transported silver particles, filaments are formed from the gold surface. We found that the energy required for silver nanofilament formation depends critically on the thickness and electrostatic property of the molecular layer, while the energy required for the dissolution of silver nanofilaments is virtually molecule-independent. I will discuss what our results tell us about chemical reactions in the nanoscale, and the practical application of our results in the area of electronic memory and chemical sensors.

[1]This work was supported by a grant provided by the FedEx Institute of Technology

9:12AM H34.00005 Bias dependent shot noise measurement in STM style Au junction at room temperature , RUOYU CHEN, PATRICK WHEELER, AMANDA WHALEY, DOUGLAS NATELSON, Rice University — Shot noise in nanoscale junctions is suppressed strongly near certain conductance values because of nearly fully transmitted modes. Using a gold tip in a STM style motion as the source, combining with high-frequency techniques, we simultaneously measured the conductance and the mean square current noise in nanoscale junctions at a series of voltage biases at room temperature. We have observed peaks in the conductance histogram and related shot noise suppression at different biases near integer multiples of the conductance quantum G0, especially the first three. It demonstrates that quantized electronic transport through quantum channels takes place. We will discuss the relevant noise processes and their evolution with bias across the junctions.

9:24AM H34.00006 Large bandwidth measurements of break junctions for molecular electronics at microwave frequencies , GABRIEL PUEBLA-HELLMANN, ANDREAS WALLRAFF, Quantum Device Lab, ETH Zurich — The controlled breaking of a thin gold wire, by mechanical stress or by electromigration, has not only been successfully employed to produce the nm-spaced electrodes necessary for creating single molecule devices, but has also attracted attention as the means to produce optical field enhancement for surface enhanced Raman scattering on the few to single molecule level. Although frequently employed, such break junctions usually have a low bandwidth when performing electrical transport measurements of single molecule devices. We investigate such junctions and single molecule devices by using microwave reflectrometry, where a break junction is integrated into a superconducting impedance matching circuit. This allows the impedance and thus the state of the junction to be deduced from the measured reflection coefficient with a bandwidth of 10-100 MHz. We electrically characterize such impedance matching circuits at microwave frequencies as well as gold break junctions at DC. We also show measurement results of the combined system, where the break junction is formed either by electromigration or by mechanical means. This setup will be used to study the transport properties of single molecule devices with a bandwidth larger than that of standard low frequency techniques.

9:36AM H34.00007 Shot Noise Measurements in Individual Electromigrated Nanoscale Jsunctions , PATRICK WHEELER, DOUGLAS NATELSON, Department of Physics and Astronomy Rice University — Shot noise provides insight into the correlated motion of electrons in nanostructures. Previous measurements have examined shot noise in mechanically controlled break junctions (MCBJs), looking at a large ensemble of junction configurations. Electromigrated, lithographically created Au structures at liquid nitrogen and helium temperatures allow for the shot noise measurement of individual junction configurations. High frequency excess noise is amplified by a rf amplifier chain and measured in combination with lock-in techniques simultaneously with the dc conductance. Preliminary noise measurements across bias and temperature are compared to previous experiments preformed with MCBJs at room temperature, with an emphasis on the dependence of the noise on bias conditions.

9:48AM H34.00008 Entanglement dynamics within the micro-canonical approach to transport , MASSIMILIANO DI VENTRA, UCSD, CHIH-CHUN CHIEN, MICHAEL ZWOLAK, Los Alamos National Lab — When a central barrier is located between two biased electrodes, the tunneling of electrons may build a quasi steady-state current and the entanglement entropy between the two sides increases. We study these quantities using the micro-canonical picture of transport [1]. The quasi steady-state current from our simulations agree with that obtained from single-particle scattering theory. In addition, we find that the entanglement entropy increases linearly in time and with bias, so long as the barrier is only partially transmitting, which agrees qualitatively with previous results derived under restrictive assumptions. The micro-canonical approach also allows us to investigate this system highly out-of-equilibrium and under a range of conditions. We present further results on barriers with different tunneling probabilities, biases, and time-dependent fields.

[1] M. Di Ventra and T. N. Todorov, J. Phys. Cond. Matt. 16, 8025 (2004).

10:00AM H34.00009 The number of transmission channels through a single-molecule junction , STAFFORD CHARLES, JUSTIN BERGFIELD, JOSHUA BARR, University of Arizona — We calculate transmission eigenvalue distributions for Pt-benzene-Pt and Pt-butadiene-Pt junctions using realistic state-of-the-art many-body techniques. An effective field theory of interacting pi-electrons is used to include screening and van der Waals interactions with the metal electrodes. We find that the number of dominant transmission channels in a molecular junction is equal to the degeneracy of the molecular orbital closest to the metal Fermi level. Thus for Pt-benzene-Pt junctions we predict two dominant transmission channels, and for Pt-butadiene-Pt junctions only one. Pt-buckyball-Pt junctions are predicted to exhibit up to five dominant transmission channels.

10:12AM H34.00010 Vibrational heating in molecular junctions , DANIEL WARD, DAVID CORLEY, JAMES TOUR, DOUGLAS NATELSON, Rice University — Energy injection, distribution and dissipation are of great important in understanding molecular electronics. One method of characterizing the distribution of energy in a system is to measure the effective temperature. Using surface-enhanced Raman spectroscopy (SERS) of molecular nanojunctions, we measure the effective vibrational temperatures of a molecular nanojunction as a function of bias. We observe significant mode-specific vibrational pumping by both optical excitation and DC current, with effective temperature changes exceeding several hundred Kelvin. These measurements provide direct information about heat generation and dissipation in molecular-scale junctions and allow direct comparisons with theories of nanoscale heating.

10:24AM H34.00011 Effective field theory of interacting pi electrons in molecular junctions , JOSHUA BARR, JUSTIN BERGFIELD, CHARLES STAFFORD, University of Arizona — We present an effective field theory that allows the two-body Hamiltonian for a π electron system to be expressed in terms of three effective parameters: the π orbital quadrupole moment, the on-site repulsion, and a dielectric constant. As an application of this theory, we present a model of screening in single-molecule junctions based on the image charge method, and use this technique to calculate the van der Waals interaction between a neutral molecule and a metallic conductor.

10:36AM H34.00012 Temperature dependence of charge transport in conjugated single molecule junctions[1] , EEK HUISMAN, MASHA KAMENETSKA, LATHA VENKATARAMAN, Columbia University — Over the last decade, the break junction technique using a scanning tunneling microscope geometry has proven to be an important tool to understand electron transport through single molecule junctions. Here, we use this technique to probe transport through junctions at temperatures ranging from 5K to 300K. We study three amine-terminated (-NH_2) conjugated molecules: a benzene, a biphenyl and a terphenyl derivative. We find that amine groups bind selectively to undercoordinate gold atoms gold all the way down to 5K, yielding single molecule junctions with well-defined conductances. Furthermore, we find that the conductance of a single molecule junction increases with temperature and we present a mechanism for this temperature dependent transport result.

[1]Funded by a Rubicon Grant from The Netherlands Organisation for Scientific Research (NWO) and the NSEC program of NSF under grant # CHE-0641523.

10:48AM H34.00013 Charge transport in mechanically controlled single-molecule break-junctions , YOUNGSANG KIM, FLORIAN STRIGL, HANS-FRIDTJOF PERNAU, ELKE SCHEER, University of Konstanz, Germany, HYUNWOOK SONG, TAKHEE LEE, Gwangju Institute of Science and Technology, Korea, THOMAS HELLMUTH, FABIAN PAULY, Karlsruhe Institute of Technology, Germany, LINDA A. ZOTTI, JUAN CARLOS CUEVAS, Universidad Autónoma de Madrid, Spain — We present inelastic electron tunneling spectroscopy (IETS) measurements carried out on single molecules incorporated into a mechanically controllable break-junction (MCBJ) at low temperature. The single molecules contacted with a MCBJ or with a STM show various conductance values under stretching depending on the contact geometry and the molecular conformation (*e.g.*, *trans* or *gauche*). In such single-molecule devices, the metal of electrodes (*e.g.*, gold or platinum) and anchoring groups (*e.g.*, thiol (-SH) or amine (-NH_2)) can also significantly influence the charge transport through the single molecules. Here we demonstrate how these individual aspects influence the conductance properties of single-molecule junctions.

Tuesday, March 22, 2011 8:00AM - 11:00AM –
Session H35 DCMP: Topological Insulators: General C140

8:00AM H35.00001 ABSTRACT WITHDRAWN –

8:12AM H35.00002 Topological Insulators as Substrates for CO Oxidation Catalysis by Ultrathin Au Films[1] , HUA CHEN, U of Tennessee-Knoxville, WENGUANG ZHU, U of Tennessee-Knoxville; Oak Ridge National Laboratory, DI XIAO, Oak Ridge National Laboratory, ZHENYU ZHANG, Oak Ridge National Laboratory; U of Tennessee-Knoxville; ICQD/HFNL, USTC — We propose a novel application of three dimensional topological insulators (3DTIs) in heterogeneous catalysis based on first- principles calculations within density functional theory. We use a Bi_2Se_3 substrate as the support of an ultrathin Au film, and show that the Au adatoms are strongly bound to and able to wet the surface of Bi_2Se_3. More importantly, we find the topological surface states of Bi_2Se_3 are robust against Au deposition, and it can enhance the interaction between Au and CO, O_2 molecules by acting as an "electron bath". The present study may broaden the potential technological applications of 3DTIs, and shine some new light on the understanding of the role of surface states in heterogeneous catalysis.

[1]Supported by DMSE/BES of USDOE, USNSF, and NNSFC

8:24AM H35.00003 Topological insulators on the ruby lattice[1] , XIANG HU, MEHDI KARGARIAN, GREGORY FIETE, The University of Texas at Austin — We study a tight-binding model on the two-dimensional ruby lattice. This lattice supports two types of second neighbor spin-dependent hopping parameters in an s-band model that preserves time-reversal symmetry. We discuss the phase diagram of this model for various values of the hopping parameters, and note an interesting interplay between the two spin-orbit terms that individually would drive the system to a Z2 topological insulating phase. The fidelity of each phase is also calculated.

[1]We gratefully acknowledge funding from ARO grant W911NF-09-1-0527

8:36AM H35.00004 Extension of the Kitaev model on the square lattice , RYOTA NAKAI, Department of Physics, The University of Tokyo, AKIRA FURUSAKI, Condensed Matter Theory Laboratory, RIKEN, SHINSEI RYU, Department of Physics, University of California at Berkeley — We study an extension of the Kitaev model [1] on the square lattice, where two types of Gamma matrices on neighboring sites have interaction that respects time reversal symmetry. A family of Kitaev models can be classified as the topological insulator/superconductor when described by Majorana fermions [2]. Our model is in class DIII in Altland-Zirnbauer classification, and thus a Z_2 invariant characterizes two distinct phases. There appear helical Majorana edge modes in the topological phase. The same model on the one-dimensional ladder is also studied.

[1] A. Kitaev, Annals of Physics 321, 2 (2006).
[2] S. Ryu, Phys. Rev. B 79, 075124 (2009).

8:48AM H35.00005 Electrical manipulation and measurement of spin properties of quantum spin Hall edge states , TEEMU OJANEN[1], JUKKA VAYRYNEN, Low Temperature Laboratory, Aalto University, Finland — The existence of the quantum spin Hall state has been confirmed in a series of experiments performed in HgTe quantum wells but a quantitative observation of the helical edge structure is still lacking. We study an electrical manipulation and measurement of helicity properties of the edge states by employing the Rashba spin-orbit interaction (SOI). Specifically, we show that a spatially uniform Rashba SOI, controllable by the gate voltage, can be utilized in tuning the spin orientation of the edge modes (J. I. Väyrynen and T. Ojanen, arXiv:1010.1353). We introduce a point-contact geometry where helicity of the edge modes can be accessed by two- terminal conductance measurements.

[1]Aalto University was previously known as Helsinki University of Technology.

9:00AM H35.00006 Electronic Transport in Exfoliated Bismuth Selenide[1] , ANDREW BESTWICK, JAMES WILLIAMS, PATRICK GALLAGHER, DAVID GOLDHABER-GORDON, JAMES ANALYTIS, IAN FISHER, Stanford University — Recent theoretical and experimental work has identified bismuth selenide as a promising candidate for studies of three-dimensional topological insulators due to its large bulk semiconducting gap crossed by topological Dirac surface states. We report on the fabrication and measurement of mesoscale exfoliated bismuth selenide devices, including the effects of electric-field-effect gating and magnetic field on transport and possible signatures of topological states. We will also discuss fabrication strategies to mitigate surface disorder and doping

[1]The authors acknowledge support from the Keck Foundation.

9:12AM H35.00007 Approaching the insulating state in Ca-doped Bi_2Se_3 nanodevices[1] , PENG WEI, ZHIYONG WANG, JING SHI, Department of Physics and Astronomy, University of California at Riverside — We report a systematic tuning of the carrier density in Ca-doped Bi_2Se_3 nanodevices. A clear transition from the metallic to insulating state is observed as both the Ca-concentration and the gate voltage are tuned. At high temperatures, the devices behave metallic as indicated by the linear temperature dependence of the electrical resistivity as the devices are initially cooled. As the temperature is lowered, the resistivity shows a minimum then increases. This insulating behavior can be modeled by a thermal activated conductivity, which is taken over by saturation at the lowest temperatures. At 1.5 K, the resistivity undergoes a $\sim$5-fold increase as a gate voltage is swept from -60 V to 60 V. The field-effect mobility is found to be about $\sim$ 5000 cm2/Vs. We have also observed a systematic evolution of the magnetoresistance as the chemical potential is tuned via the gate voltage. The combination of the chemical and electronic dopings provides an effective way to access the low carrier density gap states in Bi2Se3 topological insulator nanodevices. This work was supported in part by DOE and NSF.

[1]This work was supported in part by DOE and NSF

9:24AM H35.00008 Topological Response Theory of Doped Topological Insulators , MAISSAM BARKESHLI, Stanford University, XIAOLIANG QI — We generalize the topological response theory of three-dimensional topological insulators (TI) to metallic systems – specifically, doped TI with finite bulk carrier density and a time-reversal symmetry breaking field near the surface. We show that there is an inhomogeneity-induced Berry phase contribution to the surface Hall conductivity that is completely determined by the occupied states and is independent of other details such as band dispersion and impurities. In the limit of zero bulk carrier density, this intrinsic surface Hall conductivity reduces to the half-integer quantized surface Hall conductivity of TI. Our theory is directly related to the TI materials currently under experimental investigation, which have finite residual bulk carrier densities.

9:36AM H35.00009 Topological states in one dimensional solids and photonic crystals , TIMOTHY ATHERTON, HARSH MATHUR, Case Western Reserve University — We show that the band structure of a one-dimensional solid with particle-hole symmetry may be characterized by a topological index that owes its existence to the non-trivial homotopy of the space of non-degenerate real symmetric matrices. Moreover we explicitly demonstrate a theorem linking the topological index to the existence of bound states on the surface of a semi-infinite one dimensional solid. Our analysis is a one-dimensional analogue of the analysis of topological insulators in two and three dimensions by Balents and Moore; our results may be relevant to long molecules that are the one dimensional analogue of topological insulators. We propose the realization of this physics in a one-dimensional photonic crystal. In this case the topology of the bandstructure reveals itself not as a bound surface state but as a Lorentzian feature in the time delay of light that is otherwise perfectly reflected by the photonic crystal.

9:48AM H35.00010 Robustness of topologically protected surface states in layering of Bi_2Te_3 thin films[1] , KYUNGWHA PARK, JEAN HEREMANS, VITO SCAROLA, DJORDJE MINIC, Virginia Tech — Recently, topological insulators with time-reversal symmetry have drawn great attention due to their topologically protected states. Topological insulators differ from band insulators in that a bulk energy gap opens up due to strong spin-orbit coupling and that metallic surface states reside in the energy gap. The surface states of topological insulators are topologically protected in that impurities preserving time-reversal symmetry neither destroy the surface states nor impact the topological nature of the surface states. Recently, bulk bismuth-based alloys were shown to be topological insulators. Thin films offer valuable probes of topological insulators as well as device applications. Additionally, bismuth-based thin films of a thickness of a few nanometers were fabricated on substrates or suspended across trenches. We investigate surface states of Bi_2Te_3(111) thin films of one to six quintuple layers using density-functional theory including spin-orbit coupling. We construct a method to identify topologically protected surface states of thin film topological insulators. Applying this method to Bi_2Te_3 thin films, we examine the topological nature of the surface states as a function of the film thickness and compare our results with experimental data and other theoretical reports.

[1]Supported by NSF DMR and DOE.

10:00AM H35.00011 Spin and Charge Transport on the Surface of a Topological Insulator , ANTON BURKOV, DAVID HAWTHORN, University of Waterloo — We derive diffusion equations, which describe spin-charge coupled transport on the helical metal surface of a three-dimensional topological insulator. The main feature of these equations is a large magnitude of the spin-charge coupling, which leads to interesting and observable effects. In particular, we predict a new magnetoresistance effect, which manifests in a nonohmic correction to a voltage drop between a ferromagnetic spin-polarized electrode and a nonmagnetic electrode, placed on top of the helical metal. This correction is proportional to the cross-product of the spin polarization of the ferromagnetic electrode and the charge current between the two electrodes. We also demonstrate tunability of this effect by applying a gate voltage, which makes it possible to operate the proposed device as a transistor.

10:12AM H35.00012 Spin and Charge Transport in Thin Films of Topological Insulators , ALEXANDER ZYUZIN, ANTON BURKOV, University of Waterloo — We develop a theory of spin-charge coupled transport in thin films of topological insulator materials, when the top and bottom surfaces of the sample hybridize. We find significant differences from the case of transport on unhybridized surfaces. In particular, we find significant reduction of the spin relaxation rates, which enhances all the spin-related transport effects, compared to the case of a single surface. We also find that the out-of-plane component of the spin, which is absent from the hydrodynamic transport equations in the single surface case, reappears when the surfaces are hybridized.

10:24AM H35.00013 Conductance of a helical edge liquid coupled to a magnetic impurity , YOICHI TANAKA, AKIRA FURUSAKI, Condensed Matter Theory Laboratory, RIKEN, K.A. MATVEEV, Argonne National Laboratory — In a quantum spin Hall system, which can be realized in HeTe/(Hg,Cd)Te semiconductor quantum wells [1], helical edge states carry a current and the conductance takes the universal value of $2e^2/h$. This is because an impurity without internal degrees of freedom cannot backscatter an electron at the edge in the presence of time-reversal symmetry [2]. On the other hand, backscattering by a magnetic impurity is allowed. We study the effect of backscattering from a magnetic impurity on the conductance of a quantum spin Hall system [3], and obtain the correction $\delta G(\omega)$ to the electrical conductance as a function of frequency ω. We find that the correction $\delta G(\omega)$ vanishes in the dc limit ($\omega \to 0$), when our model conserves the total spin S_z. Another interesting transport property is the thermal conductance, which is affected by the coupling to the magnetic impurity even at $\omega \to 0$. We find that the temperature dependence of the thermal conductance shows a non-monotonic behavior with a minimum occurring at the Kondo temperature.

[1] M. Konig *et al.*, Science 318, 766 (2007).
[2] C. Wu, B. A. Bernevig and S. C. Zhang, Phys. Rev. Lett. 96, 106401 (2006); C. Xu and J. E. Moore, Phys. Rev. B 73, 045322 (2006).
[3] J. Maciejko *et al.*, Phys. Rev. Lett. 102, 256803 (2009).

10:36AM H35.00014 Design Principles and Coupling Mechanisms in the 2D Quantum-Well Topological Insulator HgTe/CdTe[1] , JUN-WEI LUO, ALEX ZUNGER, National Renewable Energy Lab, SOLID STATE THEORY TEAM — We present atomistic band structure calculations revealing a different mechanism than recently surmised via $\mathbf{k} \cdot \mathbf{p}$ calculations about the evolution of the topological state (TS) in HgTe/CdTe. We show that *2D interface* (not *1D edge*) TS are possible. We find that the transitions from a topological insulator at critical HgTe thickness of $n = 23$ ML (62.5 Å) to a normal insulator at smaller n is due to the crossing between two interface localized states: one derived from the S-like Γ_{6c} and one derived from the P-like Γ_{8v} light-hole, not because of the crossing of an interface state and an extended QW state. These atomistic calculations suggest that a 2D TS can exist in a 2D system, even without truncating its symmetry to 1D, thus explaining the otherwise surprising similarity between the 2D dispersion curves of the TS in HgTe/CdTe with those of the TS in 3D bulk materials such as Bi_2Se_3. Ref: J.W. Luo and A. Zunger, Phys. Rev. Lett. **105**, 176805 (2010).

[1]Funded by DOE-SC-BES-MSED under Contract No. DE-AC36-08GO28308 to NREL.

10:48AM H35.00015 Towards Quantum Spin Hall Effect in InAs/GaSb Quantum Wells , IVAN KNEZ, RUI-RUI DU, Rice University, GERRARD SULLIVAN, Teledyne Scientific Co. — Recently, it has been proposed that inverted InAs/GaSb composite quantum wells (CQWs) should exhibit the Quantum Spin Hall Effect (QSHE), characterized by the energy gap in the bulk and gapless edge modes which are protected from backscattering by time reversal symmetry. We have successfully fabricated a double-gated device on high-quality MBE-grown InAs/GaAs CQWs in the inverted regime, in which we were able to vary the band structure via an electrical field, and tune the Fermi level into mini-gap regime. We observed clear evidence for an energy gap in the inverted regime, with values of the gap consistent with those theoretically predicted; however, the mini-gap exhibits residual conductivity of non-trivial origin, which complicates transport investigation of proposed edge channels. We note that the InAs surface states around the sample edges may play a role in the observed resistivity features. In ongoing work, we pursue Cooper pair injection experiments by proximity to an s-wave superconductor, which should provide a novel probe of the proposed helical edge modes. We will discuss our progress towards observing QSHE in this unique material system. The work at Rice was supported by grants from NSF, Keck Foundation, and Hackerman Advanced Research Program.

Tuesday, March 22, 2011 8:00AM - 11:00AM –
Session H36 GERA: Photovoltaics: Compound Semiconductors and Organics C142

8:00AM H36.00001 Effects of doping on the band gap of iron pyrite[1] , JUN HU, YANNING ZHANG, MATT LAW, RUQIAN WU, University of California, Irvine — Iron pyrite (FeS_2), a highly abundant materials in Earth's upper continental crust, is of great interests in photovoltaic and photo-electrochemical applications, due to its wide band gap of 0.9 - 0.95 eV and large absorption coefficient of $\alpha > 10^5$ cm-1 for $\lambda < 10^3$ nm. However, its electron/hole mobility is typically very low, caused by the presence of sulfur deficiency in crystalline FeS_2 bulks or nanostructures. In principle, doping electrons or holes by exotic elements may not only compensate sulfur deficiency but also create mobile carriers. In this work, we systematically studied the dopabilities of N, P, F and Cl in bulk FeS_2, by using the first-principles calculations. First of all, we found that these elements substitute S under sulfur poor condition in the FeS_2 bulk and nanostructures. While N, P and F dopants merely induce deep localized defect levels, doping 1.6% Cl not only generates a 0.996 μ_B local magnetic moment per Cl and but also increases the carrier density by $3x10^{18}/cm^{-3}$. The defect states are delocalized and hence doping of Cl also improve the carrier mobility in FeS_2. We found that incorporation of Cl also leads to significant structural distortions around Cl atom.

[1]We thank the NSF SOLAR Program (Award CHE-1035218).

8:12AM H36.00002 The reason FeS_2 is not a good PV absorber[1] , LIPING YU, S. LANY, A. ZUNGER, NREL, H.A.S. PLATT, R. KYKYNESHI, B. PELATT, R. RAVICHANDARIN, D.A. KESZLER, J.F. WAGER, Oregon State University — FeS_2 is representative of an ideal earth-abundant candidate absorber for thin film PV, because of its appropriate band gap, high absorption coefficient and good electron/hole mobility. Yet, despite ∼15 years of research, the promise of FeS_2 as an absorber layer has been unrealized, manifesting as a low open circuit voltage which has been attributed to E_f pinning arising from bulk sulfur vacancies. Our first-principles calculations and experimental thermogravimetirc analyses, however, show that S vacancies and other point defects have rather high formation energies. Hence, they are unlikely to form and pin E_f. We find that the widely observed S deficiency in FeS_2 is accommodated by phase-coexistence of a few $Fe_{1-x}S$ compounds, rather than S vacancies. These minority phases are metallic and detrimental for PV. We find select ternary Fe sulfides do not have thermodynamically-mandated phase-coexistence like FeS_2, yet they retain optimal band gaps and high absorption strengths comparable to FeS_2. These properties and associated surface-defect calculations will be discussed.

[1]Funded by DOE through EFRC Center for Inverse Design.

8:24AM H36.00003 Direct measurement of the built-in potential in a nanoscale heterostructure

, ANNA ZANIEWSKI, MATTHIAS LOSTER, Department of Physics, University of California at Berkeley, Berkeley, CA 94720 U.S.A, BRYCE SADTLER[1], A. PAUL ALIVISATOS, Department of Chemistry, University of California at Berkeley, Berkeley, CA 94720 U.S.A, A. ZETTL, Department of Physics, University of California at Berkeley, Berkeley, CA 94720 U.S.A — Recently synthesized heterostructured nanorods are a promising material for applications such as photovoltaics. Understanding the electronic structure of these materials is both an interesting scientific question and vitally important for applications. We present the measurement of the built-in potential across individual Cu2S-CdS heterostructured nanorods by combining transmission electron microscopy with electrostatic force microscopy. This represents the first experimental determination of the electrostatic potential across an isolated nanostructure. We observe a variation of built-in potentials, ranging from 100 to 920 mV, with an average of 250 mV. Nanorods of a uniform composition with no heterojunction do not show built-in potential, as expected.

[1]Present address: Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125 U.S.A.

8:36AM H36.00004 First Principles Calculation of Optical Properties of Ternary Semiconductors Cu_3PSe_4 and Cu_3PS_4

, DAVID FOSTER, GUENTER SCHNEIDER, Oregon State University — The ternary semiconducting compounds Cu_3PSe_4 and Cu_3PS_4 are of interest as potential optoelectronic materials. Of particular interest for solar photovoltaic devices is Cu_3PSe_4, as its band gap lies in the desired 1.0 to 1.6 eV range for an absorber. We have theoretically calculated the optical properties of these materials using density functional theory with GGA and hybrid exchange-correlation functionals, as well as with the GW_0 approximation from many-particle theory. We find that Cu_3PSe_4 has a direct band gap with relatively strong optical absorption above 2 eV, indicating that this compound is a candidate photovoltaic absorber. Cu_3PS_4 has a larger band gap of approximately 2.4 eV, placing it outside consideration as a solar absorber.

8:48AM H36.00005 Crystalline ordered states and local surface potential variations of photovoltaic $Cu(In,Ga)Se_2$ thin-films[1]

, A.R. JEONG, R.H. SHIN, WILLIAM JO, Ewha Womans University — Structural and electrical properties of $CuInSe_2$(CIS), $Cu(In,Ga)Se_2$ (CIGS) and $CuGaSe_2$ (CGS) grown by co-evaporation were studied. Intriguing morphology and grain growth behaviors were found in the surface of the films. X-ray diffraction of the films exhibited phase formation of the stoichiometric chalcopyrite while Cu_2Se and $CuSe_2$ were observed. Using Raman scattering spectroscopy, shift of A_1 mode was observed from 177 cm^{-1} for CIS to 189 cm^{-1} for CGS as Ga content increased. It is very interesting that two different crystalline ordered states with chalcopyrite (CH) and CuAu structure (CA) were found. Effects of the grain boundaries on local electrical properties of the films with different chemical contents were examined. Local current mapping and surface potential distribution were obtained in the film by conductive atomic force microscopy and Kelvin probe microscopy. Minority carrier transport behaviors and local variations of potential values on and near the grain boundaries were characterized. These results suggested that a local built-in potential is possibly formed on positively charged grain boundaries.

[1]Support from the General R/D Program of DGIST, funded by MEST of the Republic of Korea.

9:00AM H36.00006 Minority-Carrier Lifetimes in GaInP

, LINDA FRITZ, NREL and Franklin & Marshall College, JERRY OLSON, National Renewable Energy Laboroatory, DARIUS KUCIAUSKAS, National Renewable Energy Laboratory — Minority-carrier lifetimes are very important to the performance of photovoltaic materials and are quite sensitive to the structure of the material. The impact of lifetimes can be readily illustrated using computer modeling of cell performance, and a brief discussion of the results of our modeling will be given. AlInP/GaInP double heterojunctions of varying thickness and doping concentration were grown on GaAs substrates by metallorganic chemical vapor deposition (MOCVD). Lifetimes were measured using time-resolved photo-luminescence. Carrier concentrations were determined using capacitance-voltage measurements. Here we report on the minority carrier lifetime as a function of active layer thickness and doping concentration for n-type and p-type GaInP that is lattice-matched to the substrate.

9:12AM H36.00007 Photvoltaic effects in ferroelectrics due to nonlinear optical processes

, STEVE YOUNG, ANDREW RAPPE, Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania — The physical mechanism for the bulk photovoltaic effect that appears in noncentrosymmetric materials, especially in ferroelectric devices, is not well understood. A promising candidate for a truly bulk photovoltaic effect is non-linear optical processes – most notably "shift current," which describes the net motion of coherently excited electrons in the absence of inversion symmetry, and has been described analytically several times in the literature. Shift current is also of interest due to the appearance of a gauge invariant phase describing the carrier mobility. We have developed an expression for shift current suitable for efficient computation and analysis utilizing wavefunctions of arbitrary origin, and calculated the response for several prominent ferroelectrics – including $LiNbO_3$, $BaTiO_3$, and $PbTiO_3$ – using KS eigenstates. The calculated short-circuit currents appear to be in rough agreement with available experimental results where they exist. Furthermore, they indicate a more subtle relationship between polarization and band gap than has heretofore been presumed, with strong implications for the materials design process, as well as shift current's overall viability as a mechanism for efficiently harvesting solar energy.

9:24AM H36.00008 Nanostructured multiferroic materials for optoelectronics and energy-related nanodevices

, RIAD NECHACHE, NAST Center & Department of Chemical Science and Technology, U. of Rome Tor Vergata, ENRICO TRAVERSA, International Research Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), SILVIA LICOCCIA, NAST Center & Department of Chemical Science and Technology, U. of Rome Tor Vergata, FEDERICO ROSEI, Centre Énergie, Matériaux et Télécommunications, INRS — Combining properties into multifunctional materials is one of innovative ways explored by the modern technology to achieve high miniaturization of integrated devices. In this context, besides their exciting physics, multiferroic materials hich combine two or more ferroic order offer opportunities for potential applications in emerging fields of spintronics, optoelectronics and data storage. For such applications, successful integration of these multifunctional materials needs to develop adequate fabrication processes and to the coexistence in singe phase of robust properties at room temperature (RT). Furthermore, a synergistic interaction between magnetic and electric orders leads to additional freedom for designing related devices. Here we review recent progress of our group in growth and nanopatterning of multiferroic thin films developed to overcome those drawbacks. We will present the fabrication of RT-multiferroic Bi_2FeCrO_6thin films. Successful nanopatterning of these complex oxides by a versatile and generic approach and their photovoltaic properties will be also discussed.

9:36AM H36.00009 Energy Transfer in Organic Photovoltaic Cells and its Impact on Measurements of the Exciton Diffusion Length

, RUSSELL HOLMES, University of Minnesota — In order to generate photocurrent from an organic photovoltaic cell (OPV), the optically generated exciton must be dissociated into its constituent charge carriers. This process is carried out at the interface between electron donating and accepting materials. Consequently, photocurrent is generated only at the donor-acceptor (D-A) interface, and exciton diffusion to the interface is a critical step in the photoconversion process. The focus of this work is on the development of methods that permit the accurate measurement of the exciton diffusion length, and realizing architectures that demonstrate enhanced exciton harvesting. In measuring the exciton diffusion length, emphasis is placed on quantifying the role of excitonic energy transfer in the dissociation process by explicitly measuring the Förster radius between donor and acceptor materials. Many of the techniques currently used to estimate the exciton diffusion length incorrectly ignore these effects, potentially leading to overestimates. Efforts to overcome the short diffusion length are focused on small molecule OPVs that contain a continuously graded D-A film composition as a means to simultaneously optimize both exciton diffusion and charge collection. In a properly optimized graded heterojunction OPV, power conversion efficiencies >4% can be realized, exceeding the performance of conventional planar and uniformly mixed structures.

9:48AM H36.00010 Effect of Thin Polymer Layers on the Performance of ZnO/Cu_2O Solar Cells[1]

TALIA GERSHON, KEVIN MUSSELMAN, ANDREW MARIN, JUDITH MACMANUS-DRISCOLL, University of Cambridge — Transition metal oxides are a class of stable, non-toxic, and inexpensive semiconductors with great potential in low-cost photovoltaics (PV) applications. Cu_2O is a versatile p-type oxide that absorbs visible light and can be solution-processed at low temperatures. ZnO is a wide-E_g n-type material with good electronic properties and has already been widely incorporated into other low-cost PV technologies such as organic and dye-sensitized solar cells. While ZnO/Cu_2O devices have large theoretical efficiencies (as high as 20%) [1], practical devices do not reach their full potential due to poor charge collection and recombination. ZnO/Cu_2O PV's can be improved by optimizing deposition conditions, such as solution pH and temperature, and device geometry, such as layer thickness [2]. This talk, however, will discuss how semiconducting polymer layers can further enhance performance for scalable device fabrication. In particular, polymer type and the Cu_2O/polymer interface will be discussed as routes to better performance.

[1] J. Nelson. *The Physics of Solar Cells*. Imperial College Press, 2003
[2] Musselman et al., unpublished

[1]This work was funded in part by the International Copper Association

10:00AM H36.00011 Nanoscale Morphology and Charge Transport in Hybrid Solar Cells by Conducting Probe Atomic Force Microscopy

, JIEBING SUN, SEAN R. WAGNER, DANIEL ENDERICH, PHILLIP DUXBURY, PENGPENG ZHANG, Physics and Astronomy Department and Center of Research Excellence in Complex Materials, Michigan State University — Measurements of the dependence of photoactive response on nanoscale morphology provide essential insights to further improve processing and achieve morphologies with enhanced device performance. To study the correlation between local morphology and photoactive response, we have fabricated hybrid polymer/zinc oxide thin films and have characterized their electrical properties at nanoscale resolution with conducting probe atomic force microscopy (c-AFM). The charge carrier mobilities were extracted based on local IV characteristics. The surface morphology and current mapping were recorded simultaneously under various illumination and biasing conditions, enabling direct study of morphology dependent transport processes in these photoactive devices.

10:12AM H36.00012 Development of Phase Stable Organic Photon Upconverters[1]

, YOICHI MURAKAMI, Tokyo Institute of Technology — Recently, high efficiency photon upconversions (UCs) utilizing triplet-triplet annihilation (TTA) in aromatic hydrocarbon molecules, applicable to sunlight intensity, have been actively studied for the purpose of improving external quantum efficiencies of photovoltaics. These studies have been using volatile organic solvents as media in order for TTA to occur, which are currently hindering its applications. I have discovered that those aromatic molecules can be stably dispersed by a simple method within certain class of ionic liquids (ILs), which are non-volatile and thermally stable up to several hundred degree C, to form unprecedented organic photon upconverters with improved phase stability [1,2]. The proposed mechanism for the molecular stabilization in ILs as well as the UC quantum efficiencies is presented.

[1] Y. Murakami and I. Sato, Patent 2010-230938JP (pending)
[2] Y. Murakami et al., submitted.

[1]The author thanks Prof. I. Sato for his valuable advice. This work was supported by the MEXT program "Promotion of Environmental Improvement for Independence of Young Researchers".

10:24AM H36.00013 Charge transport and absorption study of metal nanoparticle plasmonics for organic photovoltaics[1]

, MEI XUE, JINFENG ZHU, HUAJUN SHEN, SEONGKU KIM, JACK J. HO, UCLA, HUSSAM ALDEEN S. QASEM, ZAID S. AL OTAIBI, KANG L. WANG, DEVICE RESEARCH LABORATORY, UCLA TEAM, KACST/CALIFORNIA INSTITUTE OF EXCELLENCE ON GREEN NANOTECHNOLOGY TEAM — A hybrid plasmonic nanostructure of an optically sensitive heterojunction organic film incorporating metal nanoparticles is fabricated. From the Charge Extraction in Linearly Increasing Voltage (CELIV) measurements, the mobility of this hybrid plasmonic nanostructure has been experimentally extracted to be at least one order of the magnitude higher than that of the organic film without metal nanoparticles. The measured absorption spectrum also shows the increasing of the intensity by around 28% as well as the broadening of the spectrum. The theoretical calculation confirms this broadband optical absorption enhancement results from localized surface plasmon resonance. The optimization of the density of the metal nanoparticles has been done to achieve the best performance for the photovoltaic devices.

[1]This work is supported in part by KACST/California Institute of Excellence on Green Nanotechnology.

10:36AM H36.00014 The Effect of a Self Assembled Monolayer in Small Molecule Organic Solar Cells

, ALEXANDER COOK, KAMIL MIELCZAREK, ANVAR ZAKHIDOV, The University of Texas at Dallas Physics Department — We have previously found that a Self Assembled Monolayer (SAM) of Flouroalkyl TrichloroSilane (FTS) molecules on Single-Walled and Multi-Walled Carbon Nanotubes (SWCNT & MWCNT) can greatly improve the conductivity [1]. In present work we have studied the effect of SAM modified carbon nanotubes in Small molecule organic photovoltaic cells. (OPV) We have fabricated and characterized OPV of the general structure: CNT(FTS)/CuPC/C60/BCP/Al. We observed improvement of the performance of the OPV with CNT anodes with FTS SAM both for SW and MW CNT. The major effect is an improvement of the open circuit voltage and also small improvements in both short circuit current and filling factor. The increase in open circuit voltage is likely due to modifications of the carbon nanotube work function by the strong dipole moments of the FTS molecules. The improvements in short circuit current and filling factor is probably due to improved active layer morphology and removal of absorbed water from the substrate.

[1] Cook, Alexander; Lee, Bumsu; Kuznetsov, Alexander; Podzorov, Vitaly; Zakhidov, Anvar. Self Assembled Dipole Monolayers on CNTs: Effect on Transport and Charge Collectio. Oral Presentation APS March Meeting 2010

10:48AM H36.00015 Inverted Polymeric Photovoltaic Cells and Parallel Tandems with Transparent Single Wall Carbon Nanotubes Interlayer[1]

, KAMIL MIELCZAREK, ALEX COOK, ANVAR ZAKHIDOV, University of Texas at Dallas, ANTTI KASKELA, ALBERT NASIBULIN, ESKO KAUPPINEN, Aalto University, Finland — We demonstrate an organic photovoltaic (OPV) monolithic multi junction cell in a parallel electrical configuration utilizing polymers with complementary absorption spectra and transparent single wall CNT (SWCNT) as an interlayer electrode (IE). Parallel tandem cells are of importance because they can append to the limited spectral coverage of available polymers and because there is no need balance current as is the case with in-series configurations. Devices comprise of polymeric sub cells where one is inverted using ZnO nanoparticles and a MoO_3 buffer layers, this inverted structure allows for the SWCNT IE to function as a cathode. Each sub cell is characterized independently and the short circuit current of the tandem device is shown to increase. Overall increase in efficiency is observed and attributed to enhanced spectral coverage by spectrally complimentary polymers and the effective use of parallel tandem architecture. We also demonstrate a semi transparent inverted OPV structure with a SWCNT electrode and a efficiency of over 3%.

[1]Supported by AFRL/Rice and Welch AT 16-17 grants.

Tuesday, March 22, 2011 8:00AM - 11:00AM –

Session H37 DMP: Focus Session: Graphene Structure, Dopants, and Defects: Transport I

C146

8:00AM H37.00001 Probing the nature of impurity scattering in graphene , HELENE BOUCHIAT, LPS CNRS Univ. Paris Sud — Since the very first investigations of the electronic properties of graphene the nature of defects has been shown to play an essential role in determining the carrier density dependence of the conductance. Impurity scattering is characterized by two different times the transport and elastic scattering times which are sensitive to the mass less energy dispersion of graphene. The analysis of the ratio between these two times gives insight on the nature (neutral or charged) and range of the scatterers. We will discuss how to extract these two times from magneto-transport measurements in macroscopic samples and analyze their differences in monolayer and bilayer Graphene in relation with the different symmetry properties of their band structure and wave functions.

"Transport and Elastic Scattering Times as Probes of the Nature of Impurity Scattering in Single-Layer and Bilayer Graphene" M. Monteverde, C. Ojeda-Aristizabal, R. Weil, K. Bennaceur, M. Ferrier, S. Guéron, C. Glattli, H. Bouchiat, J. N. Fuchs, and D. L. Maslov Phys. Rev. Lett. **104**, 126801 (2010).

8:36AM H37.00002 ABSTRACT WITHDRAWN –

8:48AM H37.00003 Transport and optical measurements on Graphene - hBN heterostructures , LEI WANG, CORY DEAN, ANDREA YOUNG, ZHEYUAN CHEN, INANC MERIC, KEN SHEPARD, LOUIS BRUS, PHILIP KIM, JAMES HONE — Placing graphene on hexagonal BN (hBN) substrates has recently been shown to lead to improved device quality. In addition, the planar nature of the h-BN allows for the realization of novel device architectures with high mobility graphene, including dual-gated devices. I will discuss recent transport and optical measurements on such graphene-hBN heterostructures, focusing on high mobility dual gated bilayer graphene, in which the carrier density and the band-gap can be tuned independently.

9:00AM H37.00004 Fabrication and transport characterization of Graphene/Hexagonal Boron Nitride sandwich structures , JIAN-HAO CHEN, KWANPYO KIM, WILL REGAN, WILLIAM GANNETT, KRIS ERICKSON, MICHAEL ROUSSEAS, ALEX ZETTL, Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — High quality, large size hexagonal Boron Nitride (h-BN) thin films and single layer graphene were grown on metal substrates via the chemical vapor deposition method (CVD) and transferred to form Graphene/h-BN sandwich structures. High resolution transmission microscopy (TEM) was performed on Graphene and h-BN, confirming highly-ordered crystalline structures of both. The electronic transport properties of various sandwich configurations were investigated at low temperature and high magnetic field.

9:12AM H37.00005 Tunable band gaps in bilayer graphene-BN heterostructures , ASHWIN RAMASUBRAMANIAM, University of Massachusetts Amherst, DORON NAVEH, ELIAS TOWE, Carnegie-Mellon University — We investigate band-gap tuning of bilayer graphene between hexagonal boron nitride sheets, by external electric fields. Using density functional theory, we show that the gap is continuously tunable from 0 to 0.2 eV, and is robust to stacking disorder. Moreover, boron nitride sheets do not alter the fundamental response from that of free-standing bilayer graphene, apart from additional screening. Our calculations suggest that graphene-boron nitride heterostructures could provide a viable route to graphene-based electronic devices.

9:24AM H37.00006 Dielectric thickness dependence of carrier mobility in graphene with Al_2O_3 and HfO_2 top dielectrics , BABAK FALLAHAZAD, SEYOUNG KIM, University of Texas at Austin, LUIGI COLOMBO, Texas Instrument, EMANUEL TUTUC, University of Texas at Austin — We study the carrier mobility in graphene with high-k top dielectrics, as a function of the dielectric thickness and temperature. Metal-oxide high-k films, Al_2O_3 (k ~8.4) and HfO_2 (k ~16), are deposited on graphene by atomic layer deposition (ALD), at deposition temperatures of 200-250 $^\circ$C. A considerable (~50%) mobility drop is observed after the deposition of the first 2-4 nm of dielectric. For thicker dielectrics the mobility is relatively insensitive to thickness. The carrier mobility has a weak temperature dependence, which indicates that phonon scattering is not the primary mobility limiting factor in these devices. Our results suggest that Coulomb scattering caused by fixed charged impurities located in the high-k dielectric, and in proximity to the graphene layer plays a significant role in mobility degredation. The ALD grown high-k films are inherently oxygen deficient, and oxygen vacancies form donor levels which become positively charged in the proximity of the graphene layer. We speculate that Coulomb scattering due to charged point defects is the mobility limiting mechanism in graphene devices with Al_2O_3 or HfO_2 high-k dielectrics.

9:36AM H37.00007 Coulomb Drag in Independently Contacted Graphene Bilayers[1] , SEYOUNG KIM, INSUN JO, JUNGHYO NAH, YAO ZHEN, SANJAY BANERJEE, EMANUEL TUTUC, The University of Texas at Austin — Two graphene layers placed in close proximity, and electrically isolated, offer a unique system to investigate interacting electron physics. In such graphene bilayer, the interlayer spacing can be reduced to values much smaller than otherwise achievable in semiconductor heterostructures. Moreover, the zero energy band-gap allows the realization of coupled hole-hole, electron-hole, and electron-electron two-dimensional systems in the same sample. Here we demonstrate the realization of independently contacted graphene bilayers. We probe the resistance and density of each layer, and quantitatively explain their dependence on the back-gate bias. We experimentally measure the Coulomb drag between the two graphene layers, by flowing current in one layer and measuring the voltage drop in the opposite layer. The drag resistivity gauges the momentum transfer between the two layers, which in turn probes the interlayer coupling. The temperature dependence of the Coulomb drag above temperatures of 77K reveals that the ground state in each layer is a Fermi liquid. Below 77K we observe mesoscopic fluctuations of the drag resistivity, as a result of the interplay between coherent transport in the graphene layer and interlayer interaction.

[1]We thank NRI and NSF for support.

9:48AM H37.00008 Probing charge scattering mechanisms in suspended and supported graphene by varying dielectric environment , A.K.M. NEWAZ, KIRILL I. BOLOTIN, Vanderbilt University — The electronic properties of graphene are drastically affected by its environment, such as the substrate underneath it and the impurities near it. To elucidate the effect of scattering due to the environment, we used the Hall probe technique to study the electronic transport properties and the quantum capacitance of single layer graphene devices in environments with different dielectric susceptibility κ. We have varied the susceptibility by i) using solvents of different dielectric constants, ii) mixing two miscible solvents of different dielectric strengths and iii) varying the temperature of the solvent. To eliminate the effects due to a substrate, we have also studied suspended graphene devices. We have observed enhancement in the Hall mobility and reduction in the minimal conductivity in both supported and suspended devices as the static dielectric constant is increased from $\kappa \sim 2$ to $\kappa \sim 30$. This suggests stronger screening of charge scattering in higher κ dielectric environment. Our results support the conjecture that the dominant scattering mechanism in graphene is the long range Coulomb interaction due to the charge impurities.

10:00AM H37.00009 Charge transport studies in graphene devices: a focus on mobility behavior[1] , ARCHANA VENUGOPAL, WILEY KIRK, LUIGI COLOMBO, ERIC VOGEL, University of Texas at Dallas — Graphene has been the subject of extensive electrical characterization since 2004. As in semiconductor based FETs, mobility (μ) is used as the parameter to gauge and compare the device performance. Typically reported is the effective mobility, μ_{eff}, extracted from $I_d - V_g$ characteristics or the channel mobility (μ_H) extracted from Hall measurements, which can be especially illuminating when more than one carrier type is participating in the charge transport process. The dependence of the mobility on parameters such as applied field, dielectric type, underlying oxide thickness, channel dimensions and temperature is not well understood. A study of μ_H and the accompanying magnetoresistance as a function of the above mentioned parameters in low to moderate magnetic fields was performed, as well as μ_{eff} on the same devices, the results of which will be compared and presented. The dependence on graphene type (grown vs. exfoliated) will also be discussed.

[1]SRC-NRI Southwest Academy for Nanoelectronics

10:12AM H37.00010 Graphene nanoelectronics from ab initio theory[1] , JESSE MAASSEN, McGill University, WEI JI, HONG GUO — We employ atomic first principles theory to study the properties of realistic graphene nanoelectronic systems. We focus on the role of different contact materials and their effect on the transport properties at the graphene/metal junction. The current-voltage characteristics were calculated using density functional theory (DFT) combined with non-equilibrium Green's functions (NEGF).

[1]NSERC, FQRNT and CIFAR

10:24AM H37.00011 Charge transport in two-terminal graphene junctions with bonding metal contacts , BARRAZA-LOPEZ SALVADOR, M. Y. CHOU, School of Physics. Georgia Institute of Technology — One has to attach graphene to metal leads to measure charge transport characteristics. In a number of experiments a thin Ti film is grown on top of graphene and additional metal leads (e.g., Au or Al) are created on top of this film. Ti forms covalent bonds with graphene, destroying the linear dispersion at the Ti/graphene contact. For practical reasons (i.e., the use of Hamiltonians with a linear dispersion) most theoretical approaches either consider only the effects of the inhomogeneities caused by the insulating substrate, or, when two-terminal calculations exist, use assumptions that preclude quantitative modeling. These assumptions include: (i) extremely large bias steps separating the leads and the central region of the device, or (ii) unusually large imaginary contributions to the self-energies representing metal leads. We depart from these models and follow an atomistic approach to compute transmission characteristics of Ti/graphene/Ti junctions. From these calculations we identify the key physical ingredients determining the transport features, and extract parameters to be used in a quantitative effective model that describes accurately the electronic structure and the transmission probabilities of charge carriers. This work complements our previous results in metal/graphene/metal junctions where the metal does not bond covalently to graphene (PRL **104**, 076807 (2010)).

10:36AM H37.00012 Transport in Metal/Graphene Tunnel Junctions , CHRIS MALEC, DRAGOMIR DAVIDOVIC, Georgia Tech — We present a technique to fabricate thin oxide barriers between graphene and Al and Cu to create tunnel junctions and directly probe graphene in close proximity to a metal. We map the differential conductance of our junctions versus probe and back gate voltage, and observe fluctuations in the conductance that are directly related to the graphene density of states. We develop a simple theory of tunneling into graphene to extract experimental numbers, and take into account the electrostatic gating of graphene by the tunneling probe. Results of measurements in magnetic fields will also be discussed, including evidence for incompressible states in the Quantum Hall regime.

10:48AM H37.00013 Quantum transport in high-quality Bilayer Graphene pnp Junctions , YONGJIN LEE, LEI JING, JAIRO VELASCO JR., PHILIP KRATZ, GANG LIU, WENZHONG BAO, MARC BOCKRATH, CHUN NING LAU, Department of Physics, University of California, Riverside, California 92521 — Using high-quality bilayer grapheme pnp junctions with suspended top gates, we perform transport measurements. At a magnetic field B=0, by an applied perpendicular electric field, band gap opens at 260mK. Within the band gap, we demonstrate the conductance decreases exponentially by 3 orders of magnitude with increasing electric field and this can be explained by variable range hopping with a gate-tunable density of states, effective mass, and localization length.

Tuesday, March 22, 2011 8:00AM - 10:48AM –
Session H38 DCP DBP: Focus Session: Quantum Coherence in Biology I A130/131

8:00AM H38.00001 Indicators of quantum coherence in light-harvesting dynamics , ALEXANDRA OLAYA-CASTRO, Department of Physics and Astronomy, University College London — Characterizing quantum dynamics of electronic excitations in a variety of light-harvesting systems is currently of much interest [1]. In particular, it is important to identify measures that appropriately quantify the strength of coherent dynamics and its impact on different time scales of the light-harvesting process. In this talk I will discuss quantum transport performance measures that are defined based on the probability for the dynamics to successfully distinguish different initial photo-excitation conditions. I will also discuss how initial state distinguisability can provide information on spatially correlated phonon fluctuations as well as on the non-markovian character of the quantum dynamics. The prototype systems considered here are cryptophyte light-harvesting antennae isolated from marine algae [2, 3]. Experimental quantification of state distinguishability can be realized by monitoring the evolution of selected off-diagonal density matrix elements and therefore it could be achieved with current two-dimensional spectroscopy techniques.

[1] A. Olaya-Castro and G. D. Scholes, "Energy transfer from Förster-Dexter theory to quantum coherent light-harvesting", to appear in Int. Rev. Phys. Chem. (2010)
[2] E. Collini, C.Y. Wong, K.E. Wilk, P.M.G. Curmi, P. Brumer and G.D. Scholes, "Coherently wired light-harvesting in photosynthetic marine algae at ambient temperature" Nature, 463, 644-647 (2010)
[3] A. Kolli, A Nazir, F. Fassioli, R. Dinshaw, G D Scholes, and A Olaya-Castro, "Energy transfer dynamics in cryptophyte antennae proteins", submitted for publication (2010)

8:36AM H38.00002 Phonon-mediated path-interference in electronic energy transfer , HODA HOSSEIN-NEJAD, University of Toronto, ALEXANDRA OLAYA-CASTRO, University College London, GREGORY D. SCHOLES, University of Toronto — Motivated by the recent observations of quantum coherence in light-harvesting antennae, we present a formalism to quantify the contribution of path-interference in phonon-mediated electronic energy transfer. The transfer rate between two molecules is computed by considering the quantum mechanical amplitudes associated with pathways connecting the initial and final sites. This includes contributions from classical pathways, but also terms arising from their interference. By treating the vibrational modes of the molecules as a non-Markovian harmonic oscillator bath, we compute the first-order path-interference correction to the classical transfer rate. We show that the correction due to path-interference may have either a vibrational or an electronic character, and may exceed the contribution of the indirect classical pathways.

8:48AM H38.00003 Efficiency of the energy transfer in the FMO complex using hierarchical equations on Graphics Processing Units , TOBIAS KRAMER, CHRISTOPH KREISBECK, University of Regensburg, Germany, MIRTA RODRIGUEZ, IEM CSIC, Madrid, Spain, BIRGIT HEIN, University of Regensburg, Germany — We study the efficiency of the energy transfer in the Fenna-Matthews-Olson complex solving the non-Markovian hierarchical equations (HE) proposed by Ishizaki and Fleming in 2009, which include properly the reorganization process. We compare it to the Markovian approach and find that the Markovian dynamics overestimates the thermalization rate, yielding higher efficiencies than the HE. Using the high-performance of graphics processing units (GPU) we cover a large range of reorganization energies and temperatures and find that initial quantum beatings are important for the energy distribution, but of limited influence to the efficiency. Our efficient GPU implementation of the HE allows us to calculate nonlinear spectra of the FMO complex. References see www.quantumdynamics.de

9:00AM H38.00004 Efficient GPU calculation of 2D-echo spectra of excitonic energy-transfer in systems with large reorganization energy , BIRGIT HEIN, CHRISTOPH KREISBECK, TOBIAS KRAMER, University of Regensburg, Germany, MIRTA RODRIGUEZ, IEM, CSIC, Madrid, Spain — Using the Fenna-Matthews-Olson light harvesting complex as example, we calculate the two dimensional echo spectra (2D echo) of a multi-site system coupled to phonon baths using the propagation scheme suggested by Ishizaki and Fleming in 2009 which works for large system-bath couplings. We study the anti-correlations in the shapes of the 2D spectrum peaks which are seen as evidence for exciton energy transfer. This computationally demanding calculation uses 2.6 h GPU (graphics processing unit) time compared to 2.8 weeks time on a high performance conventional CPU cluster. The efficient implementation of the exact hierarchical equations obliterates the need for approximative methods and facilitates the interpretation and comparison of theory and experiment for systems with large reorganization energies. References see www.quantumdynamics.de

9:12AM H38.00005 Simulation of dissipative quantum dynamics in the presence of strongly-interacting and structured environments: a many-body approach to memory effects , ALEX CHIN, Ulm University, JAVIER PRIOR, Universidad Politécnica de Cartagena, SUSANA F. HUELGA, MARTIN B. PLENIO, Ulm University — Quantum systems which interact strongly with complex and structured environments are receiving increasing attention due to their importance in contexts such as solid-state quantum information processing and bio-molecular quantum dynamics. Unfortunately, these systems are difficult to simulate as the system-bath interactions cannot be treated perturbatively, and standard approaches are invalid or inefficient. Here we combine time-dependent density matrix renormalization group methods with techniques from the theory of orthogonal polynomials to provide an efficient method for simulating open quantum systems at zero and finite temperatures. Using this technique we demonstrate a number of novel dynamical effects which result from long bath memories induced by either sharp spectral structures or strong coupling, and comment on how these can be exploited to drive efficient transport in small networks. We also show how our technique can be used to find the equilibrium properties of excitations in strongly renormalizing environments, and present some results on the quantum phase transition in the sub-Ohmic spin-boson model.

9:24AM H38.00006 Optimal Excitation energy transfer dynamics in light-harvesting systems[1] , JIANLAN WU[2], JIANSHU CAO, ROBERT SILBEY, Chemistry Department, MIT — With the facilitation of surrounding protein environments, excitation energy transfer (EET) in photosynthetic systems can be highly efficient and robust. This talk compares different descriptions of dissipative exciton dynamics, discusses the generic mechanism of optimal energy transfer, and explores its implications for light-harvesting systems. (i) The generalized Bloch-Redfield equation provides a reliable description of exciton dynamics over a broad range of parameter space. (ii) The generic mechanism of optimal efficiency allows us to examine the interplay of quantum coherence, dynamics noise, and static disorder in a unified conceptual framework. (iii) The topological symmetry and network structures in photosynthetic systems reveal useful insights for the optimal design of artificial energy transfer systems.

[1]This work was supported by the MIT Energy Initiative (MITEI) Seed Grant, the MIT Center for Excitonics funded by DOE (Grant Number DE-SC0001088), and ARO DOD (Grant Number W911NF-091-04880).
[2]Physics Department, Zhejiang University, PR China

9:36AM H38.00007 A quantum landscape study of energy transfer efficiency in light-harvesting complexes , ALIREZA SHABANI, Princeton, MASOUD MOHSENI, MIT, HERSCHEL RABITZ, Princeton, SETH LLOYD, MIT — Over billion years of evolution some photosynthetic complexes have turned into highly efficient light energy harvesting systems. In this work, we demonstrate optimality and robustness of energy transfer in the Fenna-Matthews-Olson (FMO) protein complex with respect to all the relevant parameters of system and environmental interactions. To this end we developed an efficient technique for studying the dynamics of energy transfer in a non-Markovian and non-perturbative regime. For the FMO protein of green sulfur bacteria we find that all the relevant natural parameters to lay within the optimal and robust regimes of energy transfer process. This suggests a peculiar interplay of internal and external forces in order to have a system that functions optimally while being robust under physiological conditions.

9:48AM H38.00008 Fast and efficient excitation transfer across disordered molecular networks , ANDREAS BUCHLEITNER, TORSTEN SCHOLAK, Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany, FERNANDO DE MELO, Instituut voor Theoretische Fysica, Katholieke Universiteit Leuven, Celestijnenlaan 200D, B-3001 Heverlee, Belgium, THOMAS WELLENS, Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany, FLORIAN MINTERT, Freiburg Institute of Advanced Studies, Albertstr. 18, 79014 Freiburg, Germany — In this talk, we will present our statistical investigations on coherent excitation transfer through finite-size disordered molecular networks. As we have found, there exist certain molecular conformations that exhibit fast and highly efficient transport – mediated by constructive quantum interference. We will discuss the properties of these optimal conformations which go along with the enhancement of efficiency. These insights may be relevant for explaining efficient energy transfer in the photosynthetic FMO complex.

10:00AM H38.00009 Regenerative quantum coherence in photosynthesis under natural conditions[1] , STEPHAN HOYER, K. BIRGITTA WHALEY, University of California, Berkeley — Recent experiments provide compelling evidence for the feasibility of quantum coherent beating in photosynthetic light harvesting complexes, even at room temperature. However, whether this coherence arises *in vivo* and its biological function (if any) have remained unclear. Here we present theoretical evidence for the creation and regeneration of electronic coherence under natural conditions. We show how such regenerated coherence may contribute to energy transfer efficiency in the Fenna-Matthews-Olson (FMO) complex of green sulfur bacteria.

[1]Support provided in part by the DARPA QuEST and QuBE programs. S.H. is a DOE Office of Science Graduate Fellow.

10:12AM H38.00010 Enhanced exciton diffusion length via cooperative quantum transport , MASOUD MOHSENI, MIT, DAMIAN ABASTO, USC, SETH LLOYD, MIT, PAOLO ZANARDI, USC — The energy transfer rate in biomolecular systems is typically calculated from the transition probability of an excitation hopping from one molecule to another using Förster energy transfer based on dipole-dipole interaction of individual molecules in the perturbative regime. However, due to strong interactions of among a group of molecules the excitation can become highly delocalized leading to an effective large dipole moment with an enhanced oscillator strength. Under certain symmetries, this could lead to an enhancement in exicton transfer rate via cooperative donation or acceptance of an excitation. Here, we explore this phenomenon in various multichromophoric geometries, under different symmetries, initial conditions, and dynamics. We study the behavior of the exciton diffusion length under the effects of disorders and environmental fluctuations and quantify the crossover from ballistic to diffusive regimes. Specifically, for a quasi-1 D array of rings containing N chromophores interacting with a bosonic bath, an interplay of time scales dictates the exciton dynamics. In the "far-field" regime, environmental interactions are dominating and the system properties are approaching those of the incoherent equilibrium Gibbs state. However, in the "near-field" the coherent interactions among dipole aggregates dominate other time scales and exciton diffusion length is enhanced by a factor of $\sqrt{N}$.

10:24AM H38.00011 Concatenated quantum codes in biological systems[1] , SETH LLOYD, Massachusetts Institute of Technology — This talk investigates how biological systems such as photosynthetic bacteria use quantum coding techniques such as decoherent subspaces, noiseless subsystems, and concatenated quantum codes to engineer long exitonic lifetimes and rapid energy transport. The existence of hierarchical structures in photosynthetic complexes is associated with concatenated quantum codes. A concatenated code is one that combines two or more codes to construct a hierarchical code that possesses features of all its constituent codes. In photosynthetic complexes, structures at the smallest level use quantum coding techniques to enhance exciton lifetimes, and structures at higher scales possess symmetries that enhance exciton hopping rates. The result is a concatenated quantum code that simultaneously protects excitons and enhances their transport rate. All known quantum codes can be described within the framework of group representation theory. This talk reviews the relationship between symmetry and quantum codes, and shows how photosynthetic bacteria and plants put quantum coding techniques to use to improve the efficiency of photosynthetic transport.

[1]Supported by the DARPA QuBE program

10:36AM H38.00012 A possible mechanisms for quantum coherence assisted ion transport in ion channels , ALIPASHA VAZIRI, Max F. Perutz Laboratories (MFPL), University of Vienna, Austria and the Research Institute of Molecular Pathology (IMP) — Recently it was demonstrated that long-lived quantum coherence exists during excitation energy transport in photosynthesis. It is a valid question up to which length, time and mass scales quantum coherence may extend, how to one may detect this coherence and what if any role it plays for the dynamics of the system. Ion-channels are involved in many physiological processes. In the nervous system their coordinated opening and closing generates action potentials that form the basis for intra-neural communication which are essential for information representation and processing. We have recently suggested that the selectivity filter of ion channels may exhibit quantum coherence which might be relevant for the process of ion selectivity and conduction. I will discuss some of our current experimental efforts in this direction and show that quantum resonances could provide a viable approach to probe these quantum coherences. The emergence of resonances in the conduction of ion channels that are modulated periodically by time varying external fields can serve as signatures of quantum coherence in such a system.

Tuesday, March 22, 2011 8:00AM - 10:36AM –

Session H39 DBP: Focus Session: Physics of Cancer A124/127

8:00AM H39.00001 Nanotechnology Approaches to Studying Epigenetic Changes in Cancer , ROBERT RIEHN, NC State University — Placing polyelectrolytes into confined geometries has a profound effect on their molecular configuration. For instance, placing long DNA molecules into channels with a cross-section of about 100 nm^2 stretches them out to about 70% of their contour length. We are using this effect to map epigenetic changes on single DNA and chromatin strands. This mapping on single molecules becomes central in the study of the heterogeneity of cell population in cancer, since rapid change of epigenetic makeup, propagated through rare cancer stem cells, is a hallmark of its progression. We demonstrate the basic building blocks for the single-molecule epigenetic analysis of genomic sized DNA. In particular, we have achieved the mapping of methylated regions in DNA with heterogeneous 5-methyl cytosine modification using a specific fluorescent marker. We further show that chromatin with an intact histone structure can be stretched similar to DNA, and that the epigenetic state of histone tails can be detected using fluorescent antibodies.

8:36AM H39.00002 Cancer Evolution under Drug-Induced Stress-Gradients[1] , GUILLAUME LAMBERT, ROBERT H. AUSTIN, Princeton University — The lack of long term success in eliminating cancer cells while avoiding the evolution of drug resistance indicates that our understanding of how cells evolve in response to stress is still incomplete. We interpret this not as a failure of the current approaches, but rather as an indication that new research venues should be undertaken, where conventional wisdom is challenged in order to drive forward our understanding of cancer. Of particular importance, we believe that the powerful role of evolution in the origin of drug resistance is ill-understood. We do not ask whether evolution occurs, but rather how. We do not describe molecular mechanisms underlying drug resistance at the single cell level, but rather ask how does resistance spread in cancerous tissues and metastatic lesions. We attempt to answer these questions by studying the population-wide dynamics of drug evolution and the collective stress response of cancer cells in a microfluidics device. We use microfluidics technologies to impose high levels of stress on cancer cell metapopulation by create smoothly varying gradients of either oxygen, chemotherapeutic drug, nutrient or pH. We present long-term studies of the adaptation of tumorigenic cancer cells to drug- induced stress gradients.

[1]Partially supported by and performance at NCI U54CA143803, CNF ECS-0335765, NSF PHY- 0750323, and NSERC.

8:48AM H39.00003 Are biomechanical changes necessary for tumor progression? , JOSEF A. KAS, ANATOL FRITSCH, TOBIAS KIESSLING, DAVID K. NNETU, STEVE PAWLIZAK, FRANZISKA WETZEL, MAREIKE ZINK, University of Leipzig — With an increasing knowledge in tumor biology an overwhelming complexity becomes obvious which roots in the diversity of tumors and their heterogeneous molecular composition. Nevertheless in all solid tumors malignant neoplasia, i.e. uncontrolled growth, invasion of adjacent tissues, and metastasis, occurs. Physics sheds some new light on cancer by approaching this problem from a functional, materials perspective. Recent results indicate that all three pathomechanisms require changes in the active and passive cellular biomechanics. Malignant transformation causes cell softening for small deformations which correlates with an increased rate of proliferation and faster cell migration. The tumor cell's ability to strain harden permits tumor growth against a rigid tissue environment. A highly mechanosensitive, enhanced cell contractility is a prerequisite that tumor cells can cross its tumor boundaries and that this cells can migrate through the extracellular matrix. Insights into the biomechanical changes during tumor progression may lead to selective treatments by altering cell mechanics. Such drugs would not cure by killing cancer cells, but slow down tumor progression with only mild side effects and thus may be an option for older and frail patients.

9:00AM H39.00004 A cellular automaton model for tumor growth in heterogeneous environment[1] , YANG JIAO, Physical Science in Oncology Center, Princeton University, SAL TORQUATO, Dept. Chemistry, Princeton University — Cancer is not a single disease: it exhibits heterogeneity on different spatial and temporal scales and strongly interacts with its host environment. Most mathematical modeling of malignant tumor growth has assumed a homogeneous host environment. We have developed a cellular automaton model for tumor growth that explicitly incorporates the structural heterogeneity of the host environment such as tumor stroma. We show that these structural heterogeneities have non-trivial effects on the tumor growth dynamics and prognosis.

[1]Y. J. is supported by PSOC, NCI

9:12AM H39.00005 Microfabricated Tepui: probing into cancer invasion, metastasis and evolution in a 3D environment[1] , LIYU LIU, Princeton University — Cancer metastasis and chemotherapeutic resistance are the major reasons why cancer remains recalcitrant to long-term therapy. We are interested to know: 1. How cancer cells invade tissues and metastasize in a 3D spatial environment? 2. How cancer cells evolve resistance to chemotherapeutic therapy? Answering these fundamental questions will require spatially propagating cancer cells in a 3D *in vitro* micro environment with dynamically controlled chemical stress. Here we attempt to realize this micro environment with a three-dimentional topology on a micro-chip which consist of isolated highlands (Tepui) and deep lower lands. Cancer cells are patterned in the lower lands and their spatial invasion to the mesas of Tepui is observed continuously with a microscope. Experiments have demonstrated that the cell invasion potential is time dependent, which is not only determined by cell motility, but also cell number and spatial stress. Quantitative analysis shows that the invasion rate fits logistic equation. Further more, we have also imbedded collagen based Extracellular Matrix (ECM) inside these structures and established a robust chemical gradient in a vertical space. With merit of real-time confocal imaging, cell propagation, metastasis and evolution in the 3D environment are studied with time as a model for cell behavior inside tissues.

[1]NCI grant: U54CA143803

9:48AM H39.00006 Study of breast cancer cell behavior under chemical stress using microfluidic gradient generator[1] , AMY WU, KEVIN LOUTHERBACK, GUILLAUME LAMBERT, LIYU LIU, ROBERT AUSTIN, JAMES STURM, PRINCETON PSOC TEAM — Understanding the behavior of cancer cells in gradients of chemotherapeutic agents is important in studying the evolution of cancer drug resistance. Compared to traditional in-vitro methods, microfluidic gradient generators better control temporal and spatial profile of gradients. However, maintaining chemical gradients requires high flow rate of liquid (10ul/hr) in microfluidic chip while culturing mammalian cells demands slow flow rate of liquid (1ul/hr). In this paper, we modify a microfluidic gradient generator (Jeon et al, Langmuir, 2001) to overcome the challenge of maintaining slow flow rate and stable gradients simultaneously based on numerical simulations, and culture metastatic breast cancer cell line (MDA-MB-231) in the chip. To characterize the stability of gradients, we visualize the gradient profile by infusing fluorescein. Finally, we will report the response of the on-chip culture under the stress of chemical gradients, observing for cellular phenotypic changes including death, proliferation, morphology, and migration.

[1]National Institute of Health

10:00AM H39.00007 Superficial dose distribution in breast for tangential radiation treatment of breast cancer , ROUMIANA CHAKAROVA, MAGNUS GUSTAFSSON, ANNA BAECK, NINNI DRUGGE, ASA PALM, ANDREAS LINDBERG, MATTIAS BERGLUND, Sahlgrenska University Hospital, Dept. of Medical Physics and Biomedical Engineering, Gothenburg, 413 45 Sweden — The superficial (0-2 cm) dose distribution in a cylindrical phantom is examined theoretically and experimentally when irradiated by tangential photon beams. The lateral superficial part of the phantom is shown to receive full dose beyond 2 mm whereas the build-up region is up to 7 mm where the beams enter. Eclipse AAA calculations agree well with the experimental and Monte Carlo data while Eclipse PBC underestimates the entrance dose the first 3-4 mm and fails to give a correct lateral dose close to the surface up to 10 mm depth. The performance of the Eclipse algorithms is evaluated in a number of clinical cases with Monte Carlo results. Examples are given to illustrate how differences in geometrical presentation of the body structure in the treatment planning system and the Monte Carlo simulation as well as the patient voxelization may affect the evaluation results.

10:12AM H39.00008 Origin of using cisplatin over transplatin for cancer treatment: An ab initio study[1] , SA LI, PURU JENA, Virginia Commonwealth University, DEPARTMENT OF PHYSICS, VIRGINIA COMMONWEALTH UNIVERSITY TEAM — Eventhough cisplatin has been used as a chemotherapy anti-cancer drug for over 40 years the thermodynamics and kinetics of the reactions are still largely unknown. Cisplatin molecules are known to be attacked by water molecules before they react with DNA. As a result, two Cl atoms are eliminated. The active piece in the cell, therefore, is not cisplatin but $(NH_3)_2Pt^{2+}$. To explain why only cisplatin but not transplatin functions as anticancer drug, we used first principles method to study the dechlorination process in cis- and transplatin. Although transplatin molecule is more stable than cisplatin by 0.52 eV, we found cisplatin to be more favorable for reaction due to the following reasons: 1) the energy cost to remove a Cl atom is less from cisplatin than transplatin. 2) cis-form $(NH_3)_2Pt^{2+}$ derived from cisplatin with N-Pt-N angle of 97° is lower in energy than trans-form derived from transplatin with N-Pt-N angle of 180°. The rotation barrier for N-Pt-N changing from 180° to 97° is about 1.0 eV. 3) When cis-form of $(NH_3)_2Pt^{2+}$ reacts with two Guanines in DNA, the two N atoms in Guanines can readily bind to the Pt atom in cisplatin. The transplatin due to steric reasons does not provide that opportunity.

[1]This work is supported by grants from the Department of Energy

10:24AM H39.00009 Actinomycin D binding mode reveals the basis for its potent HIV-1 and cancer activity , THAYAPARAN PARAMANATHAN, IOANA D. VLADESCU, MICAH J. MCCAULEY, Northeastern University, Boston, MA, IOULIA ROUZINA, University of Minnesota, Minneapolis, MN, MARK C. WILLIAMS, Northeastern University, Boston, MA — Actinomycin D (ActD) is one of the most studied antibiotics, which has been used as an anti-cancer agent and also shown to inhibit HIV reverse transcription. Initial studies with ActD established that it intercalates double stranded DNA (dsDNA). However, recent studies have shown that ActD binds with even higher affinity to single stranded DNA (ssDNA). In our studies we use optical tweezers to stretch and hold single dsDNA molecule at constant force in the presence of varying ActD concentrations until the binding reaches equilibrium. The change in dsDNA length upon ActD binding measured as a function of time yields the rate of binding in addition to the equilibrium lengthening of DNA. The results suggest extremely slow kinetics, on the order of several minutes and 0.52 ± 0.06 μM binding affinity. Holding DNA at constant force while stretching and relaxing suggests that ActD binds to two single strands that are close to each other rather than to pure dsDNA or ssDNA. This suggests that biological activity of ActD that contributes towards the inhibition of cellular replication is due to its ability to bind at DNA bubbles during RNA transcription, thereby stalling the transcription process.

Tuesday, March 22, 2011 8:00AM - 10:12AM –

Session H40 DBP: Multi-cellular Processes and Development A122/123

8:00AM H40.00001 Dynamics of asexual reproduction in planarians , EVA-MARIA SCHOETZ, BRYAN LINCOLN, SOFIA QUINODOZ, Princeton University — Planaria research is experiencing a resurgence due to the development of molecular tools, the Planarian genome project and database resources. Despite the resulting progress in planarian biology research, an extensive study of their physical properties remains to be undertaken. We developed a method to collect a large amount of data on the dynamics of clonal reproduction in the freshwater planarian S.mediterranea. The capability of planarians to regenerate an entire organism from a minuscule body part is based on a homogeneously distributed stem cell population that comprises 25-30% of all cells. Due to this stem cell contingent, planarians can reproduce spontaneously by dividing into a larger head and a smaller tail piece, which then will rebuild the missing body parts, including a central nervous system, within about a week. Time-lapse imaging allows us to characterize the fission process in detail, revealing the stages of the process as well as capturing the nature of the rupture itself. A traction force measurement setup is being developed to allow us to quantify the forces planarians exert on the substrate during reproduction, a macroscopic analog to the Traction Force Microscopy setups used to determine local cellular forces. We are particularly interested in the molecular processes during division and the interplay between tissue mechanics and cell signaling.

8:12AM H40.00002 Quantifying cell behaviors during embryonic wound healing[1] , DAVID MASHBURN, XIAOYAN MA, SARAH CREWS, HOLLEY LYNCH, W. TYLER MCCLEERY, M. SHANE HUTSON, Vanderbilt University — During embryogenesis, internal forces induce motions in cells leading to widespread motion in tissues. We previously developed laser hole-drilling as a consistent, repeatable way to probe such epithelial mechanics. The initial recoil (less than 30s) gives information about physical properties (elasticity, force) of cells surrounding the wound, but the long-term healing process (tens of minutes) shows how cells adjust their behavior in response to stimuli. To study this biofeedback in many cells through time, we developed tools to quantify statistics of individual cells. By combining watershed segmentation with a powerful and efficient user interaction system, we overcome problems that arise in any automatic segmentation from poor image quality. We analyzed cell area, perimeter, aspect ratio, and orientation relative to wound for a wide variety of laser cuts in dorsal closure. We quantified statistics for different regions as well, i.e. cells near to and distant from the wound. Regional differences give a distribution of wound-induced changes, whose spatial localization provides clues into the physical/chemical signals that modulate the wound healing response.

[1]Supported by the Human Frontier Science Program (RGP0021/2007 C).

8:24AM H40.00003 Keeping track of embryo development: new insights in the coupling between local and global changes , TIMON IDEMA, PHILIP NELSON, ANDREA LIU, University of Pennsylvania, JULIEN DUBUIS, LISA MANNING, THOMAS GREGOR, Princeton University — Modern imaging techniques allow us to study biological systems such as Drosophila in vivo during early development. Between the ninth and fourteenth cell cycles of the Drosophila embryo, nuclei are positioned at the embryo's surface and are observed to divide at the end of each cycle in a highly synchronized fashion. We have implemented a new tracking technique that allows us to determine the shapes of the nuclei as they elongate and divide, and to follow their motion on the surface. We find that during each cycle, the nuclei shapes evolve with time in a consistent way from nucleus to nucleus. These shape changes spread as waves with a well-defined wave velocity through the embryo, coupling local (nucleus) and collective (entire embryo) development. The waves in turn induce collective motions of the nuclei, not just after division but also before it.

8:36AM H40.00004 A cellular Potts model of germband retraction and dorsal closure[1] , M. SHANE HUTSON, JASON ROHNER, SARAH CREWS, W. TYLER MCCLEERY, W. BRADLEY ROBINSON, Vanderbilt University — Germband retraction and dorsal closure are critical morphogenetic events in fruit fly embryogenesis. Both involve the coordinated reshaping of two epitheloid tissues – germband (GB) and amnioserosa (AS). The GB is initially curled into a U-shape with the AS between the arms of the U. Retraction leaves the embryo's dorsal surface covered by AS cells which then contract to pull lateral parts of the GB up to cover the dorsal surface. We have simulated these events using a cellular Potts model. The model is 3D with several generalized cell types: a central yolk; a surrounding monolayer of AS and GB cells with epithelial polarization; and an outer vitelline membrane enclosing the cells and a perivitelline fluid. The model also incorporates several critical cell behaviors: polarized apical constriction of AS cells; controlled relaxation of stretched GB cells; and differentiation of GB cells at the GB-AS interface so that these cells then contract a supracellular purse-string and extend filopodia that reach across the AS and zip together the GB's approaching lateral flanks. We will discuss how all of these components are necessary to reproduce normal tissue motions and those observed during laser microsurgery experiments.

[1]Supported by NSF Grant IOB-0545679.

8:48AM H40.00005 Developmental and Metabolite Transport Strategies to Optimize the Growth of Filamentous Cyanobacteria , AIDAN BROWN, ANDREW RUTENBERG, Department of Physics, Dalhousie University, Halifax, Nova Scotia, Canada — Individual cells of filamentous cyanobacteria share nutrients through cytoplasmic and/or periplasmic connections. Under conditions of low fixed-nitrogen some cells terminally differentiate into heterocysts, which fix nitrogen for the remaining photosynthetic vegetative cells. Heterocysts are observed to occur in a regular pattern separated by clusters of vegetative cells. Using a quantitative model of nitrogen uptake, consumption and transport together with vegetative cell growth and division, we explore how the overall growth rate of the filament depends on different heterocyst positioning patterns and on particular strategies of nitrogen transport.

9:00AM H40.00006 Elasticity of developing cardiac tissue , STEPHANIE MAJKUT, JOE SWIFT, CHRISTINE KRIEGER, DENNIS DISCHER, University of Pennsylvania — Proper development and function of the heart from the tissue to cellular scale depends on a compliant ECM. Here we study the maturation of embryonic cardiac tissue mechanics in parallel with the effects of extracellular mechanics on individual cardiomyocyte function throughout early development. We used micropipette aspiration to measure local and bulk elastic moduli (E) of embryonic avian heart tissue from days 2-12. We observe stiffening of the early heart tube from E = 1 kPa at day 1 to E = 2 kPa at day 4, reaching neonatal values by day 12. Treating heart tubes with blebbistatin led to 30% decrease in E, indicating a significant but partial actomyosin contribution to mechanics at these stages. We performed a proteomic analysis of intact and decellularized 2-4 day heart tubes by mass spectrometry to quantify the ECM present at these stages. Isolated cardiomyocytes from 2-4 day chick embryos were cultured on collagen-coated PA gels of various stiffnesses. Beating magnitude was modulated by substrates with E = 1-2 kPa, similar to physiological E at those stages.

9:12AM H40.00007 ECM ordering effects as a marker for early tissue formation on artificial substrates - a sum-frequency-generation spectroscopy study , PATRICK KOELSCH, MARK-OLIVER DIESNER, Karlsruhe Institute of Technology, BIOINTERFACES TEAM — The in situ monitoring of the interphase between a substrate and a cellular layer is of great interest as it allows determination of changes in surface properties and extracellular matrix (ECM) organization. The latter is an early indicator of major cellular processes like migration, adhesion, proliferation, metastasis, tissue formation, and gain or loss of differentiation. We demonstrated recently that vibrational sum-frequency-generation (SFG) spectroscopy can be used to probe the layer between living cells and a solid substrate. In this contribution we will report on the investigation of ordering phenomena within the ECM of fibroblasts allowing to track early stages of tissue formation. SFG spectroscopy offers a unique way to observe these correlated changes of order in real-time without the need of labeling or disruption.

9:24AM H40.00008 Distinguishing Pattern Formation Phenotypes: Applying Minkowski Functionals to Cell Biology Systems[1] , ERIN RERICHA, CAN GUVEN, University of Maryland, College Park, CAROLE PARENT, National Cancer Institute, National Institutes of Health, WOLFGANG LOSERT, University of Maryland, College Park — Spatial Clustering of proteins within cells or cells themselves frequently occur in cell biology systems. However quantifying the underlying order and determining the regulators of these cluster patterns have proved difficult due to the inherent high noise levels in the systems. For instance the patterns formed by wild type and cyclic-AMP regulatory mutant *Dictyostelium* cells are visually distinctive, yet the large error bars in measurements of the fractal number, area, Euler number, eccentricity, and wavelength making it difficult to quantitatively distinguish between the patterns. We apply a spatial analysis technique based on Minkowski functionals and develop metrics which clearly separate wild type and mutant cell lines into distinct categories. Having such a metric facilitated the development of a computational model for cellular aggregation and its regulators.

[1]Supported by NIH-NGHS Nanotechnology (R01GM085574) and the Burroughs Wellcome Fund

9:36AM H40.00009 Measuring the viscosity of embryonic epithelia *in vivo* by magnetic tweezers[1] , XIAOYAN MA, M. PAULA ANGARITA, MERSHARD FRIERSON, DREW SHELDON, M. SHANE HUTSON, Vanderbilt University — During early development, sheets of epithelial cells are reshaped by cellular forces. Several recent investigations in fruit fly (*Drosophila*) embryos have used laser microsurgery and video force microscopy to measure these forces; however, these measurements are actually limited to force/viscosity ratios because the effective viscosity of epithelial cells in a living embryo is largely unknown. This effective viscosity may vary spatially within the embryo and temporally as development progresses. To address this issue, we use microinjection, magnetic tweezers and confocal microscopy to measure the effective viscosity of epithelial cells in fruit fly embryos *in vivo*. We inject fluorescent magnetic beads (2-μm diameter) into GFP-labeled embryos at the multi-nuclear syncytial blastoderm stage. The beads are pulled to embryo's surface by a permanent magnet and become engulfed by individual epithelial cells during cellularization. During later stages of development, we supply current pulses to an electromagnet to apply force pulses to the beads with a magnitude of $\sim$100 pN. The effective viscosity is inferred from the movement of these beads as tracked by confocal microscopy. We will report initial results on amnioserosa cells during dorsal closure.

[1]This Work Supported by NSF Grant IOB-0545679.

9:48AM H40.00010 Modeling of Endothelial Glyccalyx via Dissipative Particle Dynamics , MINGGE DENG, Univ. of Science & Technology of China and Brown University, HAOJUN LIANG, Univ. of Science & Technology of China, GEORGE KARNIADAKIS, Brown University — We employ Dissipative Particle Dynamics (DPD) to simulate flow in small vessels with the endothelial glycocalyx attached to the wall. Of particular interest is the quantification of the slip velocity at the edge of glycocalyx and of the increased pressure drop at different crafting densities, stiffness and height of the glycocalyx. Results will be presented for capillaries and small arterioles, and interactions with discrete red blood cells will be included in the modeling. In addition to the physical insight gain for this important but relatively unexplored bioflow, simple models for the slip velocity will be proposed that can be used in continuum simulations of blood flow in micro-vessels.

10:00AM H40.00011 An approach to collective behavior in cell cultures: modeling and analysis of ECIS data , DAVID RABSON, EVAN LAFALCE, DOUGLAS LOVELADY, University of South Florida, CHUN-MIN LO, National Yang-Ming University — We review recent results in which statistical measures of noise in ECIS data distinguished healthy cell cultures from cancerous or poisoned ones: after subtracting the "signal," the $1/f^{\alpha}$ noise in the healthy cultures shows longer short-time and long-time correlations. We discuss application of an artificial neural network to detect the cancer signal, and we demonstrate a computational model of cell-cell communication that produces signals similar to those of the experimental data. The simulation is based on the q-state Potts model with inspiration from the Bak-Tang-Wiesenfeld sand-pile model. We view the level of organization larger than cells but smaller than organs or tissues as a kind of "mesoscopic" biological physics, in which few-body interactions dominate, and the experiments and computational model as ways of exploring this regime.

Tuesday, March 22, 2011 8:00AM - 10:36AM –

Session H41 Irving Langmuir Prize Session: Ultrafast Dynamics A115/117

8:00AM H41.00001 Irving Langmuir Prize in Chemical Physics Talk: Attosecond Electron Dynamics[1] , STEPHEN LEONE, University of California Berkeley — Isolated attosecond pulses are produced by the process of high order harmonics, and these pulses are used as a soft X-ray probe in wavelength-dispersed transient absorption. Inner shell core-level spectroscopic transitions are thus used to analyze the chemical and electronic environment of specific atomic states as a function of time following ionization and dissociation. High field ionization processes, using 800 nm pulses, result in spin-orbit electronic state populations, alignment, and electronic wave packet superpositions, all of which are investigated by the spectrally-resolved X-ray probe. By using isolated attosecond pulses as the probe, high field ionization events on a subfemtosecond timescale are investigated. The generality of the transient absorption method for attosecond dyamics is described, as well as the challenges during the pump-probe pulse overlap time period. The results are compared to theoretical calculations by collaborators.

[1]Supported by DOE, NSF and AFOSR.

8:36AM H41.00002 Time- and Angle-Resolved Photoemission Spectroscopy: Ultrafast Dynamics of Electronic Structure , JONATHAN A. SOBOTA, PATRICK S. KIRCHMANN, SHUOLONG YANG, ZHI-XUN SHEN, Stanford University — Angle-resolved photoemission spectroscopy (ARPES) is a powerful experimental tool for condensed matter systems as it measures the single-particle spectral function. Using femtosecond laser pulses in a pump-probe scheme, ARPES can be extended into the time domain. Here we report the construction of a time-resolved ARPES (trARPES) system. We utilize a Ti:Sapphire oscillator to produce infrared pump pulses, while ultraviolet probe pulses are generated by frequency quadrupling. A hemispherical electron analyzer measures the photoemission spectrum as a function of pump-probe delay. We present results on Gallium Arsenide, which displays hot electron dynamics on two distinct timescales in the unoccupied states. Interestingly, the signal in the occupied states has high temporal contrast, resembling a step-function with dynamics at negative delays. These properties make Gallium Arsenide a versatile tool for trARPES system characterization, allowing for calibration of pump-probe temporal and spatial overlap, as well as determination of time resolution.

8:48AM H41.00003 Beyond the Frontiers of Time-Resolved Spectroscopy[1] , THOMAS PFEIFER, Max-Planck Institut fuer Kernphysik — Time-resolved spectroscopy experiments typically require the measurement of at least two ("pump" and "probe") interactions of a field (e.g. a laser pulse) with the spectroscopic target system (e.g. atom, molecule) at variable but known temporal delays. It is often assumed that the shortest dynamics measurable with such techniques is on the order of the pulse duration of the pump and probe events. In this talk, it will be shown that attosecond electron wavefunction beating can, in principle, be resolved by employing a nonlinear interferometry concept with phase-stabilized femtosecond pulses that does not require attosecond pulses for pumping nor probing. The perfectly coherent and reproducible electric fields of the pump and probe pulses thus seem the ultimate technical goal to achieve the highest temporal resolution in science. By contrast, however, it will be shown that statistically varying (colored-noise) partially coherent pulses typically produced at free-electron lasers (FELs) can be beneficial in resolving dynamics beyond their average pulse duration. These findings may carry general implications for the future development of time-resolved spectroscopy.

[1]Support from the MPRG program of the Max-Planck Gesellschaft ist gratefully acknowledged.

9:24AM H41.00004 Quantitative imaging of ultrashort photoelectron pulse dynamics[1] , ZHENSHENG TAO, HE ZHANG, PHILLIP DUXBURY, MARTIN BERZ, CHONG-YU RUAN, Michigan State University — Understanding and mitigating the space charge effects is a pressing issue in the development of ultrafast electron diffraction and imaging. Using a novel ultrafast projection imaging technique, quantitative imaging of transient space charge effects in the generation of high density ultrashort electron pulses is performed, which offers a means to directly compare with multi-electron calculations. We establish that the pulse width exhibits a fractional power-law scaling with the sheet density of the emitted electron pulses. By comparing to multi-electron simulations, the initial longitudinal phase space of the photoelectrons is extracted, demonstrating a strong dependence of the initial momentum spread on the sheet density. Multielectron effects are treated using a simple extension of single electron photoemission theory yielding qualitatively correct estimates of the quantum efficiency.

[1]This work was supported by Department of Energy under Grant No. DE-FG02-06ER46309 and MSU Foundation.

9:36AM H41.00005 Electron and ion dynamics in the melting of two-dimensional charge density waves[1] , TZONG-RU HAN, Michigan State University, CHRISTOS MALLIAKAS, Northwestern University, S.D. MAHANTI, Michigan State University, MERCOURI KANATZIDIS, Northwestern University, CHONG-YU RUAN, Michigan State University — The cause of local lattice distortion in the formation of charge density waves (CDW) in 1D materials is often attributed to the Peierls mechanism, while for 2D system, such as CeTe3, it is not precisely known, due to imperfect nesting of the Fermi surface and a rather large CDW gap observed. Using ultrafast electron crystallography, the femtosecond electronic melting and recrystallization of CDW is investigated by following the superlattice peaks (order parameter) originated from the long-range charge ordering and the accompanying lattice distortion. We find that the reconstitution of CDW is subject to a bottleneck effect that can be attributed to the distinctively separated dynamical properties of electrons and ions in the short time scale, revealing the complexity of 2D CDW formation.

[1]This work is supported by DOE under DE-FG02-06ER46309 and NSF under NSF-DMR 0703940.

9:48AM H41.00006 Nonperturbative Rydberg excitations triggered by electrons or photons[1] , CHRIS H. GREENE, University of Colorado — Recently investigated processes with autoionizing Rydberg atoms or molecules will be discussed. In one class of processes, two or more Rydberg state are dressed by a laser field that couples them nonperturbatively, after which the coupled states are subsequently probed by XUV photons in a transient absorption experiment. This class will be discussed in the context of two recent experiments involving doubly-excited autoionizing states of atomic helium. In the second class of processes, the Rydberg states are initially created when electrons collide with molecular ions in a plasma environment, then get trapped temporarily in a high Rydberg state after giving up part of their energy to vibrational or rotational degrees of freedom. The Rydberg molecules then have competitive decay pathways, via photon emission, autoionization, or dissociation. The theory will be discussed in the context of experiments that bear on this second class of dynamical processes, which have been performed in Berkeley and also in Prague.

[1]Supported by the DOE Office of Science

10:24AM H41.00007 Molecular structures studied using laser induced electron diffraction , YUNFEI LIN, Department of Chemistry, Wayne State University, Detroit, MI, 48202, SUK KYOUNG LEE, LU YAN, WEN LI — In a strong laser field, the field ionized electrons from molecules can be returned to the parent molecules by the laser field. These electrons are then scattered off their parent ions. Such phenomena can be used to study molecular structures like the conventional electron diffraction technique, with much better temporal resolution (a few femtoseconds). In this study, we demonstrated its capability to retrieve static structures of molecules using a simple experimental setup. We obtained electron diffraction patterns from spatially aligned oxygen, nitrogen and carbon dioxide in a strong laser field with intensity around $7*10^{13}$ W cm^{-2}. Excellent energy and angular resolutions were achieved by using velocity map imaging detection of electron momentum. The analysis shows that in order to extract the structure information, two kinds of interferences have to be considered: in the first kind, the electrons are ionized and scattered from the same atom; in the second kind, they are ionized from one atom but scattered off another atom in the molecule. We were able to account for the main features in the diffraction patterns of all three molecules and thus obtained the internuclear distances. In the future, we will apply this technique to retrieve structures of polyatomics and also plan to study molecular dynamics exploiting its superb temporal resolution.

Tuesday, March 22, 2011 8:00AM - 11:00AM –

Session H42 DMP DPOLY GERA: Focus Session: Polymers for Energy Storage and Conversion – Physics of Ion Conductivity in Polymers A302/303

8:00AM H42.00001 Polymer Physics Prize Break –

8:36AM H42.00002 Broadband Dielectric Spectroscopy and Quasi-Elastic Neutron Scattering on Single-Ion Polymer Conductors , CHRISTOPHER SOLES, HUA-GEN PENG, KIRT PAGE, CHAD SNYDER, NIST Polymers Division, ASHOUTOSH PANDY, YOUMI JEONG, JAMES RUNT, Pennsylvania State University, NIST POLYMERS DIVISION COLLABORATION, PENNSYLVANIA STATE UNIVERSITY COLLABORATION — The application of solid polymer electrolytes in rechargeable batteries has not been fully realized after decades of research due to its low conductivity. Dramatic increases of the ion conductivity are needed and this progress requires the understanding of conduction mechanism. We address this topic in two fronts, namely, the effect of plasticizer additives and geometric confinement on the charge transfer mechanism. To this end, we combine broadband dielectric spectroscopy (BDS) to characterize the ion mobility and quasi-elastic neutron scattering (QENS) to quantify segmental motion on a single-ion model polymer electrolyte. Deuterated small molecules were used as plasticizers so that the segmental motion of the polymer electrolyte could be monitored by QENS to understand the mechanism behind the increased conductivity. Anodic aluminum oxide (AAO) membranes with well defined channel sizes are used as the matrix to study the transport of ions solvated in a 1D polymer electrolyte.

8:48AM H42.00003 A Quasi Elastic Neutron Scattering study of polymer dynamics in PEO based sulfonate ionomers: Effect of ion content and ion identity , KOKONAD SINHA, JANNA MARANAS, The Pennsylvania State University — We present Quasi Elastic Neutron Scattering (QENS) data for characterizing dynamics in ion containing polymers (ionomers) with varying ion content (cation to ether oxygen ratio) and ion identity. To remove electrode reverse polarization, the anion is immobilized by covalently bonding it to the PEO backbone through an 'ionizable' isophthalate co-monomer unit and only the cation contributes to the conductivity. We vary the ion content in two ways: changing the ratio of neutral to ionized co-monomer units, and changing the length of the PEO spacer separating the co-monomer units. In neutral ionomers, we observe two segmental processes; PEO segments in the spacer midpoint are one order of magnitude faster than those near the isophthalate groups. In ionized samples, cross-linking between ionic groups considerably slows the dynamics of PEO segments near the isophthalate group. The extent of cross linking depends on the ion content and spacer length. This effect is also ion dependent, which indicates that cations have different binding capacities and formation of this complex controls the availability of free cations for conduction.

9:00AM H42.00004 Structure and Dynamics of Proton-Conducting Azoles Confined within Metal-Organic Frameworks , JAMIE FORD, University of Pennsylvania, JASON SIMMONS, NIST Center for Neutron Research, TANER YILDIRIM, University of Pennsylvania/NIST Center for Neutron Research — Efficient polymer electrolyte membrane (PEM) fuel cells are one of the most promising candidates to power our vehicles of the future. Hydrated sulfonated polymers are currently the preferred membrane material because of their excellent conductivity and gas diffusion characteristics. The intrinsic water dependence in these systems limits the operating temperature to 100 C, leading to reduced electrode kinetics and increased CO poisoning. If water can be replaced by a small molecule with a higher boiling point, the overall efficiency of the system can be improved. To this end, we have investigated a set of new host/guest materials based on metal-organic frameworks (MOFs) loaded with a variety of azoles. The thermally and chemically stable frameworks provide a well-defined porous structure that accommodates the proton conduction pathways formed by the azole networks. We will present the structure of the azole networks as well as insight into the proton motion dynamics as a result of a variety of neutron scattering experiments.

9:12AM H42.00005 Ion solvation thermodynamics in polymer blends and block copolymers , ZHEN-GANG WANG, California Institute of Technology — There is much current interest in ion-containing polymers as materials for energy applications. For example, a promising system for rechargeable battery applications consists of diblock copolymers of an ion-dissolving block, typically polyethylene oxide (PEO) and a nonconducting block such as polystyrene. The addition of lithium salts has been shown to significantly alter the order-order and order-disorder transition temperatures, which reflects a change in the miscibility between the two polymer blocks. In this talk, I discuss some simple theoretical ideas for explaining and predicting the change in polymer miscibility due to the addition of salt ions for both polymer blends and block copolymers. A key effect is the solvation energy of the ions by the polymers, which we approximate using the Born solvation model. The difference in the Born energy of the ions between different polymers provides a driving force towards phase separation, whereas the translational entropy of the ions favors keeping the polymers mixed. In the case of lithium salts added to systems containing PEO, we develop a complexation model in which the lithium ions are tightly bound to the oxygen groups in the EO monomers, while the anions can either be free or form ion pairs with the lithium. For PEO-PS blends or block copolymers, we show that adding lithium salts leads to significant increase in the effective χ parameter between the two polymers. Our theory predicts that the effect should weaken with increasing radius of the anion, in agreement with available experimental data. Furthermore, we show that the domain spacing in microphase separated block copolymers should increase, also in agreement with experiments. We also examine the issue of ion distribution using self-consistent field theory.

9:48AM H42.00006 Understanding Ion Transport in Plasticized Polymer Electrolytes using Dielectric Spectroscopy , U. HYEOK CHOI, SIWEI LIANG, JAMES RUNT, RALPH COLBY, Penn State University — A challenge facing the development of new renewable energy storage materials is the low ionic conductivity within polymer matrices. Most materials development must overcome two main hurdles: Increase the ionic mobility and maximize the conducting ion concentration. The main role of small molecule plasticizers is not only to improve flexibility and segmental motion, which consequently lowers the T_g and increase ion mobility, but also to solvate the counterion through some specific interaction, which increase the conducting ion content. In this study, we add plasticizers to polysiloxane-based ionomers that have anions covalently attached to the polymer chain, with Li^+ counterions. Using the 1953 Macdonald model it is possible to separate the conductivity of plasticized ionomers into the number density of conducting ions and their mobility, allowing us to quantify these vital quantities as functions of plasticizer content and temperature.

10:00AM H42.00007 Ionic conductivity of mesoporous block copolymer membranes in liquid electrolyte as a function of copolymer and homopolymer molecular weight[1] , DAVID WONG, SCOTT MULLIN, GREG STONE, University of California, Berkeley, VINCENT BATTAGLIA, Lawrence Berkeley National Labs, NITASH BALSARA, University of California, Berkeley — Mesoporous block copolymer membranes have been synthesized using poly(styrene-block-ethylene-block-polystyrene) (SES). A series of symmetric SES copolymers and PS homopolymers have been studied at different blending fractions. Ionic conductivities of the porous films in a liquid electrolyte, 1.0 M $LiPF_6$ in ethylene carbonate/diethyl carbonate, compare favorably to conventional battery separators and generally increase with internal surface area, as measured by nitrogen adsorption. Characterization of the effects of pore structure and SES morphology on conductivity will be presented.

[1]Support from the U.S. Department of Energy Office of Vehicles Technologies (FCVT) under the Batteries for Advanced Transportation Technologies (BATT) Program

10:12AM H42.00008 Cation/Anion Associations and Transport in Ionic Polymer Membranes , LOUIS MADSEN, JIANBO HOU, ZHIYANG ZHANG, JING LI, Department of Chemistry and Macromolecules and Interfaces Institute, Virginia Tech — Ionic polymer membranes and ionic liquids (ILs) find fruitful applications in a range of ion conduction applications, from electromechanical "artificial muscles" to organic batteries. Various intermolecular interactions determine local structure and dynamics in these ion-dense media. In particular, ion aggregation can drastically affect ion transport, especially since neutral species (dipoles, quadrupoles...) will not be driven by electric fields. We are investigating mixtures of different ILs, ILs with water, and ILs swollen into ionomer membranes, using pulsed-gradient NMR to probe diffusion and electrophoretic mobility. We observe strong dependencies of the cation/anion diffusion coefficient ratio (ranging from 3X to 0.25X) on mixture and membrane properties, which we relate to ion association phenomena. We will further discuss NMR for transport and dynamics studies, especially regarding chemically resolved transport of various mobile species, probing a range of length and time scales, and quantifying ion aggregation.

10:24AM H42.00009 Correlation between cation conduction and ionic morphology in a PEO-based single ion conductor , KAN-JU LIN, JANNA MARANAS, Pennsylvania State University — We use molecular dynamics simulation to study ion transport and backbone mobility of a PEO-based single ion conductor. Ion mobility depends on the chemical structure and the local environment of the ions, which consequently impact ionic conductivity. We characterize the aggregation state of the ions, and assess the role of ion complexes in ionomer dynamics. In addition to solvated cations and pairs, higher order ion clusters are found. Most of the ion clusters are in string-like structure and cross-link two or more different ionomer chains through ionic binding. Ionic crosslinks decrease mobility at the ionic co-monomer; hence the mobility of the adjacent PEO segment is influenced. Na ions show slow mobility when they are inside large clusters. The hopping timescale for Na varies from 20 ns to 200. A correlation is found between Na mobility and the number of hops from one coordination site to another. Besides ether oxygens, Na ions in the ionomer also use the anion and the edge of the cluster as hopping sites. The string-like structure of clusters provide less stable sites at the two ends thus ions are more mobile in those regions. We observed Grotthus like mechanism in our ionomer, in which the positive charge migrates within the string-like cluster without the cations actually moving.

10:36AM H42.00010 Decoupling Between Ionic Conductivity and Segmental Dynamics in Polymers , ALEXANDER AGAPOV, Dept. of Polymer Science, Univ. of Akron and Dept. of Chemistry, Univ. of Tennessee, ALEXEI SOKOLOV, Dept. of Chemistry, Univ. of Tennessee and Chemical Sciences Division, ORNL — The idea of solid polymer-based electrolytes (SPE) with high ionic conductivity at room temperature is known in scientific community for more than three decades. The interest is caused by unique advantages these materials may offer: mechanical flexibility, high power density, enhanced environmental and operational safety, etc. However, even after several decades of studies, the main challenge remains – there is no "dry" SPE with conductivity of $\approx 10^{-2} - 10^{-3}$ S/cm at room temperature. Ionic conductivity is controlled by two parameters, number of ions and their diffusion. Traditional views relate the diffusion of ions in a polymer to the segmental relaxation. Thus, when segmental dynamics freeze the ion motion halts, leading to low conductivity in solid state. A very good example of a material with such behavior is poly(ethylene oxide). In this work we demonstrate that the temperature dependence of ionic conductivity and segmental relaxation can be decoupled in a material specific way. Degree of the observed decoupling exhibits strong correlation with the steepness of the temperature dependence of structural relaxation (fragility). We predict that more fragile materials can have higher ionic conductivity in the solid state than the strong polymers (e.g. PEO).

10:48AM H42.00011 Molecular dynamics simulations of ionic aggregates in a coarse-grained ionomer melt[1] , LISA HALL, MARK STEVENS, AMALIE FRISCHKNECHT, Sandia National Laboratories — Ionomers (polymers with a small fraction of covalently bound ionic groups) have potential application as solid battery electrolytes. Understanding ion transport is essential for such applications. A key question is how molecular properties affect ionic aggregation and counterion dynamics. Recent experimental advances allowed synthesis and extensive characterization of ionomers with a precise spacing of charged groups, which is ideal for comparison with simulations. We use coarse-grained molecular dynamics to simulate ionomers with charged beads placed periodically either in the polymer backbone or pendant to the backbone. The polymers, along with counterions, are simulated at melt densities. Pendant ions at low dielectric form roughly spherical aggregates with liquidlike interaggregate order, qualitatively different from the aggregate morphology of analogous linear ionomers. The effects of dielectric constant and backbone spacing of charged beads on ionic structure and diffusion will be discussed.

[1]Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration, contract DE-AC04-94AL85000.

Tuesday, March 22, 2011 8:00AM - 11:00AM –

Session H43 DPOLY: Focus Session: Thin Film Block Copolymers II A306/307

8:00AM H43.00001 Polymer Physics Prize Break –

8:36AM H43.00002 Directed self-assembly of Si-containing block copolymer thin films in topographical templates , CAROLINE ROSS, Massachusetts Institute of Technology — Block copolymer films in which one block contains Si are attractive for nanolithographic applications due to the high etch contrast and etch resistance of the Si-rich block. We describe the microphase separation of thin films of such polymers on topographic templates made either by electron-beam writing or by etching of another block copolymer film. The self-assembled morphology is governed by the commensurability between the block copolymer and the template, and both periodic and aperiodic patterns such as meanders and junctions can be directed by appropriate template designs. Different morphologies can be formed in one block copolymer film by sequential solvent anneal steps. Results for directed assembly of diblock copolymers and triblock terpolymers are understood through 3D self consistent field theory modeling.

9:12AM H43.00003 Thermal Manipulation of Block Copolymer Morphology by Focused Laser Spike (FLaSk) Annealing[1] , JONATHAN SINGER, KEVIN GOTRIK, STEVEN KOOI, CAROLINE ROSS, EDWIN THOMAS, Department of Materials Science and Engineering, Massachusetts Institute of Technology — Block copolymer (BCP) thin films have a high potential as a pattern transfer medium for ultra-fine (<10nm) features. We introduce a novel technique for performing rapid local annealing of BCP films by focused laser spike (FLaSk) heating using visible wavelengths. This process may be viewed as imposing a local instantaneous landscape in both block mobilities and interaction parameters corresponding to the temperature profile. By controlling the duration and intensity of the dose, either the rapid local perfection of the equilibrium microdomain morphology or the controlled incorporation of metastable architectures is possible. Moreover, the ultra-short FLaSk process can limit polymer degradation, allowing faster microdomain manipulation by enabling higher temperature anneals. Utilization of a direct write stage allows for deliberate control of arbitrary thermal patterns and subsequent BCP ordering, with line width near the diffraction limit. FLaSk can be applied to nearly any BCP system and performed with other ordering techniques. Direct write experiments were combined with thermal finite elements simulations to probe the various material and process parameters necessary to enhance control of spherical and cylindrical BCPs and address challenges such as the use of thicker films.

[1]This research was supported in part by ARO contract W911NF-07-D-0004. JS was supported by the DOD through the NDSEG Program.

9:24AM H43.00004 Tunable Cosolvent Annealing Affects on Block Copolymer Morphology , KEVIN GOTRIK, JEONG GON SON, ADAM HANNON, ALFREDO ALEXANDER-KATZ, CAROLINE ROSS, Massachusetts Institute of Technology — Being able to precisely and reproducibly control block copolymer (BCP) morphology is of interest for lithographic applications due to the techniques ability to result in feature sizes ranging from 10-100nm. We explore the morphological phase behavior that thin films (30-40nm) of poly(styrene-b-dimethylsiloxane) (PS-PDMS, 45kg/mol, ∼0.26 segmental Flory-Huggins interaction parameter) exhibit under different cosolvent vapors of toluene and heptane. Variation in the solvent conditions results in selective swelling of the different blocks of the copolymer depending on relative Hildebrand solubility parameters (e.g. PS- 18.5, toluene-18.3 $(MPa)^{1/2}$) resulting in cylinders, spheres, lamella, and perforatted lamella self-assembled features which can be revealed by selectively etching the PS with an oxygen plasma (50W CF4). Here we describe precision solvent vapor control while doing in situ spectral reflectometry (230-1500nm) to track swelling of the BCP films as a function of time to gain insight into this BCP system.

9:36AM H43.00005 Annealing Techniques for Obtaining Ordered Morphologies in Poly(methacrylic acid)-Poly(methyl methacrylate) Diblock Copolymer Thin Films , YAN SUN, KEVIN HENDERSON, Northwestern University, ZHANG JIANG, JOSEPH STRZALKA, JIN WANG, Argonne National Laboratory, KENNETH SHULL, Northwestern University — The microphase separation of block copolymers in thin films continues to be of great value for the fabrication of nanostructured materials. While highly ordered arrays of microdomains can be easily achieved in some block copolymers, proper processing of others are more challenging. Obtaining ordered morphologies in poly(methacrylic acid)-poly(methyl methacrylate) (PMAA-PMMA), a diblock possessing polyelectrolyte functionality, offers unique associative properties and aqueous reaction chemistries otherwise inaccessible by most other block copolymer films. Due to the limited choices of suitable solvents with sufficiently high vapor pressure and the thermal degradation temperature of PMAA being lower than its glass transition temperature, direct solvent and thermal annealing of PMAA-PMMA are not ideal for generating ordered nanostructures. Here, we begin by solvent annealing poly(tert-butyl methacrylate)-poly(methyl methacrylate) (PtBMA-PMMA) films at room temperature. We then thermally anneal the films to convert the PtBMA block to PMAA. We present results from atomic force microscopy (AFM) and grazing-incidence small-angle x-ray scattering (GISAXS) studies.

9:48AM H43.00006 High-Speed Block Copolymer Self-Assembly under Ambient Conditions , DAE UP AHN, YIFU DING, University of Colorado — Self-assembled block copolymer (BC) nanopatterns have critical application impacts on nanotemplates and scaffolds for the fabrication of nanometer scale periodic arrays, nanostructured networks and membranes for fuel cells, and high-density information storage media in computers and related devices. To achieve such application potentials, well-aligned BC nanopatterns should be reliably engineered in a thin film on a variety of functional substrates within a practical time-scale for industrial production. Here, we illustrate an exceedingly high-speed BC self-assembly under ambient conditions, which is not readily achievable in a vacuum. Only in a few seconds, BC nano-cylinders perpendicular to an energetically preferential surface have been spontaneously developed in a thin BC film under air. The time-scale for the BC self-assembly under air is at least 1000 times faster than that under vacuum. However, a micro-scale film instability that seriously impairs BC nanostructures has also rapidly evolved under air prior to the lateral self-organization of BC nano-cylinders. To suppress the evolution of micro-scale film instability and also to enhance the lateral order of BC nano-cylinders, we have imposed geometric confinements during the thermal annealing process of a thin BC film. Consequently, only in a few minutes, we have prepared hexagonally well-aligned BC nano-cylinders perpendicular to the bottom surface of geometric confinements under ambient conditions.

10:00AM H43.00007 Directed self-assembly with density multiplication of block copolymer via controlled solvent annealing , MIKIHITO TAKENAKA, Kyoto University, HIROSHI YOSHIDA, YASUHIKO TADA, Hitachi Ltd., TERUAKI HAYAKAWA, YOSHIHITO ISHIDA, Tokyo Institute of Technology, HIROKAZU HASEGAWA, GO SAKAGUCHI, KINICHIRO YAMAGUCHI, Kyoto University — We report density multiplication of chemically patterned template employing highly segregating polyhedral oligomeric silsesquioxane (POSS) containing block copolymer (PMMA-bPMAPOSS) for extending the technique to smaller dimensions than that attained by PS-b-PMMA. PMMA-b-PMAPOSS which self-assembles into hexagonally closed packed (hcp) array of dots with lattice spacing d=13nm was spin coated on the chemical template with doubled hcp lattice spacing d=26nm, and annealed under controlled CS_2 atmosphere. By tuning the swell ratio of PMMA-b-PMAPOSS, ordered array of dots with d=13nm, which correspond to 3.5Tbit/in^2 was obtained by multiplying pattern density of the chemical template in a factor of 4. This work was supported by New Energy and Industrial Technology Development Organization, Japan.

10:12AM H43.00008 Temperature Gradient effects in Directed Assembly of Block Copolymer Films via Cold Zone Annealing[1] , GURPREET SINGH, MANISH KULKARNI, Department of Polymer Engineering, University of Akron, Ohio 44325, KEVIN YAGER, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY 11973, BRIAN BERRY, Department of Chemistry, University of Arkansas at Little Rock, Little Rock, AR 72204, ALAMGIR KARIM[2], Department of Polymer Engineering, University of Akron, Ohio 44325 — Vertically oriented micro-phases of block copolymers (BCPs) are generally preferable for applications like organic photovoltaic devices and nanoscale lithography. Here we demonstrate a Cold Zone Annealing (CZA) technique that produces a very sharp thermal gradient in contrast to our previous studies that produced well-ordered parallel BCP microphases [1]. Under these conditions, initial experiments on cold zone annealed PS-b-PMMA BCP films, yielded long range vertical orientation order in PMMA cylinders. GISAXS analysis indicates that the vertical morphology is maintained throughout the film thickness. Comparison of the CZA with conventional oven annealed samples show a magnitude of improvement in the ordering of BCP phases.

[1] Berry et al., *Nano Lett.*, **7**, pg 2789 (2007)

[1]Acknowledgement: Work supported by NSF DMR-1006421

[2]Corresponding Author

10:24AM H43.00009 The dynamics of lamellar re-orientation in free-standing diblock copolymer films: flipping the morphology from edge-on to flat-on , ROBERT D. PETERS, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, L8S 4M1 — Many exquisite structures formed by diblock copolymers have been studied rigorously over the past two decades. Using a symmetric polystyrene-poly(methyl methacrylate) diblock copolymer, we prepare thin films on a substrate which form lamellae oriented perpendicular to the film interfaces. These "edge-on" samples are subsequently transferred, by floating onto water, to produce free-standing films with a symmetric boundary condition. Upon annealing these free-standing films, the lamellae switch from edge-on, to "flat-on" such that the domains are oriented parallel to the interface. Using atomic force microscopy, we study the dynamics of pattern formation as lamellae flip from the edge-on to flat-on morphology.

10:36AM H43.00010 New approaches to directing self-assembly and alignment of block copolymer , HANQIONG HU, PAWEL MAJEWSKI, CHINEDUM OSUJI, Yale University, OSUJI LAB TEAM — Directed self-assembly of block copolymers (BCPs) has been explored extensively using a variety of methods to simultaneously develop long-range order and exert orientational control over microphase separated structures. Here we propose two new routes for directing self-assembly in BCPs. First we discuss solvent vapor permeation which is based on pressure driven transport of a solvent vapor through a free-standing film. We demonstrate that alignment of BCP interfaces parallel to the vapor flux may be achieved rapidly in mm-scale thick films of high molecular weight BCP. Secondly, we present the use of electrospray for controlled deposition of block copolymer thin films. We speculate that morphology can be dictated by thermal equilibration in the presence of a pre-existing pattern or substrate template and that the ultra-slow growth afforded by electrospray permits persistence of this pattern beyond the 1 micron scale where conventional surface directed morphologies degenerate.

10:48AM H43.00011 A novel approach to achieve perpendicular long range order alignment in lamella PS-b-PEO system , PARVANEH MOKARIAN- TABARI, Dept of Chemistry, University College Cork; Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College, Ireland, TIMOTHY W. COLLINS, Department of Chemistry, University College Cork, Cork, Ireland, JUSTIN D. HOLMES, MICHAEL A. MORRIS, Dept of Chemistry, University College Cork; Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College, Ireland — Here, we introduce a novel approach for obtaining perpendicular alignment in lamella forming PS-b-PEO system. The vertical alignment of layers in diblock copolymer thin films has great potential for producing nanowires used in nanofabrication of electronic devices. However, due to selective surface interaction of the polymers with the substrate, perpendicular alignment usually requires neutralisation of the surface by means of brushes or making pre-pattern substrates which could be complicated and time consuming. Applying our novel approach named "combinatorial annealing" which consists of two stages of thermal and solvent annealing process, we have successfully created parallel lines (without a brush). After selective etching of one block, the remaining template is pattern transferred to a silicon substrate leading to manufacturing of sub 20 nm silicon nanowires.

Tuesday, March 22, 2011 8:00AM - 11:00AM –

Session H44 DPOLY: Surfaces, Interfaces, and Polymer Thin Films I A309

8:00AM H44.00001 Polymer Physics Prize Break –

8:36AM H44.00002 Diffusion and Filtration Properties of Self-assembled Close-packed Nanocrystal Membranes , JINBO HE, The University of Chicago, XIAO-MIN LIN, Argonne National Laboratory, LELA VUKOVIC, HENRY CHAN, PETR KRAL, University of Illinois at Chicago, HEINRICH JAEGER, The University of Chicago — Small dyes are known to be able to penetrate through randomly packed nanoparticle monolayers, but a detailed understanding of the mechanisms for transport through the interstices between nanoparticles is still lacking. We report on systematic measurements of molecular transport across monolayers of close- packed, 5 nm diameter gold nanocrystals ligated with dodecanethiol. For water we find a filtration coefficient two orders of magnitude larger than for polymer-based nanofiltration membranes, while the self-diffusion coefficient is more than 100x smaller than in films of pure hydrocarbons. As we confirm by molecular dynamics simulations, larger molecules (tested molecular weight range: 200 - 43000) are unable to diffuse through the ligands. Instead, they most likely move through nm-sized regions of reduced ligand density, which are formed by slight variations in the local packing configuration and orientation of neighboring nanocrystals. In this intermediate size range we also find a pronounced dependence of the rejection rate on the molecules' charge. Molecules with cross-section above 2 nm are totally rejected.

8:48AM H44.00003 Diffusion of Small Penetrants in Polybutadienes , AHMED E. ISMAIL, RWTH Aachen University, FLINT PIERCE, GARY S. GREST, Sandia National Laboratories — The diffusion coefficient D in the dilute limit for three different penetrants—oxygen, water, and methanol—in three different conformations of polybutadiene (all cis-1,4, all trans-1,4, and a random copolymer containing 50% trans-1,4, 40% cis- 1,4, and 10% vinyl-1,2 repeat units) has been computed using molecular dynamics simulations for temperatures in the range $T = 300$–$400\,\mathrm{K}$. Simulations runs of 25 and 50 ns made for each of the 45 combinations of penetrant, conformation, and temperature studied. Over this temperature range the density of the all-cis-1,4 conformation is higher than that of the all-trans-1,4 and random copolymer conformations, which are approximately equal. For all three conformations, D for oxygen and water are comparable and larger than that of methanol. However, for a given penetrant, strong differences were observed in the rate of increase of D for the three conformations. We find that the activation barriers for the three penetrants are generally between 20 and 30 kJ/mol, in agreement with experimental results. The magnitude of the activation energy is directly proportional to the size, rather than the mass, of the penetrant molecule. (Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.)

9:00AM H44.00004 Control dispersion of water in thin films of semi-fluorinated polymer/POSS nanocomposites , DILRU RATNAWEERA, DVORA PERAHIA, Clemson University, MANISH DUBEY, JAROSLAW MAJEWSKI, Los Alamos National Laboratory — The permeation and distribution of solvents in polymer nanocomposites is governed by the way the nanoparticles (NP) associate within the matrix polymer. We have previously shown that in thin films interfacial effects affect the distribution of the NP. The current work focuses on the response of a semi-fluorinated random copolymer, Biphenyl Perfluorocyclobutane, and Polyhedral Oligomeric Silsesquioxane (POSS) NP modified with fluorinated or protonated side chains, to presence of D_2O. POSS was introduced either as a free NP or tethered to a polymer chain. We found that the presence of POSS reduces the overall uptake of D_2O. It also changes the distribution of water in the film as well. In the pristine polymer film the water mainly accumulated at the substrate/polymer interface. In the nanocomposite, the water distribution is correlated with the NP distribution, where NP at the air interface minimize water penetration.

9:12AM H44.00005 Water Desorption from Ferroelectric and Dipole-Oriented Polymers , CAROLINA ILIE, LILLIE GHOBRIAL, GREGORY MASLAK, MARK STEWART, MICHAEL EVANS, Dept. of Physics, SUNY Oswego, LUIS G. ROSA, Dept. of Physics and Electronics, University of Puerto-Rico - Humacao, PETER A. DOWBEN, Dept. of Physics and Astronomy, University of Nebraska at Lincoln — Herein we compare the water absorption/ adsorption on three different polymer films: the ferroelectric co-polymer poly(vinylidene fluoride with trifluoroethylene) P(VDF-TrFE), the strongly dipole oriented polymer poly(methyl vinylidene cyanide) (PMVC) [1] and the dipole oriented poly(methyl methacrylate) PMMA. We investigate the dipole-dipole interaction of the water molecule and the ferroelectric/ dipole oriented polymer films and we propose that the dipole interactions may affect the surface chemistry at these polymer surfaces. Surface dipoles can affect the binding site of water species adsorbed at the surface and sterically hinder or enhance desorption of adsorbed and absorbed water.

[1] Dowben, P.A., Rosa, Luis G., Ilie, C.C., *Zeitschrift für Physikalische Chemie* 222 (2008) 755-778.

9:24AM H44.00006 Role of Diffusion in Scaling of Polymer Chain Aggregates Found in Vapor Deposition Polymerization[1] , SAIRAM TANGIRALA[2], DAVID LANDAU[3], The University of Georgia — Linear polymer chain aggregates grown by 1+1D Monte Carlo simulations of vapor deposition polymerization (VDP) were studied. The behavior of chain length distribution $n_s(t)$ as a function of chain length (s) and deposition time (t) was examined for relevant model parameters. The scaling of $n_s(t)$ was found to be sensitive to the ratio $G = D/F$ of deposition rate (F) and free monomer diffusion (D). A systematic approach is presented to isolate the dependence of $n_s(t)$ on t, s, and G. We found power law dependence of $n_s(t)$ on t with exponent $\omega = 1.01 \pm 0.02$ that was invariant with changes in G. For small s and deposition time of $t = 1 \times 10^3$, 5×10^3, and 10×10^3, $n_s(t)$ showed a power-law decrease with s and exponent $\tau = -0.58 \pm 0.02$. We observed a strong influence of G on the rescaled $n_s(t)$ data that prevented the manifestation of unique scaling function for varying G. The dependence of scaling function of $n_s(t)$ on G was found to be a characteristic of VDP and elucidates the sensitivity of polymer chain aggregates to G.

[1]Research supported by NSF
[2]Corresponding author
[3]Ph. D advisor

9:36AM H44.00007 ABSTRACT WITHDRAWN –

9:48AM H44.00008 Structure and dynamics of dense polymer chains in 2D , HENDRIK MEYER, CNRS Institut Ch. Sadron, JOACHIM P WITTMER, ALBERT JOHNER, JORG BASCHNAGEL — Self-avoiding polymers in two-dimensional melts are known to adopt compact and segregated configurations. Compactness does obviously not imply Gaussian chain statistics nor does segregation of chains impose disk-like shapes minimizing the average perimeter length of the chains. Using scaling arguments and molecular dynamics simulations with chain length up to 2048 we show that the chain perimeters are highly irregular and characterized by a fractal line dimension 5/4. This result may be verified experimentally from the power-law scaling of the intrachain form factor in the intermediate wavevector regime in agreement with a generalized Porod law for a compact object of fractal border [1]. The dynamics of dense polymer chains exhibits two interesting features: the incompressibility induces long range correlations in the displacement auto-correlations and a relaxation channel due to friction at the fractal contours of compact sub-segments leads to relaxation faster than a Rouse model would predict [2].

[1] H. Meyer et al Phys. Rev. E 79 050802(R) (2009); J. Chem. Phys. (2010)
[2] J. Wittmer et al. Phys. Rev. Lett 105 (2010) 037802.

10:00AM H44.00009 Dynamic surface tension effects from molecular dynamics simulations , ALEX LUKYANOV, University of Reading — Effects of dynamic surface tension have been studied in a model system using molecular dynamics simulations. The model system has been made of an artificially expanding liquid droplet, with the rate of change of the external surface area being comparable with the gas-liquid interface formation characteristic time, obtained from the estimates of macroscopic theories. The size of the liquid droplet has been chosen to have about 5.000-7,000 identical molecules, each having between 10-20 beads, to obtain well developed and separated the bulk and surface phases. The methodology of surface tension evaluation has been verified against the Laplace Law in a stationary state of the liquid drop. The results of the MD simulations will be discussed in comparison with the estimations obtained from macroscopic experiments on dynamic wetting using a sharp interface formation theory for different chain length of molecules and strength of intermolecular interactions.

10:12AM H44.00010 Hierarchical roughness of sticky and non-sticky superhydrophobic surfaces , MUHAMMAD AKRAM RAZA, STEFAN KOOIJ, AREND VAN SILFHOUT, HAROLD ZANDVLIET, BENE POELSEMA, University of Twente, PHYSICS OF INTERFACES AND NANOMATERIALS TEAM — The importance of superhydrophobic substrates (contact angle $>150^\circ$ with sliding angle $<10^\circ$) in modern technology is undeniable. We present a simple colloidal route to manufacture superstructured arrays with single- and multi-length-scaled roughness to obtain sticky and non-sticky superhydrophobic surfaces. The largest length scale is provided by (multi-)layers of silica spheres (1μm, 500nm and 150nm diameter). Decoration with gold nanoparticles (14nm, 26nm and 47nm) gives rise to a second length scale. To lower the surface energy, gold nanoparticles are functionalized with dodecanethiol and the silica spheres by perfluorooctyltriethoxysilane. The morphology was examined by helium ion microscopy (HIM), while wettability measurements were performed by using the sessile drop method. We conclude that wettability can be controlled by changing the surface chemistry and/or length scales of the structures. To achieve truly non-sticky superhydrophobic surfaces, hierarchical roughness plays a vital role.

10:24AM H44.00011 Alkane Self Assembling , TOMAS CORRALES, MPI-P Mainz, Germany, PIA HOMM, PIERO FERRARI, MARIA JOSE RETAMAL, Pontificia Universidad Catolica de Chile, VALERIA DEL CAMPO, Universidad Tecnica Federico Santa Maria, Chile, ULRICH G. VOLKMANN, Pontificia Universidad Catolica de Chile — Self-assembling of organic molecules has awaken scientific and technological interest. In this work we study the self-assembling process of long chain hydrocarbons, mainly n-dotriacontane (n-C32H66). We dip-coated C32 monolayers onto silicon wafers covered by their native silicon oxide layer (Si(100)/SiO2). Our results show that withdrawing speed affects the coverage and morphology of the C32 films. For slow withdrawing speeds, alkanes formed islands with a dragon-fly shape, while for fast withdrawing alkanes assembled in stripes with widths in the order of microns. When we quantified coverage and morphology versus withdrawing speed, we found an inflection, which we associate with a transition between two film deposition kinetics. These transitions have been previously described by de Gennes [1]. For slow withdrawing, film deposition follows the Langmuir-Blodget process and above a threshold speed, solution on the solid enters a Landau-Levich regime. This work opens the possibility for growing microstructures with nanometric thickness using a very simple method. These organic microstructures could be used as templates or as grids for optical diffraction.
[1] P.G. de Gennes, Colloid & Polymer Sci. 264, 463-465 (1986).

10:36AM H44.00012 A Thermodynamic Treatment of Polymer Thin Film Glasses[1] , RONALD WHITE, JANE LIPSON, Dartmouth College — We have recently developed a mean field equation of state (EOS) approach to model the thermodynamic properties of polymer thin films. The model is analytic and transparent yielding characteristic film properties as a "whole sample" average. We focus on the properties of freestanding thin films and, parameterizing only with bulk data, demonstrate how the EOS leads to predictions of film properties as a function of film thickness under varied thermodynamic conditions. We share some thoughts on how to use this model for the prediction of the thickness-dependent depression of the thin film glass transition temperature.

[1]work supported by the National Science Foundation

10:48AM H44.00013 Non-equilibrium behavior of spin-cast films , KATHERINE THOMAS, University of Cambridge — The behavior of polystyrene films cast from various solvents using an electric field to weakly perturb the free surface of the polymer melt was examined. The effective viscosity and residual stresses of the as-spun films strongly depend on the casting solvent. As-cast films had a substantially reduced viscosity compared to annealed films, with the greatest reduction in films cast from solutions near θ-temperature. The reduced viscosity is explained in terms of non-equilibrium effects from the film formation process; rapid quenching during spin-coating results in a lower entanglement density of chains compared to an equilibrium melt. The difference in films spun from the various solvents is explained by changes in chain conformations in the initial solutions and the vitrification point. The wavelength of the instabilities in as-cast films was higher than expected, indicating a weak stabilizing pressure. This is attributed to frozen-in normal stresses resulting from an asymmetric deformation of the chains due to evaporation of residual solvent after vitrification. The results show the non-equilibrium nature of as-cast polymer films and that processing conditions strongly influence their behavior.

Tuesday, March 22, 2011 8:00AM - 11:00AM –

Session H45 DAMOP: Exotic Quantum Phases in Optical Lattices: FFLO, P-band Physics, and Beyond A310

8:00AM H45.00001 Stable Fulde-Ferrell-Larkin-Ovchinnikov pairing states in 2D and 3D optical lattices[1] , ZI CAI, The department of Physics, Univeristy of California, San Diego, YUPENG WANG, Institute of Physics, Chinese Academy of Sciences, Beijing, P. R. China, CONGJUN WU, The department of Physics, Univeristy of California, San Diego — We present the study of the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) pairing states in the p-orbital bands in both two and three-dimensional optical lattices. Due to the quasi one-dimensional band structure which arises from the unidirectional hopping of the orthogonal p-orbitals, the pairing phase space is not affected by spin imbalance. Furthermore, interactions build up high dimensional phase coherence which stabilizes the FFLO states in 2D and 3D optical lattices in a large parameter regime in phase diagram. These FFLO phases are stable with imposing the inhomogeneous trapping potential. Their entropies are comparable to those of the normal states at finite temperatures.

[1]This work is supported by NSF-DMR0804775

8:12AM H45.00002 Robust Larkin-Ovchinnikov-Fulde-Ferrell phases in a wide class of lattice models[1] , MENG CHENG, University of Maryland, College Park, CHRISTOPHER VARNEY, Georgetown University, KAI SUN, VICTOR GALITSKI, University of Maryland, College Park — We consider BCS pairing of fermions on lattice whose normal state breaks both time-reversal and spatial inversion symmetries. Due to the asymmetric band structure, unusual pairing states exist: Cooper pairs condense at finite momentum, which is known as the Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) state. A one-dimensional lattice model of spinless fermions is studied in detail and two types of FFLO states are found: (1) a FF state with spontaneous supercurrent and (2) a nodeless LO state where the amplitude of order parameter oscillates. This conclusion is obtained via mean-field theory, bosonization, and exact diagonalization. The transition between the two phases can be tuned by the filling. We also find that the FF state is a topological superconductor. We further consider a generalization to two dimensions, where similar physics is realized.

[1]Work supported by DARPA, US-ARO, JQI and JQI-NSF-PFC.

8:24AM H45.00003 Spectral Functions of FFLO states in coupled chains[1] , NANDINI TRIVEDI, KARIM BOUADIM, YEN-LEE LOH, The Ohio State University, VALERY ROUSSEAU, Louisiana State University — Polarized Fermi gases hold the possibility of an exotic and fragile modulated superfluid known as a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state. Quasi-one-dimensional systems of ultracold fermions are the ideal place to look for FFLO physics. Using various methods [1] (including determinant quantum Monte Carlo, stochastic Green function, and Bogoliubov-de Gennes methods), we study the correlation functions and quantum dynamics of polarized Fermi gases in single chains and coupled chains. Our results indicate that fluctuating domain walls lead to spectral weight near the Fermi energy in the spin-resolved density of states, that are a signature of Andreev reflections and fluctuating bound states. We derive bounds for the optimal interchain coupling to maximize the critical temperature of the FFLO state, in order to aid detection of these FFLO states in cold atom experiments [2].

[1] Y.-L. Loh and N. Trivedi, Phys. Rev. Lett. **104**, 165302 (2010).
[2] Y-an. Liao et. al Nature **467**, 567-569 (2010).

[1]ARO, DARPA grant no. W911NF-08-1-0338, and Ohio Supercomputer Center

8:36AM H45.00004 Understanding the Mass-Imbalanced Highly-Polarized Fermi Gases , MICHAEL KOLODRUBETZ, BRYAN CLARK, Princeton University — The phase diagram of spin-polarized single atomic species Fermi gases has been well-studied theoretically and experimentally. However, cold gases containing multiple atomic species open up the possibility of seeing more exotic states. Recent variational calculations (arXiv:1002.0101v2 [cond-mat.quant-gas]) suggest a complicated phase diagram for a light impurity interacting via a short-range potential with a sea of heavier fermions. In particular, at large mass ratio the polaron is expected to give way to more complicated many-body bound states, such as the trimer or the FFLO molecule. We extend these results beyond this variational ansatz, sampling over many-body states with an arbitrary number of particle-hole pairs. We will discuss the phase diagram resulting from these simulations, including implications for the stability of the trimer and FFLO phases.

8:48AM H45.00005 Spectroscopy of the soliton lattice formation in quasi-one-dimensional fermionic superfluids with population imbalance[1] , ROMAN LUTCHYN, Microsoft Station Q, MAXIM DZERO, Kent State University, VICTOR YAKOVENKO, University of Maryland — Motivated by recent experiments in low-dimensional trapped fermionic superfluids we study quasi-1D superfluid with imbalanced populations between two hyperfine states and analyze its properties using the exact mean field solution for the order parameter. When population imbalance exceeds some critical value the superfluid order parameter develops spatial inhomogeneities and can be described by a soliton lattice formation. Emergence of the soliton lattice is accompanied by the formation of the spin density wave with the majority fermions residing at the points in space where Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) order parameter vanishes. We show that the presence of the spin density wave leads to the formation of the band of the "subgap states," which serves as a hallmark of the quasi-1D FFLO state. We employ the soliton lattice description to discuss the possibilities for the experimental detection of the quasi-1D FFLO phase: elastic and inelastic optical Bragg scattering experiments and radio-frequency spectroscopy. We demonstrate that these measurements allow one to extract necessary information about the inhomogeneous superfluid phase to unambiguously identify quasi-1D FFLO state.

[1]This work was supported by JQI-NSF-PFC and Kent State University

9:00AM H45.00006 $(2k_F, 2k_F)$ density-wave orders of interacting p-orbital fermions in square optical lattice[1] , ZIXU ZHANG, University of Pittsburgh, W. VINCENT LIU, University of Pittsburgh and Kavli Institute for Theoretical Physics, University of California, Santa Barbara — We study instabilities of spinless fermionic atoms in the p- orbital bands in two dimensional optical lattices at non-integer filling against interactions. Stripe charge-density- wave or orbital-density-wave orders are found for attractive and repulsive interactions, respectively. A surprising result is that the superfluid phase, usually expected of attractively interacting fermions, is less energetically favored. Nesting quasi-one-dimensional Fermi surfaces in such systems are independent of filling, which ensures that the stripe density- wave orders occur in a large parameter regime.

[1]This work is supported by ARO (W911NF-07-1-0293) and ARO-DARPA-OLE (W911NF-07-1-0464). We also thank the KITP at UCSB for its hospitality where this research is supported in part by NSF Grant No. PHY05-51164.

9:12AM H45.00007 $U(1) \times Z_2$ transition from the Mott insulator to $p_x + ip_y$ Bose-Einstein superfluid phase , XIAOPENG LI, Department of Physics and Astronomy, University of Pittsburgh, ERHAI ZHAO, Department of Physics and Astronomy, George Mason University, W. VINCENT LIU, Department of Physics and Astronomy, University of Pittsburgh — Motivated by the recent experiment on p-band bosons in optical lattices [arXiv:1006.0509 (2010)], we study theoretically the quantum phases and phase transition of a two-dimensional extended Bose-Hubbard model with p-orbital degrees of freedom. The system features a novel superfluid phase with transversely staggered orbital current at weak interaction, and a Mott insulator phase with antiferro-orbital order at strong coupling and commensurate filling. We derive an effective theory from a microscopic model to describe the quantum phase transition from Mott to superfluid phase. We also calculate the excitation spectra near quantum critical point and find two gapless modes away from the Mott tip but four gapless modes at the tip point. We describe how the phase coherence builds up in the Mott regime when approaching the critical point.

9:24AM H45.00008 Induced p-wave superfluidity at unitarity in strongly imbalanced Fermi gases[1] , KELLY PATTON, DANIEL SHEEHY, Louisiana State University — We compute the induced interaction among the majority spin-up fermions, due to the presence of the minority spin-down fermions, in a population imbalanced Fermi gas. This interaction leads to an instability of the spin-polaron Fermi liquid, favoring a p-wave superfluid. For the majority component, near unitarity, the transition temperature is found to be within experimental reach, of order a few percent of the Fermi energy. As a probe of this phase, the radio-frequency spectroscopic line-shape is calculated for the $p_x + ip_y$ ground state.

[1]Supported by The Louisiana Board of Regents, under grant LEQSF (2008-11)-RD-A-10.

9:36AM H45.00009 Polaron Metastability , KAYVAN SADEGZADEH, University of Cambridge — We investigate the metastability associated with the first order transition from normal to superfluid phases along the BEC-BCS crossover in partially polarised Fermi gases. The momentum thresholds and rates of key decay processes involved are presented in the context of the system's phase diagram, together with metastability regions. In the limit of a single polaron, this region extends from the interaction strength at which a polarised phase of molecules becomes the groundstate ($\frac{1}{k_{F\uparrow}a}0.73$), to the value of the crossing point from a single polaron to molecule groundstate ($\frac{1}{k_{F\uparrow}a}0.9$). Finally, we propose experiments to explore the metastability of this Fermi liquid and the various decay processes, and to observe the $\frac{1}{k_{F\uparrow}a}0.9$ value.

9:48AM H45.00010 Possibility of π-Josephson junction and spontaneous current in a spin-polarized Fermi gas[1] , TAKASHI KASHIMURA, Department of Physics, Keio University, SHUNJI TSUCHIYA, Department of Physics, Tokyo University of Science, JST(CREST), YOJI OHASHI, Department of Physics, Keio University, JST(CREST) — We theoretically propose an idea to realize a π-phase in a superfluid Fermi gas, where the phase of the superfluid order parameter differs by π across a Josephson junction. When a weak nonmagnetic potential barrier is embedded in a superfluid Fermi gas with population imbalance ($N_\uparrow > N_\downarrow$, where N_σ is the number of atoms with pseudospin $\sigma =\uparrow, \downarrow$), this barrier may be $magnetized$ in the sense that some of excess atoms $N_\uparrow - N_\downarrow > 0$ are localized around it. This magnetic barrier behaves like a $ferromagnetic\ junction$ discussed in superconductivity literature, which twists the phase of superfluid order parameter by π. We confirm this idea by solving an attractive Hubbard model within the mean-field theory at $T = 0$. We also show that, when this ferromagnetic barrier is realized in a ring-shaped (or torus) trap, the system becomes the so-called π-Josephson junction, where spontaneous circulating current flows due to the phase twist at the juntion.

[1]This work is supported by the Global COE Program "High-Level Global Cooperation for Leadig-Edge Platform on Access Space (C12)."

10:00AM H45.00011 Many-body spectral moment sum rules for the Bose Hubbard model[1] , JAMES FREERICKS, Georgetown University, VOLODOMYR TURKOWSKI, University of Central Florida, HULIKAL KRISHNAMURTHY, Indian Institute of Science — Exact results for many-body interacting systems are rare. Here we derive a series of exact results for the single-band Bose-Hubbard model. In particular, we derive spectral moment sum rules for the Green's functions of the Bose-Hubbard model. Unlike the fermionic sum rules, the bosonic ones depend on complicated expectation values of the bosons that go beyond just needing to know the local particle density. Nevertheless, they can be used to benchmark the quality of different numerical calculations of spectral functions. These sum rules hold with arbitrary values of the interaction strength and even into nonequilibrium situations, similar to what is seen for the fermionic case. We present some case studies comparing the exact moments to those found with other numerical techniques like the VCA approximation.

[1]Supported under ARO Award W911NF0710576 with funds from the DARPA OLE Program.

10:12AM H45.00012 Bosonic Hubbard-Holstein model and its realization in optical lattices , MAN-HONG YUNG, Harvard University, KUEI SUN, U. of Cincinnati & U. of Illinois at Urbana-Champaign, ALAN ASPURU-GUZIK, Harvard University — The Hubbard-Holstein (HH) model describes the interplay between the Coulomb interaction and the electron-phonon coupling for fermionic systems. Motivated by the recent experimental progresses in optical lattices, we investigate a bosonic version of the HH model, where the two competing many-body interactions of the HH model become a bosonic two-body interaction and a boson-phonon coupling. In the regime of weak boson-phonon coupling, the mean-field phase diagram shows that overall effects of the phonons is to expand the domain of superfluidity. This bosonic Hubbard-Holstein (BHH) model can be realized in a pair of overlapping optical lattices, where bosonic particles trapped in one optical lattice are perturbed by more massive particles trapped in the other lattice.

10:24AM H45.00013 Number Density Distributions of Ultracold Bosons in 3D Optical Lattices[1] , JOE GARRETT, ERIC DUCHON, The Ohio State University, NANDINI TRIVEDI, The Ohio State Univesity — We calculate the probability, $P(n)$, of finding n bosons at a site and the probability of hopping in a uniform optical lattice as a function of the temperature, T, and the repulsive interaction between bosons, U/t, as a function of hopping energy. We examine the characteristic $P(n)$ distribution for the Mott Insulator, quantum critical region and superfluid and determine its behavior across thermal and quantum phase transitions using quantum Monte Carlo. The behavior of the local kinetic energy is estimated using the probability of hopping. These results illuminate number squeezing in the Mott Insulator and the quantum critical region described in [1].

[1] Y. Kato, et al., *Nature Physics* **4**, 617 (2008).

[1]This research was funded by The Ohio State University Physics Department's Harold McMaster Scholarship and ARO grand number W911NF-08-1-0338

10:36AM H45.00014 Surface Majorana modes in ultra-cold fermion systems with unconventional Cooper pairings , YI LI, CONGJUN WU, Department of Physics, University of California, San Diego — The rapid progress of dipolar fermions provides a new opportunity to investigate unconventional Cooper pairings and exotic topological properties. We study the zero energy modes for the single and multiple-component dipolar gases along the surface perpendicular to the z-direction, which are a flat band of Majorana fermions. Under time-reversal symmetry breaking perturbations, such as vortices, the degeneracy of the surface Majorana modes is lifted. We also investigated the spontaneous time-reversal symmetry breaking effect in such systems.

10:48AM H45.00015 Attractive Bose-Hubbard model with three-body constraint[1] , KWAI-KONG NG, MING-FONG YANG, Tunghai University — We numerically study the quantum and thermal phase transitions of the Bose-Hubbard model with particle numbers per site restricted to less than three. The bosons experience on-site attractions while the nearest-neighbor interactions are repulsive. Using particular two-loops algorithm in the QMC simulations, we study the exotic dimer superfluid at small hopping and low density regime. The nature of the phase transitions between the dimer superfluid and the atomic superfluid will be discussed.

[1]This work is supported by the National Center for the theoretical Science and by the NSC (R.O.C.), Grant No. NSC 97-2112- M-029-003-MY3.

Tuesday, March 22, 2011 11:15AM - 1:39PM –

Session J1 DCMP: Toward Single Spin Electronics Ballroom A1

11:15AM J1.00001 Imaging and Manipulating Single and Interacting Spins on Surfaces: Towards Atomic-Scale Spin Devices , ROLAND WIESENDANGER, University of Hamburg — Spin-Polarized Scanning Tunneling Microscopy (SP-STM) provides new insight into spin structures at a length scale and a sensitivity level which are inaccessible by other magnetic-sensitive measurement techniques [1]. The combination of atomic resolution in direct space, single spin sensitivity, and high energy resolution nowadays offers unique possibilities for probing spin-dependent states and interactions in natural or artificially created nanostructures [2]. The ultimate goal has been the combination of spin-resolved imaging with atomic resolution and magnetometry at the single-atom level in order to probe spin states and magnetic interactions of individual adatoms and nanostructures at solid surfaces quantitatively and in a most direct way. This challenging goal has been achieved by operating a SP-STM system at temperatures below 1 Kelvin and in external magnetic fields up to several Tesla. The new method of single-atom magnetometry with an unprecedented degree of magnetization measurement sensitivity is applicable to metallic [3, 4] as well as to semiconducting [5] and molecular systems [6]. The combination of single-atom manipulation techniques and single-atom magnetometry has recently led to the first demonstration of atomic-scale spin logic devices based solely on spin- rather than charge-transport for realizing computation and information transmission at the atomic level.

[1] R. Wiesendanger, Rev. Mod. Phys. 81, 1495 (2009).
[2] D. Serrate, et al., Nature Nanotechnology 5, 350 (2010).
[3] F. Meier, et al., Science 320, 82 (2008).
[4] L. Zhou, et al., Nature Physics 6, 187 (2010).
[5] A. A. Khajetoorians, et al., Nature 467, 1084 (2010).
[6] J. Brede, et al., Phys. Rev. Lett. 105, 047204 (2010).

11:51AM J1.00002 All-electric control of single atom spin states , SANDER OTTE, Delft University of Technology, The Netherlands — The quantum state of a single spin is a great candidate for forming a qubit. Spin systems in various forms are considered for the task, ranging from electrons trapped in artificial quantum dots to magnetic dopants in semiconductors and diamond. In this talk I will review recent progress towards controlling the spins of individual atoms on a surface through local access with an STM probe tip: an intriguing approach in view of the possibility to rearrange the atoms at will so as to build multi-atom structures. Magnetic d-metal atoms, separated from a metal substrate by a thin decoupling layer, are studied through inelastic electron tunneling spectroscopy (IETS): a tool by which transition energies of the spin state can be accurately followed. By addressing the atoms with a spin-filtered probe tip, controlled excitations or de-excitations can be made, effectively pumping the spin into a magnetization direction of choice. In a more recent experiment, spin pumping is performed in short pulses, opening up ways to control atomic spins in the time domain. I will discuss avenues to further develop this technique, eventually leading to coherent control of an atomic spin qubit.

12:27PM J1.00003 Quantum control and nanoscale placement of single spins in diamond[1] , DAVID D. AWSCHALOM[2], Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — Diamond is a unique solid state platform for fundamental studies of spintronics and quantum information science that has recently enabled control, readout, and storage of quantum states at the single spin level. Nitrogen-vacancy (NV) center spins can be individually addressed and have remarkably long spin coherence times at room temperature. We show that the spin of single NV centers in both the orbital ground[3] and excited state[4] can be controlled on sub-nanosecond time scales using intense microwave fields. Moreover, coherent light-matter interactions enable non-destructive spin measurement and localized single spin manipulation with near-resonant light.[5] An associated quantum memory is also demonstrated using the intrinsic nuclear spin of nitrogen.[6] Scaling these findings toward a spin network is a key challenge - to this end we present a simple method for patterning NV center formation on 50 nm length scales.[7] These results represent progress toward control, coupling, and scaling of single spins for future spin and photon based quantum information processing.

[1]Work supported by the AFOSR, ARO, and DARPA.
[2]In collaboration with G.D. Fuchs, B. B. Buckley, D.M. Toyli, P. Klimov, and G. Burkard.
[3]G. D. Fuchs, V. V. Dobrovitski, D. M. Toyli, F. J. Heremans, and D. D. Awschalom, *Science* **326**, 1520 (2009).
[4]G. D. Fuchs, V. V. Dobrovitski, D. M. Toyli, F. J. Heremans, C. D. Weis, T. Schenkel, and D.D. Awschalom, *Nat. Phys.* **6**, 668 (2010).
[5]B. B. Buckley, G. D. Fuchs, L. C. Bassett, and D. D. Awschalom,*Science Express* (DOI: 10.1126/science.1196436)
[6]G. D. Fuchs, G. Burkard, P. Klimov, and D. D. Awschalom, in preparation.
[7]D. M. Toyli, C. D. Weis, G. D. Fuchs, T. Schenkel, and D. D. Awschalom,*NanoLett.* **10**, 3168 (2010).

1:03PM J1.00004 Exploring the quantum frontier of spin dynamics , PATRICK BRUNO, ESRF, Grenoble, France — Our familiar classical concept of a *spin* is that of a system characterized by the *direction* in which the spin is *pointing*. In this picture, we may think of the dynamics of a spin as the motion of a *classical gyroscope*, wich we can aptly describe the spin dynamics as the motion of a point on a sphere. This classical description of the spin dynamics, formalized in the Landau-Lifshits-Gilbert equation, has proved extremely successful in the field micro- and nanomagnetism. However, as the size of the system is further decreased (e.g., when considering molecular magnets such as the Fe_8 or Mn_{12} systems, which have a spin S=10), *quantum* effects such as tunneling, interference, entanglement, coherence, etc., play an essential role, and one must adopt a fully quantum mechanical description of the spin system. The landscape in which the system evolves is then no longer a mere sphere, but rather it is the projective Hilbert space (wich is the projective complex space $\leq \mathrm{P}^{2S}$ for a spin S), as space of considerably greater richness and complexity than the sphere of classical spin dynamics. A very appealing tool to describe a quantum spin system is Majorana's stellar representation, which is the extension for a spin S of the Bloch sphere description of a spin $1/2$. I shall discuss how this representation can help us in improving our understanding of fundamental quantum processes and concept such as Landau-Zener transitions, Rabi oscillations, Berry phase, diabolical points and illustrate this on the example of spin dynamics of molecular magnets.

Tuesday, March 22, 2011 11:15AM - 2:15PM –
Session J2 DCMP: Force Probes of Materials' Structure and Function Ballroom A2

11:15AM J2.00001 Nanoscale Mechanical Resonators for Probing Physical Phenomena: Fluid Dynamics of High-frequency Flows[1] , KAMIL EKINCI, Boston University — With their miniscule sizes, high frequencies, and small force constants, nanoelectromechanical systems (NEMS) resonators are expected to emerge as tools for sensing a variety of analytes, for probing biological entities, and for measuring molecular-scale forces. Because many of these foreseeable applications are in fluids, it is natural to consider the operation of NEMS resonators in fluids. When immersed in a fluid, however, the NEMS resonator loses most of its vibrational energy to the fluid. In other words, the quality factor (Q) of the resonator decreases significantly. Reductions in Q result in a reduction in the resonator's sensitivity to added mass or force. In order to understand the fluid dynamics of NEMS, we have revisited a well-known fluid dynamics problem: Stokes' second problem of the oscillating plate in a fluid. At the typical frequencies of NEMS resonators, Stokes' second problem needs to be reformulated using a relaxation time approach in order to accurately describe the fluidic effects. Our experiments and theory show that the fluid relaxation time in conjunction with the resonator frequency determines the nature of the flow; linear dimension and geometry appear to have weak effects. Our results support a universality in oscillating flows and suggest a deep connection between simple and complex fluids. With this understanding, we are making progress toward reducing NEMS dissipation in water.

[1]Generous support from the US NSF through Grants CBET-0755927, CMMI-0970071 and ECCS-0643178 is acknowledged.

11:51AM J2.00002 Consistency and discrepancy between single molecule force spectroscopy experiments and theoretical models , ROBERT ROS, Department of Physics, Arizona State University, Tempe, AZ 85287-1504 — Single molecule force spectroscopy is a well-established tool to study molecular interactions in a wide range of binding affinities on the single-molecule level. Information about the strength of the molecular bond can be quantified in terms of the dissociation rate k_{off}, and the reaction length x_b (i.e., the distance between potential minimum and maximum along the direction of pulling). The analysis and interpretation of the underlying force-distance curves is still challenging and various models describing the experimental data are under discussion. In this talk, I will present experimental data for a protein-RNA interaction related to posttranscriptional regulation on the single molecule level, and the interaction between DNA bases forming two or three hydrogen bonds. I will use these examples to discuss the advantages and limitations of this technique, and the consistency and discrepancy to theoretical models.

12:27PM J2.00003 Magnetic force microscopy of superconductors: vortex manipulation and measuring the penetration depth , OPHIR AUSLAENDER, Technion - Israel Institute of Technology — We use a low temperature magnetic force microscope (MFM) to image superconductors. The interaction between the magnetic tip and individual vortices allows us to both image vortices and to manipulate them. The manipulation results depend on sample thickness and on the superconducting properties. Here I concentrate on $YBa_2Cu_3O_{6+x}$ (YBCO) samples and on $Ba(Fe_{0.95}Co_{0.05})_2As_2$, an underdoped pnictide. In thin films, if the force exerted by the tip is strong enough to overcome the pinning potential a vortex jumps as a whole to a new pinning site. The behavior in thick YBCO single crystals depends on the doping level. In a slightly overdoped sample vortices stretch rather than jump when we perturb them strongly [1]. The dragging distance in this crystal is anisotropic: it is easier to drag vortices along the Cu-O chains than across them, consistent with the tilt modulus and the pinning potential being weaker along the chains. We also find that when we "wiggle" the top of a vortex we can drag it significantly farther than when we do not, giving rise to a striking dynamic anisotropy between the fast and the slow directions of the scan pattern. In an underdoped YBCO single crystal, where superconductivity is so anisotropic that a vortex should be viewed as a stack of two dimensional pancakes, we show that vortices kink rather than tilt when we perturb them [2]. Since the discovery of the pnictides, a new family of high temperature superconductors, we have also been developing ways to determine the absolute value of the magnetic penetration depth, which is notoriously difficult to measure, as well as its dependence on temperature. For that we either use the Meissner repulsion of the magnetic MFM tip from the sample or the magnetic interaction between the tip and the magnetic field from a vortex. The temperature dependence that we find allows us to comment on the symmetry of the order parameter [3].

Work done in collaboration with Lan Luan and Kathryn A. Moler (Stanford)

[1] O. M. Auslaender et al., Nat. Phys. 5, 35 (2009).
[2] Lan Luan et al., Phys. Rev. B 79, 214530 (2009).
[3] Lan Luan et al., Phys. Rev. B 81, 100501 (2010).

1:03PM J2.00004 Nanoscale Magnetic Resonance Imaging[1] , DANIEL RUGAR, IBM Research Division — Magnetic resonance imaging (MRI), based on the sensitive detection of nuclear spins, enables three dimensional imaging without radiation damage. Conventional MRI techniques achieve spatial resolution that is at best a few micrometers due to sensitivity limitations of conventional inductive detection. The advent of ultrasensitive nanoscale magnetic sensing opens the possibility of extending MRI to the nanometer scale. If this can be pushed far enough, one can envision taking 3D images of individual biomolecules and, perhaps, even solving molecular structures of proteins. In this talk we will discuss issues related to nanoscale magnetic resonance imaging, especially its implementation using magnetic resonance force microscopy (MRFM). We will also consider the future possibility of using NV centers in diamond for detection of nanoMRI.

[1]This work was performed in collaboration with John Mamin, Mark Sherwood, Christian Degen, Martino Poggio and Ginel Hill.

1:39PM J2.00005 Histone Post-Translation Modifications Influence Chromatin Mechanical Stability , MICHAEL POIRIER, Ohio State University — Histone proteins organize the human genome into chromatin fibers while their post-translation modification (PTM) regulates genome replication, expression and repair. The mechanistic connections between histone PTMs and biological functions remain enigmatic. We find with a combination of magnetic tweezers mechanical measurements and biochemical studies that a number of histone PTMs influence the DNA mismatch repair process by mechanically destabilizing chromatin. The location of the PTM within the chromatin structure appears to determine the mechanism by which it alters the mechanical stability. These findings have direct implications for understanding the repair of the human genome.

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J3 DMP DCMP: The Kavli Foundation Special Symposium: Nobelist Perspectives on 100 Years of Superconductivity Ballroom A3

11:15AM J3.00001 Theoretical work on superconductivity up to 1956 , ANTHONY LEGGETT, University of Illinois at Urbana-Champaign — In this talk I survey some of the attempts to understand superconductivity which preceded the 1957 work of Bardeen, Cooper and Schrieffer, and conclude by asking if there are any lessons we can draw for our current efforts to understand apparently "non-BCS" superconductors such as the cuprates and ferropnictides.

11:51AM J3.00002 The Exceptional Properties of Superconductivity in Cuprates , K.A. MUELLER, Physics Institute, University of Zurich, Switzerland — Copper oxides are the only materials that have transition temperatures, T_c, *above* the boiling point of liquid nitrogen, with a maximum T_c^m of 162 K under pressure. Their structure is layered, with one to several CuO_2 planes, and upon hole doping, their transition temperature follows a dome-shaped curve with a maximum at T_c^m. In the underdoped regime, i.e., below T_c^m, a pseudogap T^* is found, with T^* always being larger than T_c, a property unique to the copper oxides [1]. In the superconducting state, Cooper pairs (two holes with antiparallel spins) are formed that exhibit coherence lengths on the order of a lattice distance *in the* CuO_2 plane and one order of magnitude less perpendicular to it. Their macroscopic wave function is parallel to the CuO_2 plane near 100% d at their surface, but only 75% d and 25% s in the bulk, and near 100% s perpendicular to the plane in YBCO. There are two gaps with the same T_c [2]. As function of doping, the oxygen isotope effect is novel and can be quantitatively accounted for by a two-band vibronic theory [3]. These cuprates are intrinsically heterogeneous in a dynamic way. In terms of quasiparticles, bipolarons are present at low doping, and aggregate upon cooling [1], so that probably ramified clusters and/or stripes are formed, leading over to a more Fermi-liquid-type behavior at large carrier concentrations above T_c^m.

[1] For an overview, see: K.A. Müller, J. Phys: Condens.Matter **19**, 251002 (2007).
[2] R. Khasanov, A. Shengelaya *et al.*, Phys. Rev.Lett. **98**, 0570007 (2007).
[3] H. Keller, A. Bussmann-Holder, and K.A. Müller, Materials Today **11**, 38 (2008).

12:27PM J3.00003 Discovery of Superconductive Tunneling , IVAR GIAEVER, Applied BioPhysics, Inc. — Some times unlikely events happens: How can a mechanical engineer from Norway end up with a Nobel Prize in Physics? I had the great fortune to receive the prize in Physics for using electron tunneling to measure the energy gap in superconductors. In this talk I will recollect some of the events that led to this discovery and hopefully be able to convey to you some of the fun and excitement of that area. My great fortune was really to be at the right place at the right time, where I had access to outstanding and helpful physicists. If you become real interested, you may look up the talk at the web site http://nobelprize.org/ .

1:03PM J3.00004 Superconductivity and particle physics , FRANK WILCZEK, MIT — I will briefly review and give a modern perspective on some classic applications of the ideas of superconductivity theory to fundamental particle physics: spontaneous chiral symmetry breaking in vacuum QCD, the Higgs mechanism in electroweak theory, and color superconductivity in dense hadronic matter; and also the confinement problem. Then I will discuss some frontier topics that carry the ideas further and in new directions: supersymmetry and the superHiggs mechanism, exotic quantum statistics of superconducting vortices.

1:39PM J3.00005 Superfluidity in an Atomic Gas of Strongly Interacting Fermions , WOLFGANG KETTERLE, MIT — What is the benefit of realizing superfluidity in a gas a million times more dilute than air? Such systems consist of well-separated atoms which can be observed and manipulated with the control and precision of atomic physics, and which can be treated with first-principles calculations. By implementing scattering resonances, we have realized the strong-coupling limit of the Bardeen Schrieffer-Cooper (BCS) mechanism and observed a normalized transition temperature of 15% of the Fermi temperature, higher than in any superconductor. By tuning the strength of the interactions, the BEC-BCS crossover is realized. When the population of the two spin states is imbalanced, pairing is frustrated; and superfluidity is quenched at the Chandrasekhar-Clogston limit. These studies illustrate a new approach to condensed-matter physics where many-body Hamiltonians are realized in dilute atomic gases.

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J4 DPOLY DBP: Interactions Between Pore Forming Peptides and Membranes Ballroom A4

11:15AM J4.00001 Membrane Disruption Mechanism by Antimicrobial Peptides , KA YEE C. LEE, The University of Chicago — Antimicrobial peptides (AMPs) are a class of small (less than100 residues) host defense peptides that induce selective membrane lytic activity against microbes. To understand the mechanism of membrane disruption by AMPs, we investigated, via atomic force microscopy, topological changes in supported phospholipid bilayers induced by protegrin-1 (PG-1). We have observed that PG-1 induces structural transformations, progressing from fingerlike instabilities at bilayer edges, to the formation of sievelike nanoporous structures and finally to a network of stripelike structures in a zwitterionic dimyristoylphosphatidylcholine (DMPC) model membrane in buffer, with increasing PG-1 concentration. Our results suggest that AMPs act to lower the interfacial energy of the bilayer in a way similar to detergents. By varying the lipid composition, temperature and using AMPs with different secondary structures, we are able to identify factors other than electrostatics that are important for the efficacy of AMPs.

11:51AM J4.00002 Deconstruction of biophysical function in the HIV fusion peptide[1] , DENNIS BONG, The Ohio State University — We have synthesized a library of variants of the 23-residue fusion peptide domain found at the N-terminus of gp-41 glycoprotein of HIV. This sequence is critical for viral infectivity and is thought to be central in the membrane fusion of viral envelope with the host endosomal membrane. There has been extensive discussion in the literature regarding the mechanism by which this viral fusion sequence initiates membrane fusion, with importance placed on glycine-content, particular oligomeric states and secondary structure; both helical and sheet structures have been proposed to be the active fusogenic structure. Our library was designed to address the biophysical importance of secondary structure, peptide flexibility, glycine content and location as well as the nature of the membrane anchor. Each member of this library also bears a positively charged hexapeptide at the C-terminus for solubility and to facilitate binding to negatively charged membranes. We assayed each peptide for its ability to induce lipid-mixing and lysis in both large and giant unilamellar vesicles, and searched for correlations between aggregated peptides and heightened activity. We find that the information encoded in the viral fusion peptide required for may be greatly simplified: glycine is not required for fusion, aggregation is not correlated with activity, and any peptide within a window of hydrophobicity can be an effective fusion catalyst. Given the wide range of sequences which may be effective in catalyzing vesicle membrane fusion, it appears highly unlikely that a particular stably folded secondary structure is important for fusion. Rather, our data show that many flexible, linear, minimally hydrophobic peptides may achieve the biophysical function of fusion.

[1]This research was supported in part by an NSF-CAREER award to D.B.

12:27PM J4.00003 Relation between amino acid sequence and peptide-induced membrane curvature , GERARD WONG, University of California Los Angeles — This abstract not available.

1:03PM J4.00004 Structural Studies of Biological Solids Using NMR , AYYALUSAMY RAMAMOORTHY, Biophysics and Department of Chemistry, The University of Michigan, Ann Arbor, MI 48109-1055 — High-resolution structure and dynamics of biological molecules are important in understanding their function. While studies have been successful in solving the structures of water-soluble biomolecules, it has been proven difficult to determine the structures of membrane proteins and fibril systems. Recent studies have shown that solid-state NMR is a promising technique and could be highly valuable in studying such non-crystalline and non-soluble biosystems. I will present strategies to study the structures of such challenging systems and also about the applications of solid-state NMR to study the modes of membrane-peptide interactions for a better assessment of the prospects of antimicrobial peptides as substitutes to antibiotics in the control of human disease. Our studies on the mechanism of membrane disruption by LL-37 (a human antimicrobial peptide), analogs of the naturally occurring antimicrobial peptide magainin2 extracted from the skin of the African frog Xenopus Laevis, and pardaxin will be presented. Solid-state NMR experiments were used to determine the secondary structure, dynamics and topology of these peptides in lipid bilayers. Similarities and difference in the cell-lysing mechanism, and their dependence on the membrane composition, of these peptides will be discussed. Atomic-level resolution NMR structures of amyloidogenic proteins revealing the misfolding pathway and early intermediates that play key roles in amyloid toxicity will also be presented.

1:39PM J4.00005 How antimicrobial peptides disrupt lipid bilayers? , DURBA SENGUPTA, University of Groningen — The molecular basis for the activity of cyclic and linear antimicrobial peptides is analysed. We performed multi-scale molecular dynamics simulations and biophysical measurements to probe the interaction of antimicrobial peptides with model membranes. Two linear antimicrobial peptides, magainin and melittin and a cyclic one, BPC194 have been studied. We test different models to determine the generic and specific forces that lead to bilayer disruption. We probe whether interfacial stress or local membrane perturbation is more likely to lead to the porated state. We further analyse the reasons that determine specificity and increase of activity in antimicrobial peptides. The results provide detailed insight in the mode of action of antimicrobial peptides.

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J5 CSWP: Hildred Blewett Scholars and their Research followed by Panel Discussion

Ballroom C1

11:15AM J5.00001 M. Hildred Blewett and the Blewett Scholarship , BARBARA WHITTEN, Physics Department, Colorado College — M. Hildred Blewett became a physicist at a time when few women were physicists. After beginning her career at General Electric, she became a respected accelerator physicist, working at Brookhaven, Argonne, and eventually CERN. Blewett was married for a time to John Blewett, another accelerator physicist, but the couple divorced without children and she never remarried. She felt that her career in physics was hampered by her gender, and when she died in 2004 at the age of 93, she left the bulk of her estate to the American Physical Society, to found a Scholarship for women in physics. Since 2005 the Blewett Scholarship has been awarded to women in physics who are returning to physics after a career break, usually for family reasons. Family/career conflicts are one of the most important reasons why young women in early careers leave physics—a loss for them as well as the physics community, which has invested time and money in their training. The Blewett Scholarship is one way for the physics community, under the leadership of CSWP, to help these young women resume their careers. I will discuss the life and work of Hildred Blewett, the Blewett Scholarship, and its benefits to the physics community.

11:27AM J5.00002 Atomically Thin Graphene Hall Cross Devices as Sensitive Magnetic Field Probes , JANICE WYNN GUIKEMA, Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD 21218 — Experimentally realized in 2004, graphene has ignited great interest in physics, material science, chemistry and engineering. Graphene is a one-atom thick sheet of carbon atoms arranged in a hexagonal lattice. This elegantly simple material has excellent electronic and mechanical properties, as well as remarkable physics resulting from its relativistic Dirac electrons. Graphene is a highly promising material for many applications, including sensors. One of my research projects has been investigating graphene for use as a nanoscale magnetic sensor. Such sensors could be used to measure small magnetic particles or as a scanning probe to map out magnetic fields. The Hall cross geometry of the devices gives a noninvasive and straightforward magnetic field probe. I fabricated Hall crosses from mechanically exfoliated single-, bi-, and multi-layer graphene with cross junction widths down to a few hundred nanometers. The devices were tested in a small applied field and the noise spectra of the Hall signal as a function of bias current and back gate voltage was measured at room and cryogenic temperatures. The best field sensitivity at room temperature obtained for a 400 nm graphene Hall cross was 15 $G/Hz^{1/2}$ at 1 Hz and 1 $G/Hz^{1/2}$ at 4 kHz, which is on par with similar crosses made from other materials in the literature. In addition, because they are made from graphene, graphene Hall probes have further advantages such as tunability with a gate, being extremely thin and at the surface, and having mechanical stability for ultra-small device fabrication.

12:03PM J5.00003 When Nano Isn't Small Enough: Lattice Quantum Chromodynamics and My Quest to Understand Particle Physics , ELIZABETH FREELAND, University of Illinois Urbana-Champaign — Although I started my research life as a condensed matter theorist (nanotribology), I now work in the field of high-energy physics. I use effective field theories and Lattice Quantum Chromodynamics (Lattice QCD) to calculate strong-interaction effects in Standard Model processes. I have worked on quark and meson mass calculations, and contributed to decay-process calculations used to probe the weak-interation. After setting the stage for this research, I will briefly describe calculations I have worked on over the past few years and give an introduction to my current research project(s).

12:39PM J5.00004 Lateral Modulation in Antimonide Superlattices[1] , REBECCA FORREST, University of Houston — Lateral modulation is the spontaneous formation of a periodic modulation in structure or alloy composition perpendicular to the growth direction in an epitaxial structure. It has been observed in many epitaxially grown III-V semiconductor alloys, occurring during both the homogenous growth of III-V alloys and in III-V superlattices. In [001] oriented zinc blende structures, lateral modulation typically occurs along one of the [110] directions and is associated with strain and growth kinetics. It begins when strain is relieved through elastic surface undulations, typically in layers much thinner than the critical thickness for dislocation formation. In a superlattice, these undulations can lead to either compositional or purely structural modulation, depending on the relative phase and amplitude of the undulations in the constituent layers. Compositional modulation is by far the most commonly observed form in superlattice structures. We report on the analysis of purely structural lateral modulation in AlSb/AlAs digital superlattices, using x-ray diffraction. This is the first report of lateral modulation in an antimonide superlattice, and a rare observation of purely structural modulation in a superlattice. InAs/Al(In)Sb digital superlattices were also studied, and exhibited no lateral modulation. The composition and strain of the structures and critical thickness for lateral modulation will be discussed.

[1]This research was supported in part by the M. Hildred Blewett Scholarship of the American Physical Society.

1:15PM J5.00005 Panel discussion on the Blewett Scholarship, and how it helps young women achieve career/family balance.[1] , SHERRY YENNELLO, Texas A&M University — This panel discussion will be preceded by talks by three women who have had career interruptions due to family reasons and have restarted their research careers with some assistance from a Blewett Scholarship. They will discuss their experience balancing career and family. Questions from the audience will be encouraged. This session should provide inspiration for young women to pursue their passions and motivation for department chairs to be flexible and accommodating of career/family balance.

[1]The Blewett Scholarship program is administered by CSWP.

Tuesday, March 22, 2011 11:15AM - 1:39PM –

Session J6 DCOMP: The Use of GPUs in Computational Physics

Ballroom C2

11:15AM J6.00001 Fully accelerating quantum Monte Carlo simulations of real materials on GPU clusters[1] , KENNETH ESLER, Stone Ridge Technology — Quantum Monte Carlo (QMC) has proved to be an invaluable tool for predicting the properties of matter from fundamental principles, combining very high accuracy with extreme parallel scalability. By solving the many-body Schrödinger equation through a stochastic projection, it achieves greater accuracy than mean-field methods and better scaling with system size than quantum chemical methods, enabling scientific discovery across a broad spectrum of disciplines. In recent years, graphics processing units (GPUs) have provided a high-performance and low-cost new approach to scientific computing, and GPU-based supercomputers are now among the fastest in the world. The multiple forms of parallelism afforded by QMC algorithms make the method an ideal candidate for acceleration in the many-core paradigm. We present the results of porting the QMCPACK code to run on GPU clusters using the NVIDIA CUDA platform. Using mixed precision on GPUs and MPI for intercommunication, we observe typical full-application speedups of approximately 10x to 15x relative to quad-core CPUs alone, while reproducing the double-precision CPU results within statistical error.[2] We discuss the algorithm modifications necessary to achieve good performance on this heterogeneous architecture and present the results of applying our code to molecules and bulk materials.[3]

[1]Supported by the U.S. DOE under Contract No. DOE-DE-FG05-08OR23336 and by the NSF under No. 0904572.

[2]K. Esler, J. Kim, L. Shulenburger, D. Ceperley, "Fully accelerating quantum Monte Carlo simulations of real materials on GPU clusters", Computing in Science and Engineering (*preprint*) DOI: 10.1109/MCSE.2010.122 (2010).

[3]K.P. Esler, R.E. Cohen, B. Militzer, Jeongnim Kim, R.J. Needs, and M.D. Towler, "Fundamental High-Pressure Calibration from All-Electron Quantum Monte Carlo Calculations", Phys. Rev. Lett. **104**, 185702 (2010).

11:51AM J6.00002 The Use of GPUs in Lattice Gauge Theory , STEVEN GOTTLIEB, Indiana University — In the past few years, GPUs have been put to use in lattice gauge theory calculations. This talk will consider the successes and challenges of this approach including such issues as how to take advantage of multiple threads, the effort involved in porting, the resulting performance and the challenge of writing multi-GPU code that scales well.

12:27PM J6.00003 Wavelet-Based DFT calculations on Massively Parallel Hybrid Architectures , LUIGI GENOVESE, CEA Grenoble — In this contribution, we present an implementation of a full DFT code that can run on massively parallel hybrid CPU-GPU clusters. Our implementation is based on modern GPU architectures which support double-precision floating-point numbers. This DFT code, named BigDFT, is delivered within the GNU-GPL license either in a stand-alone version or integrated in the ABINIT software package. Hybrid BigDFT routines were initially ported with NVidia's CUDA language, and recently more functionalities have been added with new routines writeen within Kronos' OpenCL standard. The formalism of this code is based on Daubechies wavelets, which is a systematic real-space based basis set. As we will see in the presentation, the properties of this basis set are well suited for an extension on a GPU-accelerated environment. In addition to focusing on the implementation of the operators of the BigDFT code, this presentation also relies of the usage of the GPU resources in a complex code with different kinds of operations. A discussion on the interest of present and expected performances of Hybrid architectures computation in the framework of electronic structure calculations is also adressed.

1:03PM J6.00004 Graphical Processing Units for Quantum Chemistry , TODD MARTINEZ, Stanford University — This abstract not available.

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J7 GSNP: The Dynamics of Co-Evolving and Interdependent Networks Ballroom C3

11:15AM J7.00001 Robustness of Interdependent Networks , SHLOMO HAVLIN, Bar-Ilan University — In interdependent networks, when nodes in one network fail, they cause dependent nodes in other networks to also fail. This may happen recursively and can lead to a cascade of failures. In fact, a failure of a very small fraction of nodes in one network may lead to the complete fragmentation of a system of many interdependent networks. We will present a framework for understanding the robustness of interacting networks subject to such cascading failures and provide a basic analytic approach that may be useful in future studies. We present exact analytical solutions for the critical fraction of nodes that upon removal will lead to a failure cascade and to a complete fragmentation of two interdependent networks in a first order transition [1]. Surprisingly, analyzing complex systems as a set of interdependent networks may alter a basic assumption that network theory has relied on: while for a single network a broader degree distribution of the network nodes results in the network being more robust to random failures, for interdependent networks, the broader the distribution is, the more vulnerable the networks become to random failure. We also show [2] that reducing the coupling between the networks leads to a change from a first order percolation phase transition to a second order percolation transition at a critical point. These findings pose a significant challenge to the future design of robust networks that need to consider the unique properties of interdependent networks.

[1] S. Buldyrev, R. Parshani, G. Paul, H.E. Stanley, S. Havlin, Nature, 465, 0893 (2010)
[2] R. Parshani, S. Buldyrev, S. Havlin, PRL, 105, 048701 (2010)

11:51AM J7.00002 Interconnected Financial Networks , GUIDO CALDARELLI, Institute of Complex Systems, CNR, Rome Italy — It is known that different dynamics on a network are associated to different resilient structures. In particular in the case of financial networks the fragility is associated to the kind of relation between the vertices (financial agents). Since the same agents can be connected on different networks for different financial relations, a study on the global resilience can only be obtained by considering the whole structure. Here we present our activity on this topic.

12:27PM J7.00003 Emergent phenomena in interacting networks , RAISSA DSOUZA, University of California, Davis — This abstract not available.

1:03PM J7.00004 Dynamical network approach for social interactions , GINESTRA BIANCONI, Northeastern University — This abstract not available.

1:39PM J7.00005 The Structure and Dynamics of Economic Complexity , CESAR A. HIDALGO, Massachusetts Institute of Technology — Can network science help us understand the structure and evolution of the global economy? In this talk I summarize recent research that uses networks and complexity science to describe and explain the evolution of the mix of products that countries, and cities, produce and export. First, I show how to use information on the network connecting industries to locations to measure the complexity of an economy. Using these measures I demonstrate that countries tend to approach a level of income that is dictated by the complexity of their economies. Next, I study the evolution of economic complexity by showing that it is constrained by a coordination problem that countries, and cities, deal with using three different channels: First, they move to products that are close by, in the Product Space, to the products that they already do. Second, they are more likely to develop a product if a geographical neighbor has already developed it. And third, they follow the nestedness of the network connecting industries to locations. Finally, I introduce a simple model to account for the stylized facts uncovered in the previous sections.

Tuesday, March 22, 2011 11:15AM - 2:15PM –
Session J8 FEd: Physics Education Research in Upper-division Physics Courses Ballroom C4

11:15AM J8.00001 Using research to enhance student learning in intermediate mechanics , BRADLEY AMBROSE, Grand Valley State University — For many undergraduate physics majors the sophomore/junior level course in intermediate mechanics represents their first step beyond the introductory sequence. Over the past several years research has shown that intermediate mechanics students often encounter conceptual and reasoning difficulties similar to those that arise at the introductory level. Many difficulties suggest deeply-seated alternate conceptions, while others suggest loosely or spontaneously connected intuitions. Furthermore, students often do not connect the physics to the more sophisticated mathematics they are expected to use. This presentation will highlight results from research conducted at Grand Valley State University, the University of Maine (by co-PI Michael Wittmann) and pilot sites in the *Intermediate Mechanics Tutorials* project. These results, taken from the analysis of pretests (ungraded quizzes), written exams, and classroom observations, will illustrate specific student difficulties as well as examples of guided-inquiry teaching strategies that appear to address these difficulties. (Supported by NSF grants DUE-0441426 and DUE-0442388.)

11:51AM J8.00002 A Research-Based Approach to Transforming Upper-Division Electricity & Magnetism[1] , STEVEN POLLOCK[2], CU Boulder — We present research on transforming an upper-division undergraduate electricity and magnetism course using principles of active engagement and learning theory. We build on a systematic investigation of student learning difficulties, with the goal of developing useful curricular materials and suggestions for effective teaching practices. We observe students in classroom, help-session, and interview settings, and analyze their written work. To assess student learning, we have developed and validated a conceptual instrument, the CUE (Colorado Upper-division Electrostatics) diagnostic. We collaborate with faculty to establish learning goals, and have constructed a bank of clicker questions, tutorials, homeworks, and classroom activities. We find that students in the transformed courses exhibit improved performance over the traditional course, as assessed by common exam questions and the CUE, but there is still much work to be done. Our work underlines the need for further research on the nature of student learning and appropriate instructional interventions at the upper division.

[1]Research supported by NSF DUE-0737118 , and the Colorado Science Education Initiative.
[2]Co-authors Katherine Perkins, Stephanie V. Chasteen, Rachel Pepper

12:27PM J8.00003 Investigating student understanding in an upper-division analog electronics course[1] , MACKENZIE R. STETZER, University of Washington — The Physics Education Group at the University of Washington has recently begun an in-depth investigation of student understanding of analog electronics. As part of this investigation, we have been examining student learning in an upper-division laboratory course on this subject. In particular, we have administered written questions on fundamental electric circuits concepts (typically covered in introductory physics courses) and on canonical topics in analog electronics (e.g., filters, diodes, transistors, and operational amplifiers). Drawing on the results from such questions, we are investigating the impact of the analog electronics course on student conceptual understanding. Specific examples will be used to illustrate how the findings from this investigation have implications for instruction in both introductory and upper-division courses.

[1]This work has been supported in part by the National Science Foundation under Grant No. DUE-0618185.

1:03PM J8.00004 Research on Student Learning of Upper-Level Thermal and Statistical Physics[1] , JOHN THOMPSON, University of Maine — Within the last decade, physics education researchers have begun to extend the tools and methods used at the introductory level to conduct systematic investigations of student learning of thermal and statistical physics in the upper division. Most research in thermodynamics has focused on student ideas about the first and second laws and the associated concepts (e.g., work, heat, entropy). Several studies yield insights about broader ideas, such as state functions. Research in statistical physics has focused on the concepts underlying multiplicity and related ideas in probability. Research has identified a number of conceptual difficulties with varied degrees of persistence, some of which are consistent with findings at the introductory level. Some investigations further probe connections between physics and relevant mathematics concepts in these areas, including student interpretation of canonical representations such as pressure-volume (P-V) diagrams. Results from research are guiding the development of curricular materials in order to address several known difficulties.

[1]Supported in part by NSF Grants DUE-0817282 and DUE-0837214.

1:39PM J8.00005 Improving students' understanding of quantum mechanics[1] , CHANDRALEKHA SINGH, University of Pittsburgh — Learning quantum mechanics is especially challenging, in part due to the abstract nature of the subject. We have been conducting investigations of the difficulties that students have in learning quantum mechanics. To help improve student understanding of quantum concepts, we are developing quantum interactive learning tutorials (QuILTs) as well as tools for peer-instruction. The goal of QuILTs and peer-instruction tools is to actively engage students in the learning process and to help them build links between the formalism and the conceptual aspects of quantum physics without compromising the technical content. They focus on helping students integrate qualitative and quantitative understanding, confront and resolve their misconceptions and difficulties, and discriminate between concepts that are often confused. In this talk, I will give examples from my research in physics education of how students' prior knowledge relevant for quantum mechanics can be assessed, and how learning tools can be designed to help students develop a robust knowledge structure and critical thinking skills.

[1]Supported by the National Science Foundation.

Tuesday, March 22, 2011 11:15AM - 2:15PM –
Session J9 DFD: Liquid Crystals: Nematics, Lyotropics and Vesicles D220

11:15AM J9.00001 Dynamics of chiral liquid-crystal films driven by water transport[1] , JONATHAN V. SELINGER, LENA M. LOPATINA, Liquid Crystal Institute, Kent State University — In previous experimental and theoretical research, Tabe and Yokoyama investigated Langmuir monolayers of chiral molecules on the surface of water, and found that evaporation of water induces collective precession of the molecular orientation [1]. More recently, they have found a similar effect in freely suspended films of chiral smectic liquid crystals, but with one new feature: the molecular rotation is accompanied by large- scale flow of the molecules, indicating a strong coupling between orientation and flow. To model the coupled rotation and flow driven by water transport, we construct the Lagrangian and Rayleigh dissipation function appropriate for a film in the smectic-A or smectic-C phase, derive the equations of motion, and solve these equations in geometries corresponding to the experiments. In particular, we calculate the flow patterns in terms of the viscosity coefficients of the liquid-crystal films, in order to understand the mechanisms that control this dynamic behavior. The theoretical predictions are compared with experimental results, and with related work on granular materials [2].

[1] Y. Tabe and H. Yokoyama, Nature Mat. 2, 806 (2003).
[2] J.-C. Tsai, F. Ye, J. Rodriguez, J. P. Gollub, and T. C. Lubensky, Phys. Rev. Lett. 94, 214301 (2005).

[1]This work was supported by NSF Grant DMR-0605889.

11:27AM J9.00002 Linear aggregation and liquid-crystalline order: comparison of Monte Carlo simulation and analytic theory , TATIANA KURIABOVA, University of Colorado, M.D. BETTERTON, MATTHEW A. GLASER, University of Colorado at Boulder — Many soft-matter and biophysical systems are composed of monomers that reversibly assemble into rod-like aggregates. The aggregates can then order into liquid-crystal phases if the density is high enough, and liquid-crystal ordering promotes increased growth of aggregates. Systems that display coupled aggregation and liquid-crystal ordering include wormlike micelles, chromonic liquid crystals, DNA and RNA, and protein polymers and fibrils. Coarse-grained molecular models that capture key features of coupled aggregation and liquid-crystal ordering common to many different systems are lacking; in particular, the roles of monomer aspect ratio and aggregate flexibility are not well understood. We study a system of sticky cylinders that interact primarily by hard-core interactions but can stack and bind end to end. We use Monte Carlo simulations and analytic theory. We present results for several different cylinder aspect ratios and a range of end-to-end binding energies. The phase diagrams are qualitatively similar to those of chromonic liquid crystals, with an isotropic-nematic-columnar triple point. Our analytic theory shows improvement compared to previous theory in quantitatively predicting the I–N transition for relatively stiff aggregates, but requires a better treatment of aggregate flexibility.

11:39AM J9.00003 Modeling the Kerr effect in polymer-disordered liquid crystals[1] , LENA M. LOPATINA, JONATHAN V. SELINGER, Liquid Crystal Institute, Kent State University — In the Kerr effect, an electric field applied to an optically isotropic material induces orientational order and hence induces optical birefringence. Recently, many investigators have used the Kerr effect to develop liquid-crystal displays and other electro-optic devices that can operate at high speed and with no need for aligning substrates. This application requires a large and fairly temperature-independent Kerr coefficient. One approach to achieve this goal is by using liquid-crystal blue phases, perhaps with polymer stabilization. As an alternative approach, D.-K. Yang has suggested using a nematic phase within a disordered polymer network. This structure would be disordered and optically isotropic in the absence of a field, but it would develop order and birefringence under an applied field. To assess this approach, we perform Monte Carlo simulations of a nematic liquid crystal in a disordered polymer network, and calculate the response to an applied field. We compare the results with analytic studies of liquid crystals under quenched disorder and with experiments.

[1]This work was supported by NSF Grant DMR-0605889.

11:51AM J9.00004 A nonlocal model of inhomogeneous nematic liquid crystals , PETER PALFFY-MUHORAY, Liquid Crystal Institute - KSU, XIAOYU ZHENG, Dept. of Mathematical Sciences - KSU, ROLAND ENNIS, Pressco Technology Inc. Cleveland, OH — The free energy cost of spatial inhomogeneities in nematic liquid crystals is usually described in terms of gradients of the director field or of the order parameter tensor. The origins of such gradient expansions are not clear; they can also lead to ill-posedness of the variational problem of minimizing the free energy. We propose a simple nonlocal form of the single particle potential from which the free energy may be constructed. Our model reduces to the Maier-Saupe form for homogenous systems, but describes inhomogenous systems in general. We demonstrate the validity of the model by using it to describe the electric field induced Freedericksz transition. We discuss the connection between our non-local model and gradient expansions.

12:03PM J9.00005 Freely Suspended Nematic Films[1] , WILDER IGLESIAS, JEFFREY CHOI, ELIZABETH K. MANN, ANTAL JAKLI, Kent State University — Using one of the most commonly studied synthetic molecule, 4-Cyano-4'-pentylbiphenyl (5CB), we were able to pull freely suspended membranes of different thicknesses into circular frames of up to 20mm diameter. Films pulled this way were distorted using a speaker, while a laser light was shone onto them for studying the far field reflection and learn about resonant frequency modes and subtract valuable information about the viscoelastic terms that hold the membrane stable.

[1]This work was supported by NFS, grant 0907055.

12:15PM J9.00006 Fluctuation Modes of a Bent-Core Nematic Liquid Crystal[1] , MADHABI MAJUMDAR, S. CHAKRABORTY, B. SENYUK, O.D. LAVRENTOVICH, JAMES T. GLEESON, ANTAL JAKLI, SAMUEL SPRUNT, Kent State University — We present a dynamic light scattering study of the bent-core nematic liquid crystal compound *DT6Py6E6*. We utilize a "dark" scattering geometry, which allows us to search for fluctuation modes that are not purely associated with the uniaxial director. Indeed, we observe two modes (hydrodynamic and non-hydrodynamic) in addition to the expected twist-bend director mode. We present a model for the additional modes based on fluctuations of the biaxial order parameter, which leads to an estimate of 10-100 nm for the correlation length associated with these fluctuations.

[1]Acknowledgement: DOE DE-SC0001412 and NSF DMR-0606160.

12:27PM J9.00007 Three dielectric constants and orientation order parameters in nematic mesophases[1] , HYUNG GUEN YOON, SEUNG YEON JEONG, SATYENDRA KUMAR, Kent State University, MIN SANG PARK, JUNG OK PARK, M. SRINIVASARAO, Georgia Instittue of Technology, SUNG TAE SHIN, LCD R&D Center, Samsung Electronics Corp. — Temperature dependence of the three components ε_1, ε_2, and ε_3 of dielectric constant and orientation order parameters in the nematic phase of mesogens with rod, banana, and zero-order dendritic shape were measured using the in-plane and vertical switching geometries, and micro-Raman technique. Results on the well-known uniaxial (N_u) nematogens, E7 and 5CB, revealed two components $\varepsilon_1 = \varepsilon_{||}$ and $\varepsilon_2 = \varepsilon_3 = \varepsilon_\perp$, as expected. The three dielectric constants were different for two azo substituted (A131 and A103) and an oxadiazole based (ODBP-Ph-C12) bent core mesogens, and a Ge core tetrapode. In some cases, two of the components became the same indicating a loss of biaxiality at temperatures coinciding with the previously reported N_u to biaxial nematic transition. This interpretation is substantiated by micro-Raman measurements of the uniaxial and biaxial nematic order parameters.

[1]Supported by the US Department of Energy, Basic Energy Sciences grant ER46572 and by Samsung Electronics Corporation.

12:39PM J9.00008 The interplay between fluctuations in physical structure and power consumption in electroconvecting liquid crystals , JOHN CRESSMAN, ZRINKA GREGURIC, TYRUS BERRY, TIMOTHY SAUER, George Mason University — We will present results from experiments performed on the nematic liquid crystal MBBA. We have made simultaneous measurements of the optical patterns formed in the weakly-driven electroconvective state, as well as the electrical power consumed by the sample. By performing a dimensionality reduction on the optical data we identify the dominant modes in the system and go on to elucidate the role of these modes in the measured power fluctuations. We will conclude by discussing these results in the context of the free energy derived by de Gennes for nematic liquid crystals.

12:51PM J9.00009 Magneto-optical technique for detecting biaxial nematic phase[1] , TANYA OSTAPENKO, J.T. GLEESON, S.N. SPRUNT, A. JAKLI, Kent State University — There have been numerous attempts to find a thermotropic liquid crystal that exhibits a biaxial phase. There have been findings of biaxial order in bent-core nematic liquid crystals; however, there are recent reports that call this into question. One reason for this discrepancy is the difficulty in unambiguously identifying the biaxiality. Based on a previously described electro-optical technique, we have developed a technique that uses magnetic field, thus widening its application to any bent-core nematic material. The field orients the uniaxial director along the optical path length, and we search for birefringence perpendicular to this direction. We expect one of two situations to occur: if the material is uniaxial, the induced phase difference will decrease asymptotically to zero as the field increases. However, if the material is biaxial, the induced phase will extrapolate to a non-zero value. Results on one calamitic liquid crystal show that this method yields the expected result, namely the lack of biaxial nematic phase. We also tested several bent-core nematic liquid crystals and found that none of these materials exhibits a biaxial nematic phase.

[1]This work was supported by the NSF (DMR-0606160). Work performed at NHMFL supported by the NSF, the State of Florida and the DOE.

1:03PM J9.00010 Nonlinear electrophoresis in nematics: Flows and effects of salts , ISRAEL LAZO-MARTINEZ, OLEG D. LAVRENTOVICH, Liquid Crystal Institute and Chemical Physics Interdisciplinary Program, Kent State University — Electrophoresis (EP) in a nematic liquid crystal (LC) is dramatically different from its isotropic counterpart, as the EP velocity has a component that is quadratic in the applied electric field [1]. Unlike the regular EP velocity that is linear in the field, this component does not vanish in an ac field with a zero time average, which makes the LC EP attractive for applications where the steady flows are needed. EP propulsion is caused by distortion of the LC orientation around the particles that break the fore-aft (or left-right) symmetry, leading towards an imbalance of field-induced flows around the particles. We visualize the flows and measure the EP velocity by recording 3D trajectories of passive tracers suspended in the LC under the fluorescent confocal polarizing microscope. We demonstrate that doping the LC with organic salts increases the EP velocities. The work was supported by NSF DMR 0906751.

[1] O. D. Lavrentovich, I. Lazo, O. P. Pishnyak, Nature 467, 947-950 (2010).

1:15PM J9.00011 Anisotropic Stokes Drag and Dynamic Lift on Cylindrical Colloids in a Nematic Liquid Crystal , JOEL ROVNER, CLAYTON LAPOINTE, DANIEL REICH, ROBERT LEHENY, Johns Hopkins University — Unlike isotropic fluids, nematic liquid crystals exhibit a complex assortment of hydrodynamic properties that can strongly depend on the director field and local boundary conditions set by inclusions. To understand further these characteristics, measurements were taken of the Stokes drag on magnetic nanowires suspended in nematic 4-cyano-4'-pentylbiphenyl (5CB). Effective drag viscosities for wires moving perpendicular and parallel to the nematic director were measured and were found to differ by factors of approximately 0.88 to 2.4, depending on the wire orientation and surface anchoring. Additionally, a lift force was observed when wires were forced at an oblique angle to the director resulting in motion divergent from the line of force. The lift was greater for wires with homeotropic anchoring and smaller for wires with longitudinal anchoring, suggesting that the lift force can act as a mechanism for sorting colloidal particles according to their surface chemistry.

1:27PM J9.00012 Morphology and Rheology of the Liquid Crystal-Colloid Composites , LU ZOU, CHANJOONG KIM, Liquid Crystal Institue, Kent State University — Liquid crystal (LC)-colloid composites form aggregates and are arrested in various network structures. We study viscoelastic properties and three-dimensional structure of nematic LC-colloid composites using fluorescence confocal polarized rheoscope and fluorescence microscope. We observe various morphological transformations of the composites when we cool them down below T_{NI} from the high temperature isotropic phase. We find that colloidal particles are self-organized to ferny structures, and that the morphological characteristics of the ferny structures depend on the applied shear rates, the cooling rate, the particle volume fraction and the particle size. This study may offer a new route to form novel colloidal structures using anisotopic fluid, which could not be obtained from isotropic suspensions.

1:39PM J9.00013 Structural Reorganization of Liquid Crystals Revealled by Fast Scanning Calorimeter[1] , DONGSHAN ZHOU, JING JIANG, XIAOLIANG WANG, GI XUE, Nanjing University — Liquid crystal glass of 4-Cyano-4'-octylbiphenyl is obtained by rapid cooling with rates over 2000 Kelvin per second (K/s) on the chip calorimeter. The glass can crystallize easily upon heated above its glass transition temperature. Depending on the prior cooling rate and annealing history thereafter, melting-structural reorganization-remelting behavior similar to that of semicrystalline polymer can be observed during subsequent heating. The complex melting behavior is attributed to the transformation of metastable crystal forms formed during annealing or heating induced cold crystallization. Increasing the heating rate (>15000 K/s) can suppress the transformation and, additionally, enables us to capture the multiple N-I transition. This implies the coexistence of two different types of nematic states. To avoid above complex structural reorganization, one can anneal the sample at 260K for 2 seconds to get the stable crystal form.

[1]The work is financially supported by the National Science Foundation of China (NSFC: 20504014, 20874045, 50533020, 20774041) and National Basic Research Program of China, No 2007CB925101.

1:51PM J9.00014 Parity breaking in nematic tactoids of lyotropic chromonic liquid crystals[1] , LUANA TORTORA, OLEG D. LAVRENTOVICH, Liquid Crystal Institute, Kent State University — In many colloidal systems, an orientationally ordered nematic phase emerges from the isotropic melt in the form of spindle-like birefringent tactoids. In cases studied so far, the tactoids always reveal a mirror-symmetric non-chiral structure, even when the building units are chiral, as in the case of tobacco mosaic virus [1] and fd virus [2]. We report on parity breaking in the nematic tactoids formed in molecularly non-chiral polymer-crowded solutions of lyotropic chromonic liquid crystals. The effect is manifested by twist of the director and optical activity. Fluorescent confocal polarizing microscopy reveals that the tactoids nucleate at boundaries of cells. We explain the chirality induction by the effect of geometrical anchoring [3] and by increase of the splay elastic constant in condensed nematic regions of crowded solutions.

[1] J. D. Bernal and I. Fankuchen, J. Gen. Physiol. **25**, 111 (1941);
[2] Z. Dogic, Phys. Rev. Lett. **91**, 165701 (2003);
[3] O.D. Lavrentovich, Phys. Rev. A15 **46**, R722 (1992)

[1]NSF DMR MWN 0710544

2:03PM J9.00015 Orientational order and defect structures on curved surfaces[1] , SUBAS DHAKAL, Northwestern University, FRANCISCO J. SOLIS, Arizona State University, MONICA OLVERA DE LA CRUZ, Northwestern University — We study the topological defects in a nematic liquid crystal confined to a surface. Using Monte Carlo simulations, we investigate how the position and number of defects depend on the interaction strength, the shape of the surface and other physical parameters. On a spherical surface, we find that the interaction changes the location of four $+1/2$ defects initially sitting on a great circle of the sphere to the vertices of a tetrahedron. In deformed spheres, we observe the coalescence of defects into two single $+1$ defects.

[1]We acknowledge the support of the NERC, which is a EFRC funded DOE Office of Science under Award DE-SC0000989.

Tuesday, March 22, 2011 11:15AM - 2:15PM –
Session J10 DCMP: Surface and Interfaces with Metals D221

11:15AM J10.00001 Ordered and disordered surface alloys in Au-Pt(111) and their effect on oxygen adsorption[1] , WEI CHEN, C. WOLVERTON, Northwestern University, DAVID SCHMIDT, WILLIAM SCHNEIDER, University of Notre Dame — Bimetallic surface alloys are considered a promising type of catalyst for improved activity and selectivity. Understanding surface structure and its effect on catalytic performances plays a critical role in designing catalysts from surface alloys. We have studied the surface structure and ordering of AuPt(111) using a first-principles cluster expansion based method. Even though the Au-Pt system is phase-separating in the bulk, we find a series of thermodynamically stable, laterally ordered striped structures of AuPt(111) surfaces. The formation of such ordered structures is the result of a competition between the strain relaxations from stripes and the unfavorable Au-Pt bonds at stripe interfaces. We have also investigated the oxygen adsorption on these structures. The oxygen binding energy is found to be highly correlated with the type of nearest neighbor surface atoms of oxygen.

[1]This work is supported by National Science Foundation under contract No. CBET-0730841 and No. CBET-0731020.

11:27AM J10.00002 Order-Disorder Transitions for Au/Mo(112) , KEISUKE FUKUTANI, University of Nebraska-Lincoln, YAROSLAV LOSOVYJ, NATALIA LOZOVA, Center for Advanced Microstructure and Devices, Louisiana State University, IVAN YAKOVKIN, National Academy of Science of Ukraine, Institute of Physics, NING WU, PETER DOWBEN, University of Nebraska-Lincoln — Order-disorder overlayer phase transitions are observed at the surface of Au/Mo(112) for the nominal Au coverages of 1.66 and 1.75 monolayers. These transitions are characterized by the abrupt change in the surface Debye temperature. In the search for the detailed mechanism of this phase transition, we investigated the electron-phonon coupling (EPC), in the vicinity of the Fermi level, for the surface states of Au-covered Mo(112) surface from high- resolution angle resolved photoemission data taken parallel to the surface corrugation (i.e. $<\underline{11}1>$). The changes of the widths of the surface weighted bands, induced by Au layers, are discussed in terms of electron-electron interactions, electron-impurity scattering and electron-phonon coupling. Gold overlayers suppress the mass enhancement of the Mo(112) surface band crossing the Fermi level at 0.54 $Å^{-1}$. The data indicate that significant contributions from impurity and defect scattering must be considered in any serious analysis of the imaginary part of the self energy and that there interface effects can have a profound influence on the imaginary part of the self energy.

11:39AM J10.00003 Ab initio study of Mg self-diffusion on Mg(0001) terraces and steps[1] , MARAL AMINPOUR, MARISOL ALCANTARA ORTIGOZA, TALAT RAHMAN, Department of Physics, University of Central Florida, Orlando, 32816 — The high density of states (DOS) at the Fermi level and high density of quasi-free electrons result in a singular behavior for Mg surfaces and thin films. We find, however, that the DOS around the Fermi level, surface energy and cohesive energy converge beyond 15 layers. We also show that the Friedel charge density oscillations of Mg(0001) are more complex than depicted previously by 1D and 2D plots. These oscillations are, in fact, responsible for the stacking fault of Mg adatoms and islets on Mg(0001) and also, indirectly, for the low adatom self-diffusion barrier (20 meV) on Mg(0001), which is in agreement with effective-medium theory calculations. [1] We will compare this barrier with that of Mg adatom on a narrow terrace and across the steps on Mg(0001), as well as with predictions from Kinetic Monte Carlo simulations made to fit the growth mode observed for Mg/Mg-thin-films via scanning tunneling microscopy.

[1] Z.J. Tian, U. Yxklinten, B.I. Lundqvist and K.W. Jacobsen.Surf. Sci.**258** (1991), p. 427

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

11:51AM J10.00004 Theoretical aspects of studies of high coverage oxidation of the Cu(100) surface using low energy positrons , N.G. FAZLEEV, W.B. MADDOX, J.A. REED, Department of Physics, University of Texas at Arlington — The study of adsorption of oxygen on transition metal surface is important for the understanding of oxidation, heterogeneous catalysis, and metal corrosion. The structures formed on transition metal surfaces vary from simple adlayers of chemisorbed oxygen to more complex structures which results from diffusion of oxygen into the sub-surface regions. In this work we present the results of an ab-initio investigation of positron surface and bulk states and annihilation probabilities of surface-trapped positrons with relevant core electrons at the Cu(100) missing row reconstructed surface under conditions of high oxygen coverage. Calculations are performed for various surface and subsurface oxygen coverages ranging from 0.50 to 1.50 monolayers. Calculations are also performed for the on-surface adsorption of oxygen on the unreconstructed Cu(001) surface for coverages up to one monolayer to use for comparison. Estimates of the positron binding energy, positron work function, and annihilation characteristics reveal their sensitivity to atomic structure of the topmost layers of the surface and charge transfer. Theoretical results are compared with experimental data obtained from studies of oxidation of the Cu(100) surface using positron annihilation induced Auger electron spectroscopy.

12:03PM J10.00005 Deposition of metal onto a sulfur loaded substrate , DAEHO KIM, DEZHENG SUN, WENHAO LU, ERIC CHU, JON WYRICK, ZHIHAI CHENG, LUDWIG BARTELS, University of California, Riverside — A Cu(111) surface can be loaded with sulfur to form a variety of surface patterns. In this work, we study the deposition of copper and molybdenum on a Cu(111) surface and the resultant film morphology as a function of the sulfur pre-loading of the substrate. For copper deposition, we find the formation of adstructures of different geometry depending on the sulfur decoration of the substrate. A 0.143 ML S coverage leads to rectangular structure consisting of 6 lobes while a 0.118 ML S coverage leads to 7×7 structure. Notably, annealing allows the sulfur to float up decorating the newly deposited layer. Deposition of molybdenum shows a similar pattern, with ordered MoS2 forming as a result of annealing.

12:15PM J10.00006 Oxides on Nanoscale Platinum Surfaces[1] , DANIEL HENNESSY, Materials Science Division, Argonne National Laboratory, VLADIMIR KOMANICKY, Safarik University, UPJŠ, Košice, Slovakia, MICHAEL S. PIERCE, KEE-CHUL CHANG, HOYDOO YOU, Materials Science Division, Argonne National Laboratory — We demonstrate the existence of oxide layers on nanoscale Pt interfaces annealed in an oxygen environment. The sample is a Pt single crystal cut at the midpoint between the 100 and 111 crystal directions; annealing in Ar produces a smooth surface, while annealing in air produces ∼10 nm-sized 100 and 111 facets. Synchrotron x-ray crystal truncation rod (CTR) measurements indicate a bilayer Pt oxide structure on the nanofacets. Fitted Pt occupancies are consistent with a nearest-neighbor avoidance structure of the surface oxygen atoms. Electrochemical cycling of the faceted surface in CO-saturated solution removes the oxide and leaves clean, ordered facets. Pt single crystals of 100 and 111 surface orientations prepared the same way did not support an oxide layer.

[1]Work at ANL is supported by DOE-BES and work at SU by VEGA.

12:27PM J10.00007 The amazing kinetic stability of the high temperature ($\sqrt{3} \times 6$)rect. striped structure of decanethiol SAMs on Au(111) and other interesting properties. A scanning tunneling microscopy study.[1] , LLOYD BUMM, DAMINDA DAHANAYAKA, ABHIJIT BISWAS, RONALD HALTERMAN, The University of Oklahoma — We present an STM study of the properties of the high temperature ($\sqrt{3} \times 6$)rect. phase of decanethiol SAMs on Au (111). Although this phase is known, it has not been extensively studied. We show a simple reliable way to grow the ($\sqrt{3} \times 6$) rect. phase and show that its coverage is 75% of the normal ($2\sqrt{3} \times 3$)rect. phase. Although it has lower density compared to the normal alkanethiol SAM structure, it shows a remarkable kinetic stability with respect to uptake of additional alkanethiol molecules and reversion to the normal ($2\sqrt{3} \times 3$) rect. phase. Other properties of the ($\sqrt{3} \times 6$)rect. phase will be discussed.

[1]This work has been supported by NSF CAREER grant No. CHE-0239803, NSF MRSEC No. DMR-0080054, NSF No. DMR-0805233, and AFOSR No. FA9550-06-1-0365.

12:39PM J10.00008 Epitaxial orientations of para-sexiphenyl platelets grown on alkali halide (001) surfaces , EDWARD KINTZEL, Department of Physics and Astronomy, Western Kentucky University, DETLEF SMILGIES, Cornell High Energy Synchrotron Source (CHESS), Cornell University — Thin film growth of simple aromatic molecules has been researched intensely in recent years in the burgeoning field of organic electronics. Film growth for simple rodlike molecules on the atomically well-defined and nonreactive alkali halide (001) surfaces also constitutes an archetypical model system for the study of molecular epitaxy. We have observed a surprising variety of preferential orientations of para-sexiphenyl platelets on a series of alkali halide surfaces with lattice constants ranging from 4.6 to 6.6 Angstroms. We present a metric that helps to classify the dominant epitaxial orientations and allows us to predict epitaxial orientations on other rocksalt-type substrates, and we identified surface corrugation as the driving force for these preferred relative orientations.

12:51PM J10.00009 Pentacene thin films on vicinal Ag(111) surfaces[1] , FATIH DANISMAN, Middle East Technical University, ILKER DEMIROGLU, ERSEN METE, SINASI ELLIALTIOGLU — Here we present a structural study of pentacene thin films on different vicinal Ag(111) surfaces by helium atom diffraction measurements and density functional theory (DFT) calculations. Our helium atom diffraction results suggest a step flow growth mechanism evidenced by initial slow specular reflection intensity decay rate as a function of pentacene deposition time. This is in agreement with our previous helium diffraction results on flat Ag(111) surfaces with a small miscut angle. In parallel with the experimental findings, our DFT calculations predict the step edges as the most stable adsorption site on the surface. Isolated pentacene molecules adsorb on the step edges in a tilted configuration with a binding energy of 0.615 eV. In addition a complete monolayer with tilted pentacene on the step edges is found to be more stable than one with all lying flat molecules. Hence our results suggest, in agreement with prvious predictions, that step edges can trap the pentacene molecules and act as nucleation sites for the growth of ordered thin films with a crystal structure similar to that of bulk pentacene.

[1]This work was supported by TUBITAK under Grant No 107T408.

1:03PM J10.00010 Scaled Shell-like Pattern Formation of Selenium-Based Anthracene Derivatives at a Metal Surface , LUDWIG BARTELS, UCR, ZHIHAI CHENG, JONATHAN WYRICK, DEZHENG SUN, DAEHO KIM, YEMING ZHU, MIAOMIAO LUO, ROBERT CARP, MICHAEL MARSELLA — We investigated the behavior of selenium-substituted anthracene molecules at a Cu(111) surface. In our previous work, the sulfur and oxygen counterparts of this molecule exhibited controlled diffusion on Cu(111) violating the substrate's symmetry. In contrast Diseleno-ateanthracene shows an isotropic and very high mobility suggesting very non-local substrate interactions. However, we observe pronounced sensitivity of the diffusion to the oscillation of the Cu(111) substrate surface state. In this talk, we will focus on the coverage-dependent pattern formation of this species: at coverages close to 1 ML, two kinds of hexagonal patterns with large unit cells are formed. Both of them show a shell superstructure with an identical central empty hole. The smaller of the features one molecular shell of 6 molecules the larger a double shells of 6 and 12 molecules. Another kind of rectangular pattern is also observed, which could be an intermediate superstructure between the small and large hexagonal patterns. We will compare these patterns to prior work on sulfur and oxygen based molecules.

1:15PM J10.00011 Stable Carbon Nanoarches in the Nucleation of Graphene on Cu(111)[1] , ROBERT VAN WESEP, HUA CHEN, WENGUANG ZHU, Phys Dept, U of Tennessee; Materials Science & Engineering Division, ORNL, ZHENYU ZHANG, Phys Dept, U of Tennessee; Materials Science & Engineering Division, ORNL; ICQD, USTC — To fully exploit the device potential of graphene, reliable production of large-area, high-quality samples is required. Epitaxial growth on transition metal surfaces have shown promise in this regard, but further improvement would be facilitated by a more complete understanding of the nanoscale processes involved. Using density functional theory calculations, we have investigated the energetics and kinetics of graphene nucleation and growth on a Cu(111) surface. Our calculations have revealed an energetic preference for the formation of stable 1D carbon nanoarches consisting of 3-13 atoms when compared to 2D compact islands. Our findings may provide the structural link between nucleated carbon dimers [1] and larger carbon nanodomes [2], and may also explain some recent experimental observations. We will also present results on estimating the critical cluster size that marks the transition from nanoarch dominance to island dominance in the growth sequence.

[1] Hua Chen, et al., Phys. Rev. Lett. 104, 186101 (2010).
[2] Paolo Lacovig, et al., Phys. Rev. Lett. 103, 166101 (2009).

[1]Supported by USDOE, USNSF, and NNSF of China.

1:27PM J10.00012 An *Ab Initio* Study of Bulk γ-U and the (100) Surface[1] , DAYLA MORRISON, ASOK RAY, University of Texas at Arlington — The properties of bcc γ-U have been studied using the formalisms of the generalized gradient approximation to density functional theory (GGA-DFT) and hybrid density functional theory. The computational formalism is the full potential linearized augmented plane wave method as implemented in the suite of software WIEN2k. Computations have been performed both without and with spin orbit coupling (SOC). Results indicate that GGA-DFT with SOC performs comparatively better in the description of the properties of γ-U, such as the non-magnetic ground state, lattice constant, and the bulk modulus. The predicted lattice constant and bulk modulus are 3.463 A and 114 GPa, respectively, to be compared with the experimental values of 3.467 A and 113 GPa, respectively. For the (100) surface, the monolayer exhibited significant contraction but the lattice constants tend to converge after 5 layers. Based on the results of the five layers, we predict the surface energy and the work function to be 1.46 J/m^2 and 3.24eV, respectively.

[1]This work is supported by the Department of Energy, and the Welch Foundation, Houston, Texas.

1:39PM J10.00013 Electronic Structures of Hydrogen and Oxygen Adsorbed Tungsten (3, 2, 0) and Tungsten (8, 7, 0) Surfaces[1] , ZHUO BAO, Physics Department, University of Oregon, AARON BOSTWICK, ELI ROTENBERG, Advanced Light Source, LBNL, STEPHEN KEVAN, Physics Department, University of Oregon — The Valence band electronic structues of Hydrogen adsorbed and Oxygen adsorbed Tungsten stepped surfaces, Tungsten (3, 2, 0) and (8, 7, 0) surface are investigated using angular-resolved photoemission techniques and ab-initio electronic structure calculation methods. The band features of surface states at different Hydrogen and Oxygen coverages are experimentally distinguished by using photon-energy scanning method. Quasi-one- dimensional band features are found in the surface states with saturated Oxygen coverages of both stepped surfaces. The effects of adsorbate coverages on dimensionalities of surface electronic states are studied using high-resolution band mapping methods and ab-initio calculation methods.

[1]Thanks to Department of Energy for the financial supporting of this project.

1:51PM J10.00014 The suppression surface state near a monostep of Au(111) surface studied by low temperature scanning tunneling microscopy[1] , QING LI, PETER MAKSYMOVYCH, SERGI KALININ, MINGHU PAN, Center for Nanophase Materials Scieces, Oak Ridge National Laboratory — The dynamics of electronic states on metal surfaces is a fundamental probe of electron transport and electronic interactions with practical relevance for nanodevices and reactions. In our study, series of scanning tunneling spectroscopy near a monostep of Au(111) surface are used to investigate the behavior of surface state. We found that the Shockley surface state of Au (111) was suppressed near the step. By carefully analyzing each dI/dV spectroscopy, we determined the lateral tip-step distance dependence of the lifetime of the surface electrons. The lifetime broadening of surface state shows linear decay close to the monostep, possibly due to the electron-electron interactions.

[1]This research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Division of Scientific User Facilities, U.S. Department of Energy.

2:03PM J10.00015 Low Energy Hot Electron Scattering in Nanometer Scale Metal Films Using Ballistic Electron Emission Microscopy , JOHN GARRAMONE, JOSEPH ABEL, VINCENT LABELLA, College of Nanoscale Science and Engineering, University at Albany, SUNY, Albany, New York 12203, USA — Inelastic and elastic scattering lengths of hot electrons have been measured at low energies (<2 eV) in nanometer thick silver films utilizing ballistic electron emission microscopy (BEEM). BEEM is a scanning tunneling microscopy (STM) based technique that is capable of injecting electrons a few eV above the Fermi level and utilizes a third collector contact on the semiconductor of a Schottky diode[1]. Electrons tunnel from the STM tip into the metal base layer and a small fraction of these electrons travel ballistically to the metal/semiconductor interface. Electrons with energy greater than the Schottky barrier height (SBH) are collected as BEEM current. The silver attenuation length is extracted by measuring the BEEM current as a function of the Ag overlayer thickness over a series of samples for both electron and hole injection. The relative contribution of inelastic and elastic scattering is extracted by modeling the change in attenuation length with respect to the tip bias. A drastic increase in the attenuation length is observed as energies approach the SBH, which we attribute to the ballistic nature of the electrons and holes that are collected at these energies.

[1]L. D. Bell, et al., Phys. Rev. Lett. 61 2368 (1988)

Tuesday, March 22, 2011 11:15AM - 2:03PM –
Session J11 FIAP: Fractional Quantum Hall Effect I D222

11:15AM J11.00001 The Real-Space Entanglement Spectra of Fractional Quantum Hall States , A. CHANDRAN, Princeton University, PARSA BONDERSON, Microsoft Research, Station Q, NICOLAS REGNAULT, Laboratoire Pierre Aigrain, ENS and CNRS, ANDREI BERNEVIG, Princeton University — We investigate the entanglement spectra arising from a sharp real-space cut on the topologically ordered fractional quantum hall (FQH) ground states. We find that the counting of the real-space entanglement spectra (the number of edge excitations of the liquid) is identical to the number of bulk quasihole excitations, in accordance with the bulk-boundary correspondence. The spectra of cuts with two edges display the shape and counting of counter-propagating non-interacting modes as well. Initial estimates of the topological entanglement entropy seem to be in agreement with theory. The real-space entanglement spectra also allows us to distinguish between particle-hole conjugate states, providing us with a new probe to interacting edge modes.

11:27AM J11.00002 Identification of 331 quantum Hall states with Mach-Zehnder interferometry[1] , CHENJIE WANG, D.E. FELDMAN, Physics Department, Brown University — It has been shown recently that non-Abelian states and the spin-polarized and unpolarized versions of the Abelian 331 state may have identical signatures in Fabry-Pérot interferometry in the quantum Hall effect at filling factor 5/2. We calculate the Fano factor for the shot noise in a Mach-Zehnder interferometer in the 331 states and demonstrate that it differs from the Fano factor in the proposed non-Abelian states. The Fano factor depends periodically on the magnetic flux through the interferometer. Its maximal value is $2 \times 1.4e$ for the 331 states with a symmetry between two flavors of quasiparticles. In the absence of such symmetry the Fano factor can reach $2 \times 2.3e$. On the other hand, for the Pfaffian and anti-Pfaffian states the maximal Fano factor is $2 \times 3.2e$. The period of the flux dependence of the Fano factor is one flux quantum. If only quasiparticles of one flavor can tunnel through the interferometer then the period drops to one half of the flux quantum. We also discuss transport signatures of a general Halperin state with the filling factor $2 + k/(k + 2)$.

[1] Chenjie Wang and D. E. Feldman, Phys. Rev. B **82**, 165314 (2010).

[1]This work was supported by NSF under Grant No. DMR-0544116 and BSF under Grant No. 2006371.

11:39AM J11.00003 Bulk excitonic currents in a bilayer quantum Hall system and Andreev reflection , A.D.K. FINCK, J.P. EISENSTEIN, California Institute of Technology, L.N. PFEIFFER, K.W. WEST, Princeton University — Bilayer 2D electron systems in the quantum Hall regime can support a novel interlayer coherent phase which may be viewed as a Bose condensate of interlayer excitons. While numerous experiments over the past decade have revealed a host of remarkable properties of this strongly correlated quantum fluid, heretofore none have directly demonstrated the transport of excitons across the electrically insulating bulk of the system. We report here just such an observation. Our experimental results show that excitons may be launched into the bulk of the 2D system via a process analogous to Andreev reflection. Excitons are emitted into the bulk of the bilayer when electrons are injected into one 2D layer and withdrawn from the other along a common edge of the system. Similarly, we demonstrate that excitons arriving at the edge of the Hall droplet can drive current through external circuitry connected to contacts along that edge.

11:51AM J11.00004 Phase diagram of the even-denominator fractional quantum Hall state at $\nu = 1/2$ in wide quantum wells , JAVAD SHABANI, MANSOUR SHAYEGAN, Princeton University — We have studied the fractional quantum Hall (FQH) effect in very high quality two dimensional electrons confined to GaAs single wide quantum wells. In these systems typically two electric subbands are occupied at zero magnetic field and the electron charge distribution in the quantum well is bilayer-like. For a symmetric charge distribution and appropriate electron density, a unique even-denominator FQH state emerges at filling factor $\nu = 1/2$ which has no counter-part in standard, single-layer systems [1]. We have revisited this problem by studying wide quantum well samples with narrower well widths, $47 \leq w \leq 64$ nm, and hence larger tunneling, Δ (up to 35 K). The new $\nu = 1/2$ data in these narrower samples allow us to expand the d/l_B vs. $\Delta/(e^2/4\pi\epsilon l_B)$ phase diagram for the stability of the $\nu = 1/2$ FQH state (d is the layer distance and l_B is the magnetic length). Based on this phase diagram, we find that, it is not clear whether this state has a Pfaffian or a two-component Halperin origin.

[1] Y. W. Suen et al., Phys. Rev. Lett. 72, 3405 (1994).

12:03PM J11.00005 When is the fractional quantum Hall effect stable[1] , YANG LIU, JAVAD SHABANI, MANSOUR SHAYEGAN, Dept. of Electrical Engineering, Princeton University — The fractional quantum Hall (FQH) effect, signaled by the vanishing of the longitudinal resistance and the quantization of the Hall resistance, is the hallmark of interacting two-dimensional electrons in a large perpendicular magnetic field. The effect is most prominently observed at low Landau level (LL) filling factors (ν) and is conspicuously absent for $\nu > 4$. We examine the stability of the FQH states at high fillings in a 2D electron system in a wide GaAs quantum well which we can tune the Fermi energy (E_F) to lie, at a given filling factor, in different LLs of two electric subbands. The data provide direct and definitive evidence that the stability of the FQH states is linked to the LL where E_F resides. We observe FQH states at high filling factors such as 13/3, 14/3, 16/3, and 17/3, but only when E_F lies in the ground state ($N = 0$) orbital LLs of either of the two electric subbands, regardless of the underlying, fully occupied levels.

[1]We acknowledge support through the NSF (DMR-0904117 and MRSEC DMR-0819860) for sample fabrication and characterization, and the DOE BES (DE-FG0200-ER45841) for measurements.

12:15PM J11.00006 Evolution of odd-denominator fractional quantum Hall states in a two-subband system[1] , MANSOUR SHAYEGAN, JAVAD SHABANI, YANG LIU, Princeton University — Our magneto-transport measurements reveal that the sequence of fractional quantum Hall (FQH) states observed in two-subband, wide GaAs quantum wells at high fillings ($\nu > 2$) are very different from those of a single-subband system. When the Fermi level lies in the lowest Landau level of either of the two subbands the odd-denominator FQH states following the usual, composite fermion filling sequences are observed. These include states at $\nu = 7/3$, 8/3, 12/5, 13/5, 10/3, 11/3, 17/5, 18/5, and 25/7. The evolution of these states with changing the Zeeman and subband energies is consistent with coincidences of composite fermion Landau levels.

[1]We acknowledge support through the NSF (DMR-0904117 and MRSEC DMR-0819860) for sample fabrication and characterization, and the DOE BES (DE-FG02-00-ER45841) for measurements.

12:27PM J11.00007 Negative spin wave dispersion for composite fermions[1] , U. WURSTBAUER, Columbia Univ., D. MAJUMDER, S. MANDAL, Indian Association for the Cultivation of Science, I. DUJOVNE, A. RIGOSI, T.D. RHONE, Columbia Univ., B. DENNIS, Alcatel-Lucent, K. WEST, Princeton Univ., L. PFEIFFER, Princeton Univ, J. JAIN, Pennsylvania State Univ., A. PINCZUK, Columbia Univ. — The FQHE is a result of strongly interacting electrons that can be understood as QHE of composite fermions. We use inelastic light scattering experiments to study the collective excitations of CF with 2 flux quanta focusing on filling factors $\nu = 4/9$, 3/7 and 2/5. For these fillings, the lowest collective excitation modes are spin-waves, which display a distinct spectral weight below the bare Zeeman energy indicating a negative dispersion relation. The determined energies for these "spin-wave roton minima" are in excellent quantitative agreement with numerical calculations. Using the real experimentally transferred momentum the addressed DOS and hence inelastic light scattering spectra can be modeled. We demonstrate that the observed modes are very similar for positive and negative effective magnetic field at the same CF-filling factor.

[1]Supported by NSF and AvH.

12:39PM J11.00008 Subband Engineering Even-Denominator Quantum Hall States , VITO SCAROLA, Virginia Tech, CHRISTIAN MAY, ETH Zurich, MICHAEL PETERSON, University of California, Santa Barbara, MATTHIAS TROYER, ETH Zurich — Proposed even-denominator fractional quantum Hall effect (FQHE) states suggest the possibility of excitations with non-Abelian braid statistics. Recent experiments on wide square quantum wells observe even-denominator FQHE even under electrostatic tilt. We theoretically analyze these structures and develop a procedure to accurately test proposed quantum Hall wavefunctions. We find that tilted wells favor partial subband polarization to yield Abelian even-denominator states. Our results show that tilting quantum wells effectively engineers different interaction potentials allowing exploration of a wide variety of even-denominator states.

12:51PM J11.00009 Quasiparticle tunneling amplitute in fractional quantum Hall states[1] , ZIXIANG HU, Princeton university, KIHOON LEE, APCTP, Korea, EDWARD H. REZAYI, California State Univ, Los Angeles, XIN WAN, APCTP, Korea & ZheJiang University, China, KUN YANG, NHMFL & Florida State University — We study qp tunneling in the MR state, in which qp of charge e/4 and e/2 may co-exist and both contribute to edge transport. The tunneling amplitude for charge e/2 qp is exponentially smaller than that for e/4 qh, and the ratio between them can be (partially) attributed to their charge difference. The tunneling amplitude shows some scaling behavior which originates from the propagation and tunneling of charged qhs in an effective field analysis. In the ring limit, we conjecture the exact functional form for several cases. The results for Abelian qp tunneling is consistent with the scaling anaysis; this allows for the extraction of conformal dimensions of the qps. We analyze the scaling behavior of both Abelian and non-Abelian qps in the Z_k parafermion states. Interestingly, the non-Abelian qp tunneling amplitudes exhibit nontrivial k-dependent corrections to the scaling exponent.

[1]This work was supported by DOE grant DE-SC0002140 and APCTP

1:03PM J11.00010 Extracting Excitations From Model State Entanglement , NICOLAS REGNAULT, ANTOINE STERDYNIAK, Ecole Normale Superieure, CNRS, ANDREI BERNEVIG, Princeton University — We extend the concept of entanglement spectrum from the geometrical to the particle bipartite partition. We apply this to several Fractional Quantum Hall wavefunctions on both sphere and torus geometries to show that this new type of entanglement spectra completely reveals the physics of bulk quasihole excita tions. While this is easily understood when a local Hamiltonian for the model state exists, we show that the quasiholes wavefunctions are encoded within the model state even when such a Hamiltonian is not known. As a nontrivial example, we look at Jain's composite fermion states and obtain their quasiholes directly from the model state wavefunction. We reach similar conclusions for wavefunctions described by Jack polynomials.

1:15PM J11.00011 Neutral mode heat transport and fractional quantum Hall shot noise , SO TAKEI, University of Maryland College Park, BERND ROSENOW, University of Leipzig — We study nonequilibrium edge state transport in the fractional quantum Hall (FQH) regime for states with a counter-propagation neutral mode. Focusing on the filling fraction of 2/3, we consider a setup in which the neutral mode is heated by a hot spot, and where heat transported by the neutral mode causes a temperature difference between the upper and lower edges in a Hall bar. This temperature difference is probed by the excess noise it causes for scattering across a quantum point contact (QPC). We find that the excess noise in the QPC provides evidence for counter-propagating neutral modes, and we calculate its dependence on both the temperature difference between the edges and on source drain bias. We generalize our results to the non-abelian Moore-Read quantum Hall state at filling fraction 5/2.

1:27PM J11.00012 Anisotropic quantum Hall liquids - a small system Monte Carlo study[1] , ORION CIFTJA, BRITTNEY CORNELIUS, KESHA BROWN, EMERY TAYLOR, Department of Physics, Prairie View A&M University, Prairie View, Texas 77446, USA — While no fractional quantum Hall effect states were expected to stabilize in the second excited Landau level, the discovery of extreme magneto-transport anisotropy around filling factor 9/2 was found quite surprising. A unidirectional charge density wave is a plausible candidate for the anisotropic states as indicated by the earlier theoretical work. An alternative approach that would be consistent with observed experimental facts would view the onset of anisotropy as signature of a phase transition from an isotropic to an anisotropic liquid crystalline phase. In this work we present a small-system Monte Carlo study for anisotropic quantum Hall liquid states observed at filling factor 9/2. The anisotropic electronic liquid phases are described by a broken rotational symmetry wave function and electrons interact with Landau level-projected interaction potentials. Our small-system Monte Carlo study indicates that such an anisotropic liquid crystalline quantum Hall phase with broken rotational symmetry is energetically favored relative to an isotropic liquid one.

[1]This research was supported in part by NSF Grant No. DMR-0804568.

1:39PM J11.00013 Chiral Abelian anyons from interacting non-Abelian vortices , VILLE LAHTINEN, NORDITA, JIANNIS PACHOS, University of Leeds — We demonstrate the existence of a new topologically ordered phase in Kitaev's honeycomb lattice model. This new phase appears due to the presence of a tightly packed vortex lattice and it supports chiral Abelian anyons. We characterize the phase by its low-energy behavior that is described by four Fermi points as opposed to two Fermi points in the absence of the vortex lattice. This doubling is shown to be related to an emergent vortex lattice symmetry that arises due to interactions between the anyonic vortices. By mapping the Hamiltonian of the model to a BCS one, we show that the chiral Abelian phase can be understood as two coupled p-wave superconductors, one living on the original honeycomb lattice and the other on the dual lattice that coincides with the vortex lattice. Finally, we identify two physically distinct types of topological phase transitions in the model and show that the Fermi surface evolution associated with them is described by Dirac fermions coupling to chiral gauge fields. The study of the Fermi point transport across the Brillouin zone enables us to obtain analytic results on the extended phase space.

1:51PM J11.00014 The Weakly Coupled Pfaffian as a Type I Quantum Hall Liquid[1] , S.A. PARAMESWARAN, Princeton University, S.A. KIVELSON, Stanford University, S.L. SONDHI, Princeton University, B.Z. SPIVAK, University of Washington — The Pfaffian phase of electrons in the proximity of a half-filled Landau level is understood to be a $p + ip$ superconductor of composite fermions. We consider the properties of this paired quantum Hall phase when the pairing scale is small, *i.e.* in the weak-coupling, BCS, limit, where the coherence length is much larger than the charge screening length. We find that, as in a Type I superconductor, the vortices attract so that, upon varying the magnetic field from its magic value at $\nu = 5/2$, the system exhibits Coulomb frustrated phase separation. We propose that the weakly and strongly coupled Pfaffian states exemplify a general dichotomy between Type I and Type II quantum Hall fluids.

[1] This work was supported in part by NSF grants DMR-1006608 and PHY-1005429 (SAP, SLS), DMR-0758356 (SAK) and DMR-0704151 (BZS).

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J12 GERA DMP: Focus Session: Electricity-to-Light Conversion: Solid State Lighting II D223/224

11:15AM J12.00001 Surface origin of the LO phonon feature in the Raman spectrum of InN , ESTHER ALARCON-LLADO, NATE MILLER, MARIE MAYER, JOEL W. AGER — Wurtzite InN presents an intrinsic Fermi level pinning above the conduction band edge at the surface. For this reason, a large surface electron accumulation (SEA) occurs in InN. The interaction between the free electrons at the surface and the longitudinal optical (LO) phonon has been addressed by previous studies, but questions still remain. Here, we use the insulating nature of the Helmholtz layer that forms on a surface of an object in contact with an an aqueous electrolyte to apply potentials to n-type (undoped) and p-type (Mg-doped) InN. Applying a potential to the electrolyte changes the electric field and distribution of free carriers near the surface. This enables us to perform electrolyte gated Raman spectroscopy on differently doped InN layers and while simultaneously modulating and probing the SEA region in InN. We find that the intensity of the forbidden LO Raman feature is changed by the external potential, showing that this feature is due, at least in part, to the SEA. This is the first experimental evidence of the relation between the LO feature in InN and free electron accumulation at its surface.

11:27AM J12.00002 Hydrogen incorporation in high hole density GaN:Mg[1] , M.E. ZVANUT, Y. UPRETY, J. DASHDORJ, University of Alabama at Birmingham, M. MOSELEY, W. ALAN DOOLITTLE, Georgia Institutute of Technology — We investigate hydrogen passivation in heavily doped p-type GaN using electron paramagnetic resonance (EPR) spectroscopy. Samples include both conventionally grown GaN (10^{19} cm^{-3} Mg, 10^{17} cm^{-3} holes) and films grown by metal modulation epitaxy (MME), which yielded higher Mg (1-4x10^{20} cm^{-3}) and hole (1-40x10^{18} cm^{-3}) densities than found in conventionally grown GaN. The Mg acceptor signal is monitored throughout 30 minute annealing steps in N_2:H_2 (92%:7%)) and subsequently pure N_2. N_2:H_2 heat treatments of the lower hole density films begin to reduce the Mg EPR intensity at 750 ^oC, but quench the signal in high hole density films at 600 ^oC. Revival of the signal by subsequent N_2 annealing occurs at 800 ^oC for the low hole density material and 600 ^oC in MME GaN. The present work highlights chemical differences between heavily Mg doped and lower doped films; however, it is unclear whether the difference is due to changes in hydrogen-Mg complex formation or hydrogen diffusion.

[1]The work at UAB is supported by the NSF.

11:39AM J12.00003 Enhancing erbium emission by strain engineering in GaN heteroepitaxial layers , I-WEN FENG, JING LI, ASHOK SEDHAIN, JINGYU LIN, HONGXING JIANG, Texas Tech University, JOHN ZAVADA, North Carolina State University — Rare earth doped III-nitrides have been intensively studied due to their intra-4f transitions covering the window from visible emissions to infrared wavelengths. Trivalent Erbium (Er^{3+}) has driven particular interests since the intra-4f transition from its first excited ($^4I_{13/2}$) to the ground state ($^4I_{15/2}$) gives 1.54 μm emission, which sits in the low optical loss band of silica fibers and potentially affords light emitters and optical amplifiers at optical communication wavelength. Due to the structural and thermal stability of GaN, GaN appears to be the promising candidate as the host semiconductors. We prepared Er doped GaN (GaN:Er) samples by metal organic chemical vapor deposition. GaN:Er epilayers were simultaneously grown on different templates, including GaN/Al_2O_3, AlN/Al_2O_3, GaN/Si(111), and c-GaN bulk. The effects of stress, caused by the lattice mismatch between GaN:Er epilayers and the substrates, on the intensity of 1.54 μm emission were probed. The emission intensity at 1.54 μm increased with greater tensile stress in the c-direction of GaN:Er epilayers. The correlation between stress and 1.54 μm emission will be presented. The results implied the potential to design efficient photonic devices based on GaN:Er semiconductors.

11:51AM J12.00004 Effect of electrostatic image charge effect on the photoluminescence in Gallium droplet coated AlGaAs-GaAs Single Quantum Wells , KAROL GRYCZYNSKI, University of North Texas, JIE LIN, TONY LLOPIS, ZHIMING WANG, G. SALAMO, ARKADII KROKHIN, ARUP NEOGI, UNIVERSITY OF ARKANSAS COLLABORATION, KWANGWOON UNIVERSITY, KOREA COLLABORATION — Gallium (Ga) droplets deposited on the cap layers of AlGaAs-GaAs single quantum wells (QWs) lead to a large blue shift in the observed photoluminescence of quantum wells compared to identical single wells without Ga droplets. Furthermore the intensity of the blue shifted emission peaks is enhanced with respect to the reference QWs. As the emission energies for all depths of QWs used (1.5nm to 10nm) exceed the plasmon resonance energy of the deposited Ga droplets, surface Plasmon polariton interactions cannot account for an increase in exciton recombination energy of about 20meV it is concluded that the blue shift and enhancement from the Ga droplets is not plasmonic in nature. The observed phenomena are described and modeled by applying an additional electrostatic potential to the confined excitons within the QW. An electrostatic attraction between the confined exciton and inhomogeneous nanoscale metal surfaces exert forces on the carriers both parallel and perpendicular to the surface of the well.

12:03PM J12.00005 Polarization induced doping in graded AlGaN films , MORGAN WARE, SHIBIN LI, VASYL KUNETS, MICHAEL HAWKRIDGE, PAUL MINOR, JIANG WU, GREGORY SALAMO, Arkansas Institute for Nanoscale Materials Science and Engineering, University of Arkansas — The fixed polarization field which is intrinsic to nitride based III-V semiconductors in the wurtzite crystal phase can be manipulated during growth by varying the alloy composition. We report on initial experiments to use the space charge field which results from changing the internal polarization field of graded AlGaN films in a simple p-n junction device. Our devices are fabricated from films which are graded from GaN to AlGaN then reverse graded back to GaN without the intentional addition of impurity dopants. Structural characterization of the films is reported through X-Ray diffraction rocking curves and reciprocal space maps, and the rectifying behavior of the device is demonstrated through temperature dependent I-V measurements.

12:15PM J12.00006 Electroluminescence from $n-n$ isotype heterojunctions of graded-band-gap ZnMgO:Al and ZnO films[1] , JONG-GUL YOON, SUNG WOO CHO, University of Suwon, WOO SEOK CHOI, ReCFI, Seoul National University, DAE YEOL KIM, University of Suwon, JOONHEE LEE, Seoul National University, CHANG OH KIM, Kyung Hee University, HOJOON CHANG, HEONSU JEON, Seoul National University, SUK-HO CHOI, Kyung Hee University, TAE WON NOH, ReCFI, Seoul National University — We report room temperature electroluminescence (EL) from $n-n$ isotype heterojunction composed of Al-doped graded-band-gap $Zn_{1-x}Mg_xO$ (g-ZnMgO:Al) and ZnO films fabricated on Pt/Ti/SiO_2/Si substrates. The graded-band-gap of g-ZnMgO:Al film was investigated by spectroscopic ellipsometry and found to change contiuously from 3.22 to 3.56 eV. The EL emission spectra covered visible and near infrared regions under unipolar operation condition, with g-ZnMgO:Al as positive, at the operation voltages as low as 3-5 V. Impact ionization/excitation process in a narrow region of the graded layer was suggested as a possible origin of the EL. We discussed multistep excitation process mediated by defect-related deep levels and the effect of quasi-electric field in the graded-band-gap layer in conjunction with the apparent upconversion EL in the heterojuncition device.

[1]Supported by the research programs KRF-2008-313-C00234 and NRF 2010-0008341.

12:27PM J12.00007 Efficiency Droop in III-nitride LEDs: a differential carrier lifetime analysis , AURELIEN DAVID, Soraa Inc — GaN-based LEDs suffer from a phenomenon known as efficiency droop, which causes a (non- thermal) roll-over of the IQE at high current density, and whose underlying physical origin is not well understood. Identifying the correct process is of importance, as it dictates which strategies can be employed to quench or mitigate droop. Among the most often cited hypotheses are: localization effects related to InGaN alloy fluctuations, leakage effects, and Auger scattering. In this contribution, we will present recent experimental results which aim at testing these scenarios. We will first show why droop appears to be a bulk-like phenomenon, rather than transport-related. We will present PL measurements to illustrate how droop scales with carrier density, and biased-PL measurements which quantify the magnitude of the leakage current. In a second part, we will present differential carrier lifetime measurements, which aim at characterizing the various recombination processes in InGaN heterostructures. We will review recently published results, which show that droop is caused by the onset of a high-order non-radiative process, and confirm that lifetimes are quantitatively compatible with the hypothesis of Auger scattering. Finally, we will present new lifetime measurements on QW samples with various In contents, and discuss how the variations in droop can be explained by the impact of piezoelectric fields on the carrier lifetime.

1:03PM J12.00008 MOCVD Growths of Linearly-Shaped Staggered InGaN Quantum Wells Light-Emitting Diodes , HONGPING ZHAO, JING ZHANG, TAKAHIRO TOMA, GUANGYU LIU, JONATHAN POPLAWSKY, VOLKMAR DIEROLF, NELSON TANSU, Lehigh University — High-efficiency InGaN-based quantum wells (QWs) light-emitting diodes (LEDs) play an important role in solid state lighting. However, the existence of both spontaneous and piezoelectric polarization fields in III-Nitride semiconductors leads to severe charge separation in InGaN QWs, which significantly reduces the electron-hole wavefucntion overlap (Γ_{e_hh}) in InGaN QWs. In this work, the growths of linearly-shaped (LS) staggered InGaN QWs LEDs are investigated. The InGaN QWs with LS staggered In-content profile were grown by metalorganic chemical vapor deposition (MOCVD). The use of LS staggered In-contents in InGaN QWs results in improved electron-hole wavefunction overlap (Γ_{e_hh}), in comparison to that of conventional InGaN QW. The power dependent cathodoluminescence (CL) measurement shows 2.5-3.5 times enhancement of CL intensity for LS staggered InGaN QWs as compared to that of the conventional InGaN QWs. Theoretical calculations using self-consistent 6-band **k.p** method were performed for both LS staggered InGaN QWs and conventional InGaN QWs. The experimental measurements show good agreement with the theoretical simulation.

1:15PM J12.00009 Indirect Auger recombination in nitride light emitters , EMMANOUIL KIOUPAKIS, PATRICK RINKE, KRIS T. DELANEY, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106, USA — Nitride-based light emitters suffer from an efficiency loss at high drive currents (droop), which limits their high-power performance. The origin of this efficiency droop is not fully understood, and several loss mechanisms have been suggested as its cause. One such mechanism is Auger recombination, a three-carrier non-radiative recombination process that dominates over the radiative one at high carrier densities. We have employed first-principles computational techniques to show that Auger recombination is strong in nitride materials and therefore a likely cause of the droop in nitride LEDs. The underlying microscopic Auger recombination processes occur in an indirect way, mediated by electron-phonon and alloy scattering. Our work elucidates the origin of the droop and suggests ways to improve the high-power efficiency of nitride LEDs. This work was supported by the Center for Energy Efficient Materials, an Energy Frontier Research Center funded by the U.S. DOE, by the UCSB Solid State Lighting and Energy Center, and by the NSF MRSEC Program.

1:27PM J12.00010 Micro- and Nanostructural Properties of Wide Bandgap Semiconductors , NABIL DAWAHRE, GANG SHEN, SHAWN DAVID WILBERT, NICK HARRIS, WILLIAM BAUGHMAN, LEE BUTLER, JOSEPH BREWER, SEONGSIN MARGARET KIM, PATRICK KUNG, The University of Alabama — Wide bandgap semiconductor materials based on ZnO and GaN have attracted considerable attention in recent years because of the practical applications such as green and blue light emitting and laser diodes, solid-state lighting, photovoltaics, RF and microwave electronics, and gas sensors. However, the resulting device performance strongly depends on the quality, both compositionally and structurally, of the constituent materials. Here we report the combined use of high resolution transmission electron microscopy imaging, micro-Raman and micro-photoluminescence spectroscopy, and local electrode atom probe tomography to understand the micro- and nanostructural properties of materials synthesized by chemical vapor deposition, including defects and impurities. Growth and doping process, sample preparation, and analysis results will be discussed.

1:39PM J12.00011 Auger Recombination in Defect-Free III-Nitride Nanowires[1] , MENG ZHANG, WEI GUO, PALLAB BHATTACHARYA, JUNSEOK HEO, ANIMESH BANERJEE, University of Michigan — Defect free InGaN nanowires (NWs) and InGaN/GaN dot-in-nanowires (DNWs) were grown on (001) Si by plasma assisted molecular beam epitaxy. The nanowires have a density of $\sim$ 1x10^{11}cm^{-2} and exhibit photoluminescence emission peak at λ $\sim$500 nm. The Auger recombination coefficients of these nanowires are determined by excitation power dependent photoluminescence and time-resolved photoluminescence techniques. The measured Auger coefficients are 6.1x10^{-32} cm^6·s^{-1} and 4.1x10^{-33} cm^6·s^{-1}, in the NW and DNW samples, respectively, which are nearly two orders of magnitude lower than those measured in InGaN/GaN quantum wells and agree very well with theoretical calculations. This suggests that the abnormally high Auger coefficients measured in traditional wide bandgap nitride materials is related to the high density of dislocations. InGaN NW and InGaN/GaN DNW light emitting diodes are demonstrated. The external quantum efficiency does not decrease up to an injection current density of 400A/cm^2.

[1]The work was supported by KAUST under Grant N012509-00

1:51PM J12.00012 Effects of oxygen annealing treatment on formation of ohmic contacts to n-GaN[1] , WENTING HOU, THEERADETCH DETCHPROHM, CHRISTIAN WETZEL, Rensselaer Polytechnic Institute — Low-resistance ohmic contacts are essential for the fabrication of efficient light emitting diodes (LEDs). A commonly used ohmic contact to n-type GaN is a layer sequence of Ti/Al/Ti/Au, followed by rapid thermal annealing (RTA) in nitrogen ambient at a high temperature. We present an ohmic contact on n-GaN by a surface treatment process of rapid thermal annealing (RTA) in oxygen ambient before the n-metal deposition. As deposited n-contacts are not linear. After RTA in nitrogen ambient, ohmic contact are obtained. The annealed n-contact degrades during the p-metal anneal in oxygen ambient. However, if the sample is annealed in oxygen ambient prior to the metal deposition, the as-deposited n-contact on the treated surface is ohmic, similar to or even better than processes optimized for single-type contacts. This benefit was seen for both, mesa-etched and as-grown n-GaN epi layers. Contacts improvement is also found on unintentionally doped GaN (u-GaN). Oxygen ambient is crucial in the treatment and RTA in nitrogen ambient fail to give ohmic contacts. XPS analysis of the surface shall give us more information on the mechanism of the treatment.

[1]This work was supported by a DOE/NETL Solid-State Lighting Contract of Directed Research under DE-EE0000627.

2:03PM J12.00013 Strong non-plasmonic mechanism of light emission from semiconductor quantum well , ARKADII KROKHIN, ANTONY LLOPIS, ARUP NEOGI, University of North Texas, SERGIO PEREIRA, Universidade de Aveiro, Portugal, IAN WATSON, University of Strathclyde, UK — We report a new mechanism of enhancement of light emission from InGaN/GaN quantum wells (QW). This mechanism is due to electrostatic attraction of the carriers to gold nanoparticles (NP) imbedded within a QW. Metal equally attracts electrons and holes, causing the carriers to concentrate near its surface. Since the probability of e-h recombination is proportional to carrier densities, the QW with NPs generates a stronger emission than the same QW without the NP. We observed roughly a 60% (80%) enhancement with NPs at room temperature (77K). In these nitride heterostructures, dislocations result in hexagonal pits at the surface. Gold NPs were incorporated inside the pits with no effect on the quality. The same nitride material system used to demonstrate *plasmonic* enhancement [1]. It has been shown that gold film *do not* enhance the emission because of mismatch of surface plasmon energy and the emission energy of the QW. Here we observe the enhancement caused by electrostatic mechanism that does not require energy matching. This mechanism provides another means for enhancing the efficiency of solid- state emitters. This work is supported by the DOE grant # DE-FG02-06ER46312.

[1] K.Okamoto, *et al.*, *Nature Mat.* **3**, 601 (2004).

Tuesday, March 22, 2011 11:15AM - 2:15PM –
Session J13 GSNP: Focus Session: Jamming Theory and Experiment II D225/226

11:15AM J13.00001 Jammed particulate systems are inherently nonharmonic[1] , MARK D. SHATTUCK, Levich Institute and Physics department, The City College of New York — Normal mode analysis in the harmonic approximation underlies most of solid-state physics and applies well to both ordered and dis- ordered systems. Naturally, researches apply this analysis to jammed particulate systems, such as granular media, colloids, and foams, that interact via one-sided interactions, which are nonzero only when particles overlap. However, we find that systems with one-sided repulsive interactions possess no linear, harmonic response regime for large systems ($N \to \infty$) at finite pressures P, and for all N near jamming onset $P \to 0$. We perform simulations on 2D frictionless bidisperse mechanically stable disk packings over a range of packing fractions $\Delta\phi = \phi - \phi_J$ above jamming onset ϕ_J. We apply perturbations with amplitude δ to the packings along each eigen-direction from the dynamical matrix and determine whether the response of the system evolving at constant energy remains in the original eigenmode of the perturbation. For $\delta > \delta_c$, a single contact breaks and fluctuations abruptly spread to all discrete harmonic modes. As δ increases further all harmonic modes disappear into a continuous frequency band. We find that $\delta_c \sim \Delta\phi/N$, and thus jammed particulate systems are inherently nonharmonic with no linear vibrational response regime as $N \to \infty$ over the full range of $\Delta\phi$, and as $\Delta\phi \to 0$ at any N. This breakdown of harmonic behavior dramatically affects all aspects of system response including heat capacity, density of states, elastic moduli, and energy propagation.

[1]Funding: National Science Foundation DMS-0835742, CBET-0968013.

11:51AM J13.00002 Vibrational density of states for granular solids , CARL SCHRECK, Yale University, THIBAULT BERTAND, Close École Normale Supérieure de Cachan, MARK SHATTUCK, City College of New York, COREY O'HERN, Yale University — It was recently shown that granular packings composed of frictionless particles with purely repulsive contact interactions are strongly anharmonic. When perturbed along an eigenmode of the static packing (in the harmonic approximation), energy leaks from the original mode of vibration to a continuum of frequencies even when the system is under significant compression due to the breaking of the weakest contact. In light of this, we perform numerical simulations to measure the displacement matrix averaged over fluctuations and the associated eigenspectrum of weakly vibrated frictionless packings, which possess well-defined equilibrium positions that are different than those of the nearest static packing. We find that there is an increase in the number of low-frequency eigenmodes of the displacement matrix in the harmonic approximation (over the number of low-frequency modes in the static case) and these modes provide a more accurate description of the system dynamics. We also investigate the extent to which these results hold for systems with continuous potentials with repulsive and attractive interactions.

12:03PM J13.00003 Spatiotemporally resolved granular acoustics , ELI OWENS, KAREN DANIELS, North Carolina State University — Acoustic techniques provide a non-invasive method of characterizing granular material properties; however, there are many challenges in formulating accurate models of sound propagation due to the inherently heterogeneous nature of granular materials. In order to quantify acoustic responses in space and time, we perform experiments in a photoelastic granular material in which the internal stress pattern (in the form of force chains) is visible. We utilize two complementary methods, high-speed imaging and piezoelectric transduction, to provide particle-scale measurements of the amplitude of the acoustic wave. We observe that the average wave amplitude is largest within particles experiencing the largest forces. The force-dependence of this amplitude is in qualitative agreement with a simple Hertzian-like model for contact area. In addition, we investigate the power spectrum of the propagating signal using the piezoelectric sensors. For a Gaussian wave packet input, we observe a broad spectrum of transmitted frequencies below the driving frequency, and we quantify the characteristic frequencies and corresponding length scales of our material as the system pressure is varied.

12:15PM J13.00004 Edge Effects in Jammed Systems , CARL GOODRICH, WOUTER ELLENBROEK, ANDREA LIU, University of Pennsylvania — Packings of spheres at zero temperature and shear stress exhibit a jamming/unjamming transition as a function of density. For spheres that repel when they overlap and do not otherwise interact, packings are jammed with a nonzero static shear modulus at high densities. As density decreases towards the unjamming transition, the number of interacting neighbors per particle, z, decreases towards a critical value z_c, so that at the unjamming transition the system just has the minimum number of interacting neighbors to be mechanically stable. In 2005, Wyart, et al. [1] proposed that there is a diverging length scale, l^*, associated with this transition, that can be understood from a "cutting argument." Thus, if one cuts a cluster of linear dimension L, the cluster will have zero-frequency vibrational modes (soft modes) only for $L < l^*$, where l^* scales as Δz^{-1}, where $\Delta z = z - z_c$. This cutting argument successfully describes the scaling of jammed systems. However, we find numerically that there are soft modes confined to the surface of the cut system, which should be present even in arbitrarily large cut systems. Naively, this would suggest that $l^* \to \infty$ at all packing fractions. Given this complication, we set out to generalize the cutting argument to understand its success in describing scaling properties near the jamming transition. [1] M. Wyart, S.R. Nagel, T.A. Witten, *Europhys. Lett.* **72**, 486 (2005).

12:27PM J13.00005 Dislocations jam at any density[1] , GEORGIOS TSEKENIS, NIGEL GOLDENFELD, KARIN DAHMEN, University of Illinois at Urbana-Champaign — Crystalline materials deform in an intermittent way via dislocation-slip avalanches. Below a critical stress, the dislocations are jammed due to long-range interactions and the material exhibits plastic response, while above this critical stress the dislocations are mobile (the unjammed phase) and the material fails. We use dislocation dynamics and scaling arguments to show that the critical stress grows with the square root of the dislocation density. Consequently, dislocations jam at any density, in contrast to granular materials, which only jam below a critical density.

[1]We acknowledge funding from NSF grand DMR 03-25939 ITR and computational resources by the University of Illinois and NSF TeraGrid resources by the Texas Advanced Computing Center and the National Center for Supercomputing Applications (RG-DMR090061).

12:39PM J13.00006 Jammed packings of bumpy spherical particles , DOMINIC KWOK, Department of Physics, K. VIJAY KUMAR, Department of Mechanical Engineering & Materials Science and Physics, CARL SCHRECK, Department of Physics, COREY O'HERN, Department of Mechanical Engineering & Materials Science and Physics, Yale University, New Haven, CT 06511, MARK SHATTUCK, Benjamin Levich Institute and Physics Department, The City College of the City University of New York, NY 10031 — Static packings of soft frictionless spheres are a simple model to understand the jamming transition in granular media, and have provided great insight. However, friction in granular media plays an important role in determining the structural and mechanical properties of jammed packings. In particular, the number and location of contacts near the Coulomb sliding threshold is strongly correlated with plastic rearrangements. To better understand friction, we numerically generate jammed packings of bumpy spherical particles as a function of the rms roughness of the particles without incorporating $ad\ hoc$ single contact frictional forces between particles, $i.e.$ frictional contacts in the Hertz-Mindlin (HM) model. The frictional interactions in the bumpy particle model emerge in a natural way via the interdigitation of bumps between contacting particles. We calculate the number of contacts, packing fraction, interparticle forces, eigenmodes of the dynamical matrix, and mechanical properties of jammed packings of bumpy particles and compare our results with those obtained using the HM model.

12:51PM J13.00007 Shock Waves in Jammed Solids , LEOPOLDO GOMEZ, Leiden University, ARI TURNER, UC Berkeley, MARTIN VAN HECKE, VINCENZO VITELLI, Leiden University — We study shock propagation in two-dimensional jammed packings of soft repulsive spheres with Herzian contacts. The critical amplitude above which acoustic waves propagate as shocks displays power law scaling with density and vanishes as the jamming point is approached. Thus close to jamming elastic energy is mainly propagated in the form of shock waves. We determine the characteristic speed and attenuation of the resulting shocks as a function of the amplitude of the initial impulse and applied load.

1:03PM J13.00008 Jamming: A Peek Behind the Curtain , MARTIN VAN HECKE, Leiden University — We will discuss two of the "dirty little secrets" concerning the (anomalous) scaling of the elastic moduli near jamming. First, there is no linear response near jamming, and we propose a novel scaling law for the onset of rearrangements as function of number of particles and distance to the jamming point. Second, the elastic moduli obtained from the dynamical matrix have a very broad distribution, and we discuss how to deal with packings with negative elastic moduli.

1:15PM J13.00009 Local anisotropy in globally isotropic granular packings , KAMRAN KARIMI, CRAIG MALONEY, Carnegie Mellon University — We study local stresses and elastic moduli defined at various coarse-graining scales, R, and volume fractions, ϕ, in a two dimensional (2D) mixture of frictionless granular particle packings. We measure the average deviatoric stress normalized by pressure, τ/p, and normalized anisotropic component of the shear modulus, $\delta\mu/\mu$, as a function of R. As the packings are prepared isotropically, both τ/p and $\delta\mu/\mu$ vanish at large R. However, in local regions, where single force chains dominate, the response can be quite anisotropic. We show that τ/p exhibits two power-law regimes in R with a cross-over that is only weakly dependent on ϕ. In contrast, $\delta\mu/\mu$, behaves like a pure power law up to $R \sim 640D$ (where D is the characteristic particle diameter) at all ϕ.

1:27PM J13.00010 Thermodynamic stability of dense packings of hard, regular tetrahedra , AMIR HAJI-AKBARI, MICHAEL ENGEL, SHARON C. GLOTZER, University of Michigan — The question of how densely regular tetrahedra can pack in three dimensions has attracted many researchers in recent years. In the first thermodynamic study of dense phases of the hard tetrahedron system, we recently reported the spontaneous formation of a dodecagonal quasicrystal [1]. The $(3.4.3^2.4)$ approximant of the quasicrystal, with an 82-particle unit cell, was compressed to a packing fraction of 85.03% [1]. Very shortly after, a much simpler crystal of tetrahedron dimers [2] with a slightly higher packing fraction of 85.63% was discovered [3], the current densest packing [3]. Since the dimer crystal packs more densely than the quasicrystal and its approximant, it is thermodynamically favored in the limit of infinite pressure. However, which structure is stable at finite pressures is an open question. Here, we explore the relative thermodynamic stability of these very different ordered phases as a function of packing density.

[1] Haji-Akbari A, Engel M, Keys A S, Zhang X Y, Petschek R, Palffy-Muhoray P, Glotzer S C, Nature 462: 773-777 (2009).
[2] Kallus Y, Elser V, Gravel S, Disc. Comp. Geom 44(2):245-252 (2010).
[3] Chen E R, Engel M, Glotzer S C, Disc. Comp. Geom. 44(2):253-280 (2010).

1:39PM J13.00011 Jamming of frictional tetrahedra , MAX NEUDECKER, Max-Planck-Institute for Dynamics and Self-Organization, Bunsenstr. 10, 37073 Göttingen, STEPHAN ULRICH, University Göttingen, Institute of theoretical physics, Friedrich-Hund-Platz 1, 37077 Göttingen, STEPHAN HERMINGHAUS, MATTHIAS SCHRÖTER, Max-Planck-Institute for Dynamics and Self-Organization, Bunsenstr. 10, 37073 Göttingen — We present experimental results on the packing of polypropylene tetrahedra with 7mm side length. Analysis via X-ray-tomography allows for a detailed analysis of the radial distribution function and the number and type of geometrical contacts. We focus particularly on the dependence of these packing properties on the bulk packing fraction.

1:51PM J13.00012 Rheology of Minimally Jammed Frictionless Rodpiles[1] , JAMES GRAHAM, SCOTT FRANKLIN, Rochester Institute of Technology — The ability of large aspect ratio granular particles to form solid plugs is now well-documented but, apart from a general phenomenological explanation of geometric entanglement, remains unexplained. Recent experiments on the collapse of granular columns [1] suggest that rods with even moderate aspect ratios can maintain angles of repose of 90° or larger, implying that the shear modulus increases continuously with aspect ratio. Our simulations generate minimally jammed packings of frictionless, aspect ratio 1-48 spherocylinders through an energy-minimization process. Once the minimally jammed state is reached, we continue the process to larger packing fractions in order to determine the bulk modulus. Packings are then subjected to infinitesimal strain in order to calculate the shear modulus as a function of particle aspect ratio. Shear simulations can be extended to large strain and used to investigate the long-time reordering of rod-like particles that accompanies macroscopic shear.

[1] M. Trepanier and S. V. Franklin, Phys. Rev. E **82**, 011308 (2010).

[1]This work supprted by NSF DMR #0706353.

2:03PM J13.00013 Couette Shear for Elliptical Particles Near Jamming[1] , SOMAYEH FARHADI, Duke University, ROBERT. P. BEHRINGER COLLABORATION — We have performed 2D Couette shear experiments on systems of photoelastic particles. The particles are identical ellipses with aspect ratio 2. We use the photoelastic property of the disks to obtain the forces acting on a particle. We use two cameras to simultaneously image the particle motion and the photoelastic force response. Using ellipses enables us to understand the effect of particle shape asymmetry on the large-scale behavior on the rheological behavior of granular systems near jamming. Of particular interest are the nematic ordering of the ellipses, the formation of shear bands and the nature of force transmission.

[1]DMR09-06908, NSF 0835742, ARO W911NF-07-1-1031

Tuesday, March 22, 2011 11:15AM - 2:03PM –
Session J14 GSNP: Focus Session: Physics of Active Materials D227

11:15AM J14.00001 Active Currents and Stresses on the cell surface: Clustering, Instabilities and Budding[1] , MADAN RAO, Raman Research Institute/National Centre for Biological Sciences, Bangalore — We study the contractile dynamics of a collection of active polar filaments, such as actin, on a two dimensional substrate, using a continuum hydrodynamic description in the presence of spatiotemporal noise. The steady states, characterized by a variety of phases generically consisting of a transient collection of inward pointing asters. We next study the dynamics of particles advected along these active filaments. This is relevant to the dynamics and organization of a large class of cell surface molecules. We make several predictions regarding the statistics of fluctuations of these passive advective particles which we confirm using fluorescence based experiments. We then show how such active patterning of filaments can give rise to membrane stresses leading to membrane shape deformations.

[1]In collaboration with Kripa Gowrishankar and Satyajit Mayor.

11:51AM J14.00002 Pattern formation in Active Polar Fluids[1] , ARVIND GOPINATH, MICHAEL HAGAN, Martin A Fisher School of Physics, Brandeis University, APARNA BASKARAN, Martin A Fisher School of Physics, Brandeis University — Systems such as bacterial suspensions or cytoskeletal filaments and motility assays can be described within the paradigm of active polar fluids. These systems have been shown to exhibit pattern formation raging from asters and vortices to traveling stripes. A coarse-grained description of such a fluid is given by a scalar density field and a vector polarization field. We study such a macroscopic description of the system using weakly nonlinear analysis and numerical simulations to map out the emergent pattern formation as a function of the hydrodynamic parameters in the context of two specific microscopic models - a quasi-2D suspension of cytoskeletal filaments and motor proteins and a system of self propelled hard rods that interact through excluded volume interactions.

[1]The authors thank the Brandeis MRSEC center for financial support.

12:03PM J14.00003 Non-Equilibrium Dynamics of the Metaphase Spindle , DANIEL NEEDLEMAN, JAN BRUGUES, Harvard University — A wide variety of cellular structures exist in a nonequilibrium steady-state with a constant flux of molecules and energy continuously modifying and maintaining their architecture. Understanding such self-organizing structures is not only crucial for cell biology, but also poses a fundamental challenge for physics, since these systems are materials that behave drastically differently from those that have been traditionally studied in condensed matter physics. Physical theories of active materials have been used to describe the cytoskeleton, but it is still unclear how applicable these theories are to complex biological systems *in vivo*. We are experimentally testing if such phenomenological theories of cytoskeletal behavior can be profitably used to model the metaphase spindle. Our approach is to use polarized light microscopy, spinning disk fluorescence microscopy, single molecule imaging, and magnetic tweezers to quantitatively measure spatial-temporal correlation functions of spontaneous fluctuations in the director, concentration, and internal stress in spindles. We are comparing these measurements with predictions from various continuum theories to determine how best to describe the non-equilibrium dynamics of these structures.

12:15PM J14.00004 Modeling active materials based on self-oscillating gels , VICTOR V. YASHIN, ANNA C. BALAZS, Chemical Engineering Department, University of Pittsburgh, Pittsburgh, PA, 15261 — The Belousov-Zhabotinsky (BZ) reaction in solution is a classical example of an active medium that demonstrates various chemical oscillations and waves, which can be observed visually. Grafting a ruthenium metal-ion complex, the catalyst to the BZ reaction, to a chemo-responsive polymer gel creates an active material (BZ gel), which exhibits periodic volumetric changes in the course of the reaction. The redox oscillations of the catalyst affect the polymer-solvent interactions and cause the periodic swelling and de-swelling of the gel, so that chemo- mechanical energy transduction occurs within the material. We consider a model that couples the polymer gel dynamics and the BZ reaction kinetics; the latter is described by the modified Oregonator model. The model equations are solved numerically in 2D. We demonstrate that the dynamical behavior of the BZ gel can be controlled by a heterogeneous distribution of the catalyst and by such structural features as the solvent-filled voids. The dynamics of an active membrane having the self-oscillating pores is considered as an example.

12:27PM J14.00005 Homeostatic pressure, tumor growth and fingering of epithelial tissues: Some generic physics arguments[1] , THOMAS RISLER, Institut Curie — We propose that one aspect of homeostasis is the regulation of tissues to preferred pressures, which can lead to a competition for space of purely mechanical origin and be an underlying mechanism for tumor growth. Surface and bulk contributions to pressure lead to the existence of a critical size that must be overcome by metastases to reach macroscopic sizes. This property qualitatively explains the observed size distributions of metastases, while size-independent growth rates cannot account for clinical and experimental data. It also potentially explains the observed preferential growth of metastases on tissue surfaces and membranes, suggests a mechanism underlying the seed and soil hypothesis introduced by Stephen Paget in 1889, and yields realistic values for metastatic inefficiency [1]. Treating epithelial tissues as viscous fluids with effective cell division, we find a novel hydrodynamic instability that leads to the formation of fingering protrusions of the epithelium into the connective tissue. Arising from a combination of viscous friction effects and proliferation of the epithelial cells, this instability provides physical insight into a potential mechanism by which interfaces between epithelia and stroma undulate, and potentially by which tissue dysplasia leads to cancerous invasion.

[1] M. Basan, T. Risler, J.-F. Joanny, X. Sastre-Garau, and J. Prost, *HFSP Journal*, **3**, 4, p.265

[1]In collaboration with M. Basan, J.-F. Joanny, X. Sastre-Garau and J. Prost.

1:03PM J14.00006 Hydrodynamics of an Active Smectic , TAPAN CHANDRA ADHYAPAK, SRIRAM RAMASWAMY, Indian Institute of Science, JOHN TONER, University of Oregon — We show that self-driven particles, in suspension or on a substrate, can support striped phases with long-range order in three dimensions and quasi-long-range order in two dimensions. This is in contrast to the situation for smectic phases at thermal equilibrium, which have the same spatial symmetry. We analyse the fluctuation properties of stable active smectics as well as the nature of characteristic instabilities that these systems can display. Our results apply to any active system that spontaneously develops layers, including apolar orientable cells, monolayers of rods either fluidized or shaken and, most significantly, the Rayleigh-Benard instability.

1:15PM J14.00007 Spontaneous Oscillations in Nonlinear Active Solids[1] , SHILADITYA BANERJEE, Syracuse University, TANNIEMOLA B. LIVERPOOL, University of Bristol, M. CRISTINA MARCHETTI, Syracuse University — We present a generic continuum model of a nonlinear active gel with both passive and active crosslinks. The model is relevant for actin gels with passive elasticity provided by ABPs such as filamin-A or α-actinin and dynamic active crosslinkers such as myosin-II. We consider an one dimensional continuum active solid where compressional deformations are coupled to molecular motor dynamics. Three kinds of nonlinearities are incorporated : (a) nonlinear load dependence of unbinding rate of molecular motors, (b) pressure nonlinearities stemming from excluded volume interactions, and (c) nonlinearity due to convection of bound motors along the gel. Unbinding rate nonlinearity stabilizes the oscillatory instabilities predicted by the linear theory and lead to sustained oscillations at intermediate concentrations of ATP. Pressure nonlinearity due to excluded volume interactions stabilizes the contractile instability and leads to a contracted ground state. Our work provides a generic framework for the description of the large scale properties of nonlinear isotropic active solids.

[1]This work is supported by the NSF on grants DMR-MWN-0806511 and DMR-100478.

1:27PM J14.00008 Self-diffusiophoresis in the strongly advecting regime , GARETH ALEXANDER, University of Pennslyvania, ANDREA LIU, University of Pennsylvania — Certain forms of biological motility, such as actin-based propulsion and chromosomal translocation in certain bacteria, have recently been proposed to have their physical origins in the phenomenon of self-diffusiophoresis. In diffusiophoresis, a particle in a fluid with an inhomogeneous concentration of solute will move along the concentration gradient with a well-defined velocity due to surface interactions with the solute. If the particle has the means of generating the concentration gradient itself–by catalyzing a chemical reaction on one side of its surface, for example–then self-diffusiophoresis serves as a mechanism of self-propulsion. Until now, self-diffusiophoresis has been studied under conditions of rapid diffusion, or small Péclet number, where the effects of advection on the solute dispersion can be neglected. However, in the biological examples of interest, the Péclet number is high. We present an analysis of the large Péclet number limit, where diffusion is slow and advection by the fluid flow is the primary means of solute dispersal. The resulting motion is still described in terms of a slip velocity generated in a thin boundary layer, but with a different origin, arising not from diffusion but from local outward flow to carry away the solute together with fluid continuity. A simple model is developed on this basis, contrasted with the rapid diffusion regime, and applied to provide insight into relevant biological processes.

1:39PM J14.00009 Phase transitions and solitons in a rule-based model of active particles , THOMAS IHLE, North Dakota State University — I study the Vicsek model [Phys. Rev. Lett. **75** (1995) 1226] by means of kinetic theory. In this non-equilibrium model, self-driven particles try to align their travel directions with the average direction of their neighbours. At strong alignment, rotational symmetry is spontaneously broken and a global flocking state forms. The alignment is defined by a stochastic rule, not by a Hamiltonian. The corresponding interactions are non-additive and are typically of genuine multi-body nature. Due to this and the discreteness of the time evolution, the kinetic equations are different from the usual ones found in textbooks. I derive the phase diagram for the flocking transition and show that it agrees very well with simulations at large particle velocities and is qualitatively different from the one of a continuous version of the Vicsek-model. The theory starts with the Liouville equation, the hydrodynamic equations are derived by a Chapman-Enskog expansion. These equations contain more terms than previously postulated; their coefficients are given in terms of microscopic parameters. I show how a large-wavelength instability of the flocking state leads to an inhomogeneous soliton state which is very stable and shows a first-order phase transition to the disordered state. I determine the speed of the solitons, investigate the hysteresis of the transition and estimate the system size beyond which the first order nature of the transition should be visible in computer simulations.

1:51PM J14.00010 Collective motion of vibrated polar granular disks[1] , OLIVIER DAUCHOT, DESEIGNE JULIEN, CEA-Saclay / SPEC, HUGUES CHATE, CEA-Saclay / Chate, DYCOACT COLLABORATION — In many interesting situations, the interactions among self-propelled agents lead to the spontaneous emergence of self-organized collective motion. The ubiquity of the phenomenon at all scales raises the question of the existence of some underlying universal mechanisms. Recent numerical and analytical studies have confirmed the existence of a transition from a disordered state at large noise to a state with various collective properties reflecting the local symmetry of the particles and their interactions. Though, there are still very few experimental situations where the onset of collective motion can be attributed to spontaneous symmetry breaking. Here, we report on experiments conducted with both polar self propelled and a-polar Brownian disks and by comparing the dynamics of both systems in the same experimental conditions, we demonstrate without ambiguity that collective motion emerges from the interplay of self-propulsion and hard-core repulsion only [1]. Interestingly the alignment, which has no nematic origin, is effectively induced during the collisions because of the self propulsion.

[1] Phys. Rev. Lett 105 135702 (2010)

[1]Supported by ANR DYCOACT.

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J15 DMP GMAG FIAP: Focus Session: Spins in Semiconductors - Spin Currents II

11:15AM J15.00001 Spin-Seebeck effect: Local nature of thermally induced spin currents in GaMnAs[1]

, ROBERTO MYERS, Department of Materials Science and Engineering, The Ohio State University, Columbus, Ohio — The spin-Seebeck effect refers to a spatial distribution of spins in a ferromagnetic material induced by a thermal gradient. This macroscopic spatial distribution of spins is several orders of magnitude larger than the spin diffusion length [1]. Here we describe measurements of the spin-Seebeck effect in the ferromagnetic semiconductor, GaMnAs [2]. The thermally induced spatial distribution of spins is inferred from the sign and magnitude of the inverse spin Hall voltage generated from local spin currents in platinum bars that are in electrical contact with the ferromagnetic material. From an experimental point of view, GaMnAs provides unique measurement geometries since the magnetic easy axes can be engineered in different directions and the low Curie temperature makes it convenient to perform spin-Seebeck measurements across the magnetic phase transition. Using different experimental configurations we measure either the isolated spin-Seebeck signal, the planar and transverse Nernst effect, or a combination of the spin-Seebeck and Nernst effects. One of the most intriguing aspects of the spin-Seebeck effect is the observation that the spatial distribution of spins is maintained across electrical breaks revealing that the effect does not arise from a longitudinal spin current of charge carriers.

[1] K. Uchida, S. Takahashi, K. Harii, J. Ieda, W. Koshibae, K. Ando, S. Maekawa, E. Saitoh, *Nature* **455**, 778 (2008).
[2] C. M. Jaworski, J. Yang, S. Mack, D. D. Awschalom, J. P. Heremans, R. C. Myers, *Nature Materials* **9**, 898 (2010).

[1]In collaboration with C. M. Jaworski, J. Yang, S. Mack, D. D. Awschalom, and J. P. Heremans. This work was supported by the NSF and the ONR.

11:51AM J15.00002 Theory of the Anomalous Hall Effect in the Insulating Regime

, XIONG-JUN LIU, XIN LIU, JAIRO SINOVA, Department of Physics, Texas A&M University, College Station, Texas 77843-4242, USA — The anomalous Hall effect (AHE) has been an enigmatic problem that has resisted theoretical and experimental assault for almost one century. The AHE in the metallic regime has been separated into different contributions, i.e. skew scattering side jump and intrinsic contribution. However, the recent experiments on AHE in the insulating regime discover a qualitatively different behavior described by a scaling relation which is different from that in the metallic regime. The new finding cannot be explained by available microscopic theories of metals based on impurity scattering. Here we present a theory to study the anomalous Hall conductivity (AHC) in this regime With this theory we calculate the lower and upper limits for the AHC by taking simple assumptions of the impurity distributions. Our results are quantitatively in agreement with the experimental discoveries, and thus provides the understanding of the AHE in the insulating regime.

12:03PM J15.00003 Strain manipulation of anomalous Hall response in GaMnAs micromechanical buckled Hall beam structure

, CHANUK YANG, Seoul National University, HYUNG KOOK CHOI, TAI HOON KIM, YUN DANIEL PARK — The non-magnetic manipulation of magnetic properties of diluted magnetic semiconductors (DMS) has recently received much attention, such as magnetization by electric field [1], and magnetic anisotropy by strain engineering [2]. Especially, in GaMnAs, the spin-orbit interactions (SOIs) are highly strain-dependent and the applied magnetic field plays a crucial role in determining magnetic anisotropies (MA), anisotropic magnetoresistances (AMR), and the intrinsic anomalous Hall effect (AHE) [3]. Here, we present AHE of local-strain-induced GaMnAs micro-Hallbeam by fabricating mechanical suspended structure. We observe a suppression of the AHE that varies symmetrically about the centre of the buckled beam due to strain-related SOIs.

[1] H. Ohno et al., Nature 408, 944 (2000); Y.D. Park et al. Science 295, 651 (2002)
[2] T. Dietl et al. PRB 63, 195205 (2001); M. Glunk et al., PRB 79,195206 (2009); J. Wenisch et al., PRL 99, 077201 (2007); A. W. Rushforth et al., PRB 78, 085314 (2008)
[3] Nagaosa, N. et al., Reviews of Modern Physics 82 (2), 1539 (2010).

12:15PM J15.00004 The spin-Seebeck effect in a GaMnAs/MnAs bilayer

, CHRISTOPHER JAWORSKI, Department of Mechanical Engineering, The Ohio State University, JING YANG, Department of Materials Science and Engineering, The Ohio State University, SHAWN MACK, DAVID AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, JOSEPH HEREMANS, Department of Mechanical Engineering and Department of Physics, The Ohio State University, ROBERTO MYERS, Department of Materials Science and Engineering and Department of Physics, The Ohio State University — The spin-Seebeck effect, recently discovered in ferromagnetic metals such as permalloy, semiconductors such as GaMnAs and insulators such as YIG, consists of a thermally generated spin redistribution. This effect is measured by detecting an inverse spin Hall voltage that varies spatially across a sample due to the thermally generated local spin currents. Here, we describe measurements of the spin-Seebeck effect in metallic ferromagnetic MnAs thin films grown on GaMnAs. The difference in H_c and T_c of each layer allows independent measurement of spin-Seebeck signals arising from MnAs from that of GaMnAs. We discuss the effect of the exchange bias between these layers on the spin-Seebeck effect above and below the magnetic phase transition. Work support in parts by NSF, NSF-CBET-0754023, ONR, and DMR-0820414.

12:27PM J15.00005 Magnetoresistance in Lateral GaMnAs devices with Nano-constrictions

, BHIM PAUDEL, GRANT RILEY, Miami University, LEONIDAS OCOLA, Argonne National Lab, XINYU LIU, JACEK FURDYNA, University of Notre Dame, KHALID EID, Miami University — Mn-doped GaAs (or GaMnAs) offers opportunities to demonstrate both new device concepts with added functionality and new phenomena in condensed matter physics, since it is both a ferromagnet and a semiconductor. We will present our recent results on fabricating and characterizing GaMnAs-based nano- devices. The resistance of these deep-nanoscale devices can be manipulated either by varying the applied voltage or via an external magnetic field. The nano-devices were prepared using electron-beam lithography and wet chemical etching. The magnetoresistance of the devices was as high as 50% at 4.2k and the behavior was different from previous results reported in literature.

12:39PM J15.00006 A grate field-dependent change of magnetic damping in Fe/(Ga,Mn)As

, SATOI KOBAYASHI, KEITA SUDA, HIRO MUNEKATA, Tokyo Institute of Technology — Reported here is the field dependence of the magnetic damping in the photo-induced precession of magnetization in three different samples, a simple (Ga,Mn)As, two hybrids Pt/(Ga,Mn)As and Fe/(Ga,Mn)As. The Mn content $x$is $x = 0.045$ for all cases. In (Ga,Mn)As, the precession frequency ω increases and the precession lifetime τ decreases with increasing a lateral, external field applied along the easy axis, whereas the $\omega\tau$ product is hardly changed. Similar trend is observed in Pt/(Ga,Mn)As, except that the $\omega\tau$ product is smaller than that of (Ga,Mn)As. An inverse value of the $\omega\tau$ product, so called the Gilbert damping constant α, is $\alpha = 0.1$ and 0.15, respectively, for (Ga,Mn)As and Pt/(Ga,Mn)As. The enhanced magnetic damping in Pt/(Ga,Mn)As can be understood qualitatively in terms of the spin pumping. In Fe/(Ga,Mn)As, the $\omega\tau$ product around the zero field is even smaller than that of Pt/(Ga,Mn)As, being indicative of a larger damping ($\alpha \sim 0.26$), whereas the $\omega\tau$ product increases steeply with an external field. At around 400 Oe and higher, the $\omega\tau$ product saturates at the value comparable to that of a simple (Ga,Mn)As. Taking magnetization data into account, a great field-dependent change in damping could be attributed to the spin-wave excitation at the Fe/(Ga,Mn)As interface caused by non-parallel magnetization configuration between Fe and (Ga,Mn)As in microscopic scale.

12:51PM J15.00007 Interfacial Spin Filtering at Copper/GaMnAs Contacts[1] , KHALID EID, BHIM PAUDEL, GRANT RILEY, Miami University, XINYU LIU, JACEK FURDYNA, University of Notre Dame — We determine the spin injection efficiency using a single ferromagnetic film without the need for a spin-detection layer. This is accomplished by studying the temperature dependence of the specific contact resistance (AR_C) of a copper/GaMnAs contact using a circular transmission line method. AR_C is as low as $5x10^{-8}$ Ωcm^2, and decreases slowly with decreasing temperature T. However, as T approaches Curie temperature T_C, AR_C abruptly jumps to about double its initial value. We suggest that this behavior arises from the suppression of one of the two spin conduction channels, which results in substantial spin polarization.

[1]Supported by the Research Corporation for Science Advancement.

1:03PM J15.00008 Spin-dependent Transport in GaAs/MnAs Core/shell Nanowires , J. LIANG, J. WANG, N.S. DELLAS, B.J. COOLEY, S.E. MOHNEY, R. ENGEL-HERBERT, M.H.W. CHAN, N. SAMARTH, Center for Nanoscale Science and Materials Research Institute, Penn State University, University Park PA 16802. — The integration of a metallic ferromagnet (FM) with a semiconductor (S) in axially- and radially modulated nanowires (NWs) has the potential to open up new opportunities in nanospintronics. We describe a comprehensive study of the structure, magnetism and electrical transport in hybrid core/shell S(GaAs)/FM(MnAs) NWs synthesized by molecular beam epitaxy. This is an unusual system where the competition between magnetocrystalline and shape anisotropies in the FM shell creates a magnetic ordering regime which is distinct from conventional FM metal NWs. We report four probe measurements of the temperature dependence of conductivity and the magnetoresistance (MR) in single NWs over a temperature range 0.5 K - 300 K and in magnetic fields ranging up to 80 kOe. Assuming that electrical transport is dominated by the metallic shell, we use the measured anisotropic MR in conjunction with micromagnetic simulations to gain insight into the magnetization reversal process of the FM shell. We also discuss the possible origins of a striking negative linear MR at high field which becomes more pronounced with increasing temperature. Supported by NSF-MRSEC and ONR.

1:15PM J15.00009 Ohmic spin injection from a half-metal at finite temperatures: Is the conductivity mismatch problem relevant? , JAMES GLASBRENNER, ALEKSANDER WYSOCKI, KIRILL BELASHCHENKO, University of Nebraska - Lincoln — Spin injection from a normal ferromagnet into a semiconductor requires a highly-resistive tunnel or Schottky barrier at the interface to overcome the conductivity mismatch problem. This barrier limits the current that can be achieved in a device. A half-metallic ferromagnet used as a spin injector obviously overcomes this problem at zero temperature, but the situation at finite temperatures is nontrivial. We argue that the two-current model is inapplicable to half-metals, and that Ohmic (barrierless) spin injection from a half-metal is possible even at finite temperatures. This conclusion is reached using an intuitive model which sums up multiple scatterings at the interface. To complement this model, we calculate the spin injection efficiency for a half-metallic electrode using a single-band tight-binding model with explicit statistical averaging over thermal spin fluctuations. The results are contrasted with the case of a normal ferromagnet. We also consider a practically interesting case of a CrAs electrode within the tight-binding LMTO method.

1:27PM J15.00010 MnAs/Al(AsSb)/InAs Heterostructure-Based Spin LEDs[1] , H. ZHANG, E.D. FRASER, S. HEGDE, J. KWON, J.B. HATCH, H. LUO, G.P. LINDBERG, B.A. WEINSTEIN, B.D. MCCOMBE, State University of New York at Buffalo — MnAs is a promising spin alignment material for spin-injection into InAs-based structures due to its well studied structural and magnetic properties. A well known difficulty of spin injection from a ferromagnetic metal spin aligner into a semiconductor is the so-called conductivity mismatch, which has been overcome via tunnel barrier contacts.[2,3] Lattice matching the tunnel barrier to the active region is important because a highly strained interface and resulting defects can reduce spin polarization of the injected carriers. We report development of a spin-LED structure with a lattice matched $AlAs_{0.16}Sb_{0.84}$ tunneling barrier between the MnAs spin aligner and an InAs quantum well. The composition was characterized through XRD and Raman spectroscopy. Sample growth, characterization, LED fabrication and optical polarization studies of electroluminescence in the 3 micron spectral region will be discussed.

[1]This work is supported partly by the NSF grant NSF-ECCS-0824220.
[2]B.T. Jonker *et al.*, PRB **62**, 8180 (2000).
[3]X. Jiang *et al.*, PRL **94**, 056601 (2005).

1:39PM J15.00011 Efficient injection of spin-polarized electrons from MnAs contacts into GaAs quantum well LEDs[1] , EVERETT FRASER, SHRIDHAR HEGDE, LARS SCHWEIDENBACK, ANDREAS RUSS, ATHOS PETROU, HONG LUO, University at Buffalo, The State University of New York, GEORGE KIOSEOGLOU, University of Crete — Recent studies of ferromagnetic MnAs have revealed a wide range of properties desirable for spintronic applications. In this work, ferromagnetic MnAs contacts have been used to inject spin polarized electrons into AlGaAs(n)/GaAs(i)/AlGaAs(p) light emitting diodes. The band-edge electroluminescence emitted from these devices has a saturation circular polarization of 26% at 7K. The circular polarization was found to track the out of plane magnetization of MnAs, confirming spin injection. Using optical pumping measurements, the corresponding electron spin polarization was determined to be 52%. Emission persists up to room temperature, with a saturation circular polarization of 6%. The improved performance over similar structures is attributed to the use of MnAs/AlGaAs Schottky barrier tunneling and minimal interdiffusion of Mn ions near the materials interface.

[1]Work at SUNY was supported by NSF, ONR, and the Rustgi professorship.

1:51PM J15.00012 Oscillatory spin polarization and magneto-optical Kerr effect in Fe_3O_4 thin films on GaAs(001) , YAN LI[1], WEI HAN, A.G. SWARTZ, K. PI, J.J.I. WONG, Dept. of Physics and Astronomy, UC Riverside, S. MACK, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106, R.K. KAWAKAMI, Department of Physics and Astronomy, University of California, Riverside, CA 92521 — Magnetite is an attractive material for spin injection and detection, because the theory predicts completely negative spin polarization at the Fermi level at room temperature. We fabricated high quality Fe_3O_4 films on GaAs (001) by molecular beam epitaxy. The Fermi level spin polarization of the Fe_3O_4 film was probed using the ultrafast optical measurement of ferromagnetic proximity polarization (FPP). The systematic thickness dependence of FPP and MOKE were measured on wedged Fe_3O_4 films on GaAs(001), and similar oscillatory and sign reversing behaviors were observed even though the two measurements rely on different mechanisms (spin dependent electron reflection for FPP, and optical transitions for MOKE). Quantum confinement of the t_{2g} states near the Fermi level provides an explanation for the similar thickness dependences of the FPP and MOKE oscillations.

[1]Current address: NHMFL-LANL, MS E536, Los Alamos, NM 87545

2:03PM J15.00013 TMR study of GaMnAs/AlGaAs:Be/GaMnAs trilayers[1] , JOSEPH HAGMANN, XINYU LIU, MALGORZATA DOBROWOLSKA, JACEK FURDYNA, Department of Physics, University of Notre Dame, Notre Dame, IN 46556, USA, TAEHEE YOO, SUNGWON KHYM, SANGHOON LEE, Department of Physics, Korea University, Seoul 136713, South Korea — GaMnAs/GaAs:Be/GaMnAs trilayers have recently demonstrated antiferromagnetic (AFM) coupling between the two ferromagnetic (FM) layers, mediated by holes in the spacer layer. In this work, GaMnAs/Al_xGa_{1-x}:Be/GaMnAs trilayer samples with varying Al concentrations were fabricated into magnetic tunnel junction (MTJ) devices with range of pillar diameters to measure tunneling magnetoresistance (TMR) under various conditions. SQUID measurements were use to measure the magnetization of the samples, including switching fields for parallel and antiparallel magnetization alignments of the FM layers. TMR was observed in the sample with $Al_{0.22}Ga_{0.78}As$:Be spacer, but was massively suppressed in the samples with lower Al content. The presence of holes in the spacer layer is shown to suppress TMR. This illustrates the difference in conditions for TMR and for AFM interlayer coupling.

[1]Supported by NSF Grant DMR-1005851 and OISE-1015458.

Tuesday, March 22, 2011 11:15AM - 2:15PM –
Session J16 DMP GMAG: Focus Session: Magnetic Nanostructures III D173

11:15AM J16.00001 Studies of isolated and interacting ferromagnetic gapped nanorings[1] , JIE LI, SHENG ZHANG, JASON BARTELL, CHRIS GRIGAS, Penn State University, CRISTIANO NISOLI, Los Alamos National Lab, PAUL LAMMERT, VINCENT CRESPI, PETER SCHIFFER, Penn State University — We have used micromagnetic simulation and magnetic force microscopy (MFM) to study isolated and interacting permalloy nanorings that are lithographically fabricated with gaps that prevent a rotationally symmetric magnetic state. The gapped nanorings have inner and outer radii of 200 and 300 nm respectively, and the gap has a subtended width of ∼20 degrees. The nanorings generate a strong magnetic field only in the gap, and thus the magnetization states of gapped nanorings are much more accessible to MFM imaging than complete rings. We have investigated the properties of these gapped nanorings, including the anisotropy in their coercive field and the relative alignment of the magnetic polarization in coupled pairs.

[1]We acknowledge the financial support from DOE and Army Research Office.We are grateful to Professor Chris Leighton and Mike Erickson for assistance with sample preparation.

11:27AM J16.00002 Broad-Band FMR of Patterned Square Arrays of Square Permalloy Antidots[1] , VINAYAK BHAT, University of Kentucky, JOSEPH SKLENAR, JOHN KETTERSON, Northwestern University, LANCE DELONG, University of Kentucky — We have used electron beam lithography to pattern 25-nm-thick Permalloy films with square arrays of square antidots of size D = 300, 400, 500 and 700 nm and same lattice constant d = 1000 nm, using a lift-off technique. Broadband FMR[2] was used to observe localized modes[3,4] showing four-fold rotational symmetry for in-plane DC magnetic field. We have studied FMR spectra spanning the ferromagnetic hysteresis regime around 250 MHz, up to the saturation regime ending near 14 GHz, and observe the appearance and disappearance of various FMR modes, especially at frequencies below 7 GHz. We have observed history-dependent modes below 3 GHz that may be associated with domain walls.

[1]UK research supported by U.S. DoE Grant No. DE-FG02-97ER45653.
[2]C. C. Tsai et al., Rev. Sci. Instrum **80**, 023904 (2009)
[3]C. T. Yu, M. J. Pechan, and G. J. Mankey, Appl. Phys. Lett. **83**, 3948 (2003)
[4]Minghui Yu et al., J. Appl. Phys **101**, 09F501 (2007)

11:39AM J16.00003 Broadband Magnetic Resonance Measurements on Periodic Patterned Disc and Hole Arrays , J. SKLENAR, Northwestern University, V.S. BHAT, L. DELONG, University of Kentucky, V. METLUSHKO, University of Illinois, Chicago, C.C. TSAI, Chang Jung Christian University, Taiwan, O. CHERNYASHEVSKYY, Northwestern University, K. RIVKIN, Seagate Technologies, J.B. KETTERSON, Northwestern University — We have made broadband ferromagnetic resonance measurements on patterned permalloy arrays consisting of circular dots (discs) and both square and circular anti-dots (holes). We employ a transmission meander line approach as opposed to a resonant cavity technique, and cover the frequency range 10MHz to 20GHz. Experiments are performed at a fixed frequency by sweeping the field (through positive and negative values) and at a fixed field while varying the frequency; both magnetic field and frequency modulation are employed to suppress noise and background effects. Experiments on hole arrays show two dominant resonances which from their symmetry appear to be standing spin waves centered at the X- points of the square Brillouin zone. Low field measurements on disc arrays where the field is swept over varying ranges in the region where the sample is hysteretic while tracking the history dependent disappearance and reappearance of the uniform FMR mode, allows a determination of the phase boundaries separating the single and double vortex states, and are in agreement with simulations by Rivkin.

11:51AM J16.00004 Exciton-Mn ion interaction in CdTe quantum dots[1] , ANNA TROJNAR, MAREK KORKUSINSKI, EUGENE KADANTSEV, PAWEL HAWRYLAK, Institute for Microstructural Sciences, NRC, Ottawa, Canada, K1A0R6 — We develop a microscopic theory of optical properties of quantum dots containing a single magnetic ion [1,2] which includes electron-hole correlations, short range exchange of Mn ion with electron and with heavy hole, long range electron-hole exchange, quantum dot anisotropy and external strong magnetic field. A new quantum interference (QInt) effect between electron-hole Coulomb scattering and scattering by Mn ion is obtained. Special role is played here by configurations with electron and hole on the p-shell and degenerate with it configurations with electron (hole) on s-shell and hole(electron) on a d-shell. QInt is shown to significantly reduce exciton-Mn coupling. The signature of this QInt effect in emission and absorption spectrum is discussed. The effect of strong magnetic field on the characteristic emission spectrum is discussed and the limitations of the spin model are established.

[1] S.-J.Cheng et al, Eur. Phys. Lett. 81, 37005 (2008)
[2] L.Besombes, Phys. Rev. Lett. 93, 207403 (2004).

[1]Supported by NSERC, CIFAR, NRC-CNRS CRP, QuantumWorks.

12:03PM J16.00005 Antiferromagnetic coupling in cobalt atomic clusters on (110) surface of tungsten , RENAT F. SABIRIANOV, University of Nebraska at Omaha, PAVEL LUKASHEV, AXEL ENDERS, University of Nebraska - Lincoln — We report results of the first principles calculations on the structural and magnetic properties of cobalt atomic clusters on (110) surface of tungsten. We found that for certain geometry these clusters can exhibit antiferromagnetic order. The result is unexpected, as in the bulk as well as in the thin films and free standing clusters Co always exhibits ferromagnetic structure. We compare results for Co with the ones for the analogues Fe atomic clusters. We found that Fe clusters deposited on (110) surface of tungsten tend to couple ferromagnetically similar to bcc Fe in considered geometries. In our calculations we analyzed different configurations of atomic islands, in particular N=3, 4, 5, 6, 8, 12, where N is the number of atoms in the cluster. We perform full structural and magnetic relaxation, and we show that depending on the geometry and number of cobalt atoms in the cluster, the system can be non-magnetic (N=4, 6, 8), ferromagnetic (N=3, 5) and antiferromagnetic or ferrimagnetic (N=4, 12). We present phenomenological model to explain this intriguing magnetic properties of Co atomic islands on (110) surface of tungsten.

12:15PM J16.00006 Non-liftoff block copolymer nanolithography of magnetic nanodot arrays , A. BARUTH, M.D. RODWOGIN, A. SHANKAR, M.A. TORIJA, M.J. ERICKSON, M.A. HILLMYER, C. LEIGHTON, University of Minnesota — Nanolithographic techniques based on self-assembled block copolymer templates offer exceptional potential for fabrication of large-area nanostructure arrays from a wide variety of functional materials. Despite significant progress with control of the template ordering, and development of pattern transfer schemes, significant issues exist with common techniques such as lift-off and etching. Here, we demonstrate successful execution of a nanolithographic process based on climate-controlled solvent annealing of easily degradable cylinder-forming poly(styrene-*b*-lactide) block copolymer films that avoids both lift-off and the most challenging aspects of etching. Essentially, we use an overfill/planarize/etch-back "Damascene-type" process, exploiting the large Ar ion beam etch rate contrast between polystyrene and typical metals. The process is demonstrated via formation of a large-area array of 12 nm thick, 25 $\pm$ 3 nm diameter $Ni_{80}Fe_{20}$ nanodots ($\sim$0.4 x 10^{12} dots/in^2) with hexagonally-close-packed local order. Extensive microscopy, magnetometry, and electrical measurements provide detailed characterization of the pattern formation and fidelity. We argue that this generic approach can be applied to a wide variety of materials and is scalable to even smaller feature sizes. Funded by NSF MRSEC.

12:27PM J16.00007 Investigating the origin of the magnetic switching field distribution in bit patterned media , OLAV HELLWIG, San Jose Research Center, Hitachi GST, BASTIAN PFAU, CHRISTIAN GUENTHER, Helmholtz-Zentrum Berlin, STEFAN EISEBITT, Technical University Berlin, THOMAS HAUET, Nancy University, ELIZABETH DOBISZ, XIAOYU XU, YANEY DEBORAH, San Jose Research Center, Hitachi GST — Bit patterned media (BPM) is a promising approach for extending densities in magnetic data storage. One critical challenge for BPM is a tight magnetic switching field distribution (SFD), i.e. the bit-to-bit variations in reversal field. The SFD has three components: the dipolar interactions between neighboring islands within the array, pattern non-uniformities, such as variations in island size, position or shape and the so-called intrinsic SFD of each individual island, which is due to variations in the intrinsic magnetic material properties. We use soft X-ray spectro-holography and high resolution transmission electron microscopy (TEM) to study the origin of the magnetic SFD in BPM. For this we fabricated pattern arrays with 80 nm islands by e-beam lithography and integrated these into a SiN membrane design suitable for x-ray transmission studies. After identifying individual easy and hard to switch islands in the tails of the SFD we performed plane-view TEM analysis of these islands and correlate their magnetic with their structural properties, such as misaligned grains or irregular island shapes.

12:39PM J16.00008 Control of Magnetic States of Cobalt Nanorings by an External Azimuthal Field[1] , NIHAR PRADHAN, Mount Holyoke College and UMass Amherst, MA, USA, TIANYU YANG, UMass Amherst, MA, USA, ABBEY LICHT, YIHAN LI, Mount Holyoke College, South Hadley, MA, USA, MARK TUOMINEN, UMass Amherst, MA, USA, KATHERINE AIDALA, Mount Holyoke College, South Hadley, MA, USA — Ferromagnetic nanorings attract interest due to their potential application in high density data storage and Magnetoresistive Random Access Memory (MRAM) devices. These nanorings show multidomain stable states that need to be well controlled by external in-plane or circular magnetic fields. This talk presents a new method to generate circular magnetic fields to control the magnetic states in different geometries of Cobalt nanoring structures, of varying diameter, width and thickness. A solid platinum AFM tip was used to pass current through a single nanoring, generating a circular magnetic field. In applying this field we were able to change the state of the individual ring without affecting the states of other neighboring rings. The evolution of the magnetic states of individual symmetric and asymmetric Cobalt nanorings with applied azimuthal field will be presented.

[1]The work was supported by the National Science Foundation under DMR Grant 906832 and Research Corporation Grant 7889

12:51PM J16.00009 Rotationally induced magnetic chirality in clusters of single-domain permalloy islands and gapped nanorings[1] , SHENG ZHANG, JIE LI, JASON BARTELL, PAUL LAMMERT, VINCENT CRESPI, PETER SCHIFFER, Department of Physics and Materials Research Institute, Pennsylvania State University, University Park, PA 16802 — We have studied magnetic moment configurations of clusters of single-domain ferromagnetic islands in different geometries.[2] The magnetic moments of these clusters are imaged by MFM after rotational demagnetization, following our previous protocols.[3] We observed that two types of the clusters showed a significant imbalance of their two-fold degenerate ground states after demagnetization, and this inequality is correlated to the rotational direction of the demagnetization. A similar imbalance was also found in nano-scale rings with a small gap: the chirality of their magnetic state can be precisely controlled by the rotational direction during demagnetization.

[1]We acknowledge the financial support from DOE and Army Research Office. We are grateful to Prof. Chris Leighton and Mike Erickson for assistance with sample preparation.

[2]J. Li , S. Zhang, J. Bartell, C. Nisoli, X. Ke, Paul E. Lammert, Vincent H. Crespi, and P. Schiffer, Physical Review B **82**, 134407 (2010).

[3]R. F. Wang, C. Nisoli, R. S. Freitas, J. Li, W. McConville, B. J. Cooley, M. S. Lund, N. Samarth, C. Leighton, V. H. Crespi, P. Schiffer, Nature **439**, 303 (2006).

1:03PM J16.00010 Chirality control and vortex manipulation in asymmetric Co dots[1] , KAI LIU, University of California - Davis — Magnetic vortices in sub-micron sized dots have gained considerable interests in recent years due to their fascinating physics and potential applications in information storage, spin-torque oscillators, and magnetic memory and logic devices. Reproducible control of the vortex chirality is of critical importance for these studies. Here we report on two distinctly different chirality control mechanisms in asymmetric Co dots. Arrays of Co dots were fabricated using electron beam lithography and the circular symmetry was broken by introducing a flat edge. Below a critical diameter and/or thickness, chirality control is achieved by the nucleation of a single vortex within each dot, as conventionally observed. The vortex can be manipulated to annihilate at particular sites under different field orientations and cycle sequences. Interestingly, above these critical dimensions a new chirality control mechanism is realized by the nucleation and subsequent coalescence of double vortices, resulting in a single vortex at remanence with the *opposite* chirality as found in smaller dots. Magneto-optical Kerr effect and magnetic force microscopy measurements confirm this new process. Micromagnetic simulations not only reproduce the experimentally observed behavior, but also elucidate the delicate interplay between exchange, demagnetization, and Zeeman energies and the role of fractional vortices bound to the dot edge.

[1]Work done in collaboration with Randy K. Dumas, Dustin A. Gilbert, Nasim Eibagi, Thomas Gredig, Chang-Peng Li, and Ivan K. Schuller, supported by the NSF (ECCS-0725902, ECCS-0925626, DMR-1008791), AFOSR, and CITRIS.

1:39PM J16.00011 Manipulation of Magnetization States of Permalloy Nanorings by an External Azimuthal Field[1] , TIANYU YANG, NIHAR PRADHAN, ABBY GOLDMAN, MOUREEN KEMEI, ABBEY LICHT, YIHAN LI, MARK TUOMINEN, University of Massachusetts Amherst, KATHERINE AIDALA, Mount Holyoke College — This experimental research investigates a new method of manipulating the magnetic states of ferromagnetic nanorings using a circular magnetic field directed along the ring circumference. This type of azimuthal field can naturally select a vortex magnetization of desired chirality. The understanding of the magnetization switching behavior in an azimuthal field could lead to new designs of practical magnetic data storage devices. Symmetric and asymmetric nanorings made of permalloy are fabricated by a standard technique using electron-beam lithography and e-beam evaporation. Azimuthal fields are generated by passing current through an atomic force microscope tip, which is positioned at the center of the ring. The magnetic field direction and magnitude are controlled by the current. We demonstrate control over switching from an onion state to a vortex state, and also between two vortex states, using magnetic force microscopy to image the resulting magnetic states.

[1]This work was supported by NSF grants DMR-0907201 CMMI-0531171

1:51PM J16.00012 Magnetization reversal of surface and subsurface Co/Pt multilayers in a porous matrix , B.J. KIRBY, NIST, M.T. RAHMAN, Univ. of Minnesota, R.K. DUMAS, Univ. of Gothenberg, J.E. DAVIES, NVE Corp., KAI LIU, Univ. of California - Davis, C. LAI, Tsing Hua Univ. — Deposition of magnetic multilayers onto porous host matrices has been studied as a simple and cost-effective method for fabrication of nano-patterned magnetic arrays [1]. For such structures, the magnetic reversal properties of the surface multilayer are twofold dependent on the size and depth of the host pores. First, the pore size determines the lateral size of the surface multilayer with respect to that of a single domain. Second, the pore size determines the amount and location of magnetic material within the pore - material that can exchange couple to the surface multilayer. To study these effects, we have used polarized neutron reflectometry to measure the structural and field-dependent magnetic depth profiles of a series of Co/Pt multilayers deposited on nanoporous alumina (diameter: 13, 20, or 28 nm). Despite the film porosity, we observe robust spin-dependent reflectivities, providing strong sensitivity to interfaces throughout the structure. The determined nuclear profiles show impressive agreement with cross-sectional transmission electron microscopy, and the magnetic profiles feature clearly distinct surface and subsurface magnetizations. The surface magnetization reversal and the role of exchange coupling will be discussed. [1] M. T. Rahman, et al., APL. 94, 042507 (2009).

2:03PM J16.00013 Hysteresis-Loop Overskewing , RALPH SKOMSKI, Dept. Physics & Astr. and NCMN, University of Nebraska, T.A. GEORGE, D.J. SELLMYER — The performance of permanent magnets is largely determined by the magnetostatic energy stored in free space (energy product), which depends on both materials properties and magnet geometry. The latter usually differs from laboratory shapes such as spherical samples, and demagnetizing-field corrections must be applied to compare different geometries. However, in nanostructures, especially in thin films, the macroscopic demagnetizing factors D predicted from Maxwell's equations [1] yield unphysical overskewed hysteresis loops [2]. The overskewing is probably a nanoscale effect, but its origin has remained controversial. Our explanation is that nanoscale magnetization processes violate a main condition for the applicability of macroscopy demagnetizing factors, namely the uniform character of the magnetization. In bulk magnets, the magnetization inhomogeneities effectively average to zero, but this is no longer the case if any of the dimension of the magnet becomes small. We explicitly consider granular thin films, where we find a real-structure dependent reduction D, as contrasted to the sometimes assumed infinite slope $M(H)$ at coercivity. — This research is supported by BREM (RS), ARPA-E, DOE (DJS), and NCMN. — **References:** [1] J. A. Osborn, Phys. Rev. **67**, 351 (1945); [2] R. Skomski, J.- P. Liu, and D. J. Sellmyer, Phys. Rev. B **60**, 7359 (1999).

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J17 DMP GMAG: Focus Session: Bulk Properties of Complex Oxides - Ferrites + Vanadates D174

11:15AM J17.00001 New structural phase transition in $Bi_2(Fe_{4-x}Mn_x)O_{10-x}$ complex oxides and it implications in the mullite family of materials[1] , PATRICIA KALITA, ANDREW CORNELIUS, HiPSEC & Dept. of Physics and Astronomy, University of Nevada Las Vegas, Las Vegas, NV, USA, STANISLAV SINOGEIKIN, Geophysical Lab., Carnegie Institution of Washington, Washington, DC, USA, KRISTINA LIPINSKA, OLIVER HEMMERS, Harry Reid Center for Environmental Studies, University of Nevada Las Vegas, NV, USA, MICHAEL LUFASO, ZACHARY KANN, Dept. of Chemistry, University of North Florida, Jacksonville, FL, USA, HARTMUT SCHNEIDER, Inst. of Crystallography, University of Koeln, Koeln, Germany — Complex oxides with the mullite crystal structure belong to the most important phase in both traditional (porcelains and alumino silicate refractories) and advanced ceramics (heat exchangers, shock resistant composites, optical devices). New complex oxides in the mullite family $Bi_2(Fe_{4-x}Mn_x)O_{10-x}$ were synthesized and characterized. Using synchrotron x-ray diffraction we demonstrate a new structural phase transition in $Bi_2(Fe_{4-x}Mn_x)O_{10-x}$ induced by pressure. We contrast it with the structural stability for mullite senso stricto $Al_{4+2x}Si_{2-2x}O_{10-x}$ where we did not observe any phase transition.

[1]DOE-NNSA DE-FC08-01NV14049. DOE-BES, DOE-NNSA, NSF, DOD -TACOM, the W.M. Keck Found. DOE-BES, W-31-109-ENG-38

11:27AM J17.00002 The role of charge and orbital order for the Verwey transition in Fe_3O_4 , S. DE JONG, R. KUKREJA, M. HOSSAIN, C. BACK, A. SCHERZ, D. ZHU, W. SCHLOTTER, J. TURNER, W. LEE, Y. CHUANG, R. MOORE, O. KRUPIN, M. TRIGO, L. PATTHEY, H. DÜRR, SLAC/ RSXS collaboration, N. PONTIUS, T. KACHEL, A. FÖHLISCH, M. BEYE, Helmholtz Zentrum Berlin, F. SORGENFREI, W. WURTH, Uni. Hamburg & CFEL, C. CHANG, M. DÖHLER, C. TRABANT, C. SCHÜSSLER-LANGEHEINE, Uni. Cologne — Magnetite, Fe_3O_4, displays a strong decrease in resistivity upon heating above $T_C = 123$ K: the Verwey transition. Since long it has been proposed that charge and orbital order (CO/OO), via Fe^{3+} and Fe^{2+} charge disproportionation, play a crucial role. However, the mechanism behind the Verwey transition to date remains unclear. Using pump-probe O K-edge resonant soft X-ray scattering at the new LCLS SXR beamline, we have studied the role of CO/OO for the Verwey transition on ultra-fast time-scales. We focus on the structurally forbidden (00 $^1/_2$) peak. Upon excitation, the charge gap of 200 meV is quenched on resolution limited time-scales, < 250 fs, while we still observe a residual CO/OO signal. This may indicate the existence of a new transient state of matter, displaying charge and orbital order in coexistence with metallic behavior.

11:39AM J17.00003 Pseudogap Phase of Magnetite , YOHANES PRAMUDYA, HANNA TERLETSKA, EFSTRATIOS MANOUSAKIS, VLADIMIR DOBROSAVLJEVIC, NHMFL-Florida State University — Despite extensive experimental and theoretical work, the description of the electrical transport mechanism in magnetite (Fe_3O_4) is still an unresolved issue [1]. This unusual resistivity behavior close to the Verwey transition in magnetite has long been a matter of controversy. In our study, we focus on the temperature regime above Verwey transition and far below the magnetic phase transition, where a nearly charge ordering state (due to the long-range Coulomb frustration) is expected. Here, we expect similar behavior to what has been discussed in a nearly frozen Coulomb liquid [2] with the existence of a pseudogap phase. Following this line of thought, we use extended dynamical mean field theory (EDMFT) and Monte Carlo simulation to study the simplest spinless model describing this system. Our studies do capture the main transport trends in this temperature regime with a typical pseudogap–like behavior.

[1] N. F. Mott, "Metal-Insulator Transitions", Taylor&Francis (1990).
[2] S. Pankov and V. Dobrosavljevic, Phys. Rev. Lett. **94**, 046402 (2005).

11:51AM J17.00004 Synchrotron x-ray single-crystal structure analysis of a spinel oxide FeV_2O_4 with spin and orbital degrees of freedom , YOICHI NII, HAJIME SAGAYAMA, TAKA-HISA ARIMA, IMRAM, Tohoku University , RIU SAKAI, SHINOBU AOYAGI, EIJI NISHIBORI, HIROSHI SAWA, Department of Applied Physics, Nagoya University, KUNIHISA SUGIMOTO, SPring-8/JASRI, HIROYUKI OHSUMI, MASAKI TAKATA, RIKEN SPring-8 Center — It has been reported that FeV_2O_4, which has orbital and spin degrees of freedom both in tetrahedral $Fe^{2+}(d^6)$ sites and octahedral $V^{3+}(d^2)$ sites, exhibits successive structural phase transitions, accompanying a ferrimagnetic transition. The origin of the phase transitions is supposed to be a cooperation and/or competition between the orbital and spin degrees of freedom both in Fe^{2+} and V^{3+}. By a synchrotron x-ray single-crystal structure analysis, we determined the space group and atomic coordinate of each phase (cubic- HT-tetra.- HT-ortho.- LT-tetra.). The results suggest that the HT-tetra. (a>c) and HT-ortho. phases should be ascribed to the FeO_4 local compression, whereas VO_6 elongation should be responsible for the LT-tetra. (c>a) phase. We also discuss the orbital ordering (OO) pattern assuming strong electron-lattice coupling. A conceivable OO pattern of V^{3+} at the LT-tetra. (c>a) is *ferroic* one with *yz* and *zx* orbitals occupied, which is unique among spinel-type vanadates.

12:03PM J17.00005 Single-ion Anisotropy, Dzyaloshinskii-Moriya Interaction and Negative Magnetoresistance of the Spin-1/2 Pyrochlores R2V2O7 , HONGJUN XIANG, Fudan University, ERJUN KAN, M.-H. WHANGBO, C. LEE, North Carolina State University, SU-HUAI WEI, National Renewable Energy Laboratory, X.G. GONG, Fudan University — The electronic and magnetic properties of spin-1/2 pyrochlores $R_2V_2O_7$ were investigated on the basis of density-functional calculations. Contrary to the common belief, the spin-1/2 V^{4+} ions are found to have a substantial easy-axis single-ion anisotropy. The $|D/J|$ ratio deduced from the magnon quantum Hall effect of $Lu_2V_2O_7$, where J is the nearest-neighbor spin exchange and D is the Dzyaloshinskii-Moriya parameter, is much greater than the value estimated from our calculations (i.e., 0.32 vs. 0.05). We show that this discrepancy is due to the neglect of the single-ion anisotropy of the V^{4+} ions, and the negative magnetoresistance observed for $R_2V_2O_7$ arises from a new mechanism.

12:15PM J17.00006 Stability of the $Ni_3V_2O_8$ phase diagram on substitution with magnetic and non-magnetic transition metal ions , AKILA KUMARASIRI, AMBESH DIXIT, GAVIN LAWES, Wayne State University — There is considerable interest in understanding the materials properties underlying the development of simultaneous magnetic and ferroelectric order in multiferroics. $Ni_3V_2O_8$ develops strongly coupled ferroelectric and antiferromagnetic order simultaneously at low temperatures and has a rich magnetic phase diagram due to competing magnetic interactions. We investigated how the magnetic phases of $Ni_3V_2O_8$ were affected by systematic doping by transition metal ions. For these studies, polycrystalline $Ni_3V_2O_8$ samples substituted by various concentrations of transition metal ions M (M = Zn, Cu, Co, Mn, Fe) were prepared. Heat capacity, magnetization, dielectric, AC susceptibility, and pyrocurrent measurements were used to track the change in phase transition temperatures. On doping with spin-0 Zn, the system behaves as expected for site dilution consistent with 2-D spins, where the phase transition temperatures are suppressed linearly to lower temperatures. The modifications to the phase diagram for magnetic dopants (Co, Cu, Mn and Fe) show more variation, but the multiferroic phase transition appears to persist over a range of concentrations. This suggests that the specific spin structure in $Ni_3V_2O_8$ responsible for the development of ferroelectric order is relatively robust against perturbations produced by both magnetic and non-magnetic dopants.

12:27PM J17.00007 Orbitally driven trimerization in $LiVO_2$ and $LiVS_2$: a "partial Mott transition" , HUA WU, D.I. KHOMSKII, University of Cologne, Germany — Layered triangular-lattice transition-metal compounds often display interesting magnetic and electronic properties. Here we studied the formation of the trimerized spin-singlet state of the V^{3+} (S=1) in vanadates $LiVO_2$ and $LiVS_2$ and their electronic structure with a special orbital order, using constrained LSDA+U calculations combined with lattice optimization. The obtained results show that the trimerization distortion in $LiVO_2$ increases as the effective U decreases, and the calculated distortion of $\sim$0.3 Å at the small U=1 eV agrees well with the experiments, indicating that $LiVO_2$ is close to a metal-insulator transition. The corresponding distortion in $LiVS_2$ is even stronger, being $\sim$0.4 Å at the U=1 eV, which is due to enhanced electron delocalization via increased V-S covalency, in spite of a lattice expansion. This agrees with the experimental finding that $LiVS_2$ has a metal-insulator transition. The calculated energy gain associated with the trimerization well accounts for the observed structural phase transition temperature in $LiVO_2$ and $LiVS_2$. We conclude that the trimerization in $LiVO_2$ and $LiVS_2$ is due to a partial delocalization of the orbitally ordered electrons—a "partial Mott transition," occurring not in the whole system but in small clusters (here in trimers). This situation is contrasted with that in $NaVO_2$, which is further away from the localized-itinerant crossover and thus remains insulating with different orbital ordering.

12:39PM J17.00008 Simultaneous electrical transport and Raman spectroscopic measurements on individual nanowires of $W_xV_{1-x}O_2$, TAI-LUNG WU, Department of Physics, University at Buffalo-SUNY, LUISA WHITTAKER, C.J. PATRIDGE, S. BANERJEE, Department of Chemistry, University at Buffalo-SUNY, G. SAMBANDAMURTHY, Department of Physics, University at Buffalo-SUNY — Vanadium oxide is a well-know material to study the metal-insulator transition (MIT) in correlated electron systems. Upon heating to about 340 K, VO_2 undergoes orders of magnitude drop in resistance from an insulating phase (I) to a metallic phase (M) and accompanies a lattice structural phase transition from a low-temperature monoclinical phase (M1) to a high-temperature tetragonal phase (R). We present results from combined electrical transport and Raman spectroscopic measurements to discern the effects of doping in controllably tuning the MIT in individual nanowires of single crystal $W_xV_{1-x}O_2$. The MIT temperature (T_c) in our $W_xV_{1-x}O_2$ nanowires can be tuned through a wide range from 280 to 330 K by controlling the dopant concentration. The M-I transition can also driven electrically in these nanowires. Our simultaneous measurement of electrical transport and Raman spectroscopic measurement help us understand the role of structural transition in affecting the macroscopic electrical transition in individual wires.

12:51PM J17.00009 Strain- and temperature-induced phase transitions in single crystalline VO_2 , JOANNA ATKIN, University of Colorado, Boulder, EMILY CHAVEZ, University of Washington, SAMUEL BERWEGER, University of Colorado, Boulder, JINBO CAO, WEN FAN, JUNQIAO WU, University of California, Berkeley, MARKUS RASCHKE, University of Colorado, Boulder — The metal-insulator transition (MIT) of VO_2 exhibits a rich phase behavior involving two monoclinic (M1, M2), triclinic, and tetragonal phases that can form a complex domain structure and accompany the electronic transition. The interplay between these structural variants arises from strain due to differing lattice constants, temperature-dependent phase stability, and possible external strain from the substrate; the coupling between these effects renders a systematic study of the phase behavior difficult. We report on phase mapping of the structural changes through independent control of temperature and uniaxial strain in individual single-crystal nanorods, using Raman spectroscopy and near-field imaging. This allows us to investigate the transformation between the various insulating phases, elucidating the nature of the triclinic phase as a continuously distorted variant of the M1 monoclinic phase, intermediate in the first-order transformation into the monoclinic M2 phase.

1:03PM J17.00010 Discrepancy of structural and electronic transitions in the vicinity of the Metal-Insulator-transition in V_2O_3 , HYUN-TAK KIM, ETRI and UST in Korea, JUN-HWAN SHIN, University of Science and Technology, JUNG-YOUNG CHOI, BONG-JUN KIM, ETRI — Vanadium sesquioxide (V_2O_3), representative of strongly correlated electronic system, has been known as undergoing the MIT (Metal-Insulator-Transition) which is between rhombohedral paramagnetic metallic phase and monoclinic antiferromagnetic insulating phase near the transition temperature, (T_c) ≈150 K. In order to reveal a relation between electronic and structural atomic transition, we has measured the temperature dependence of DC conductivity and structural crystallographic characterization with various temperatures from 90 K to 300 K by using low-temperature X-Ray diffraction (LTXRD). The obtained results show a discrepancy of structural and electronic transitions. This discrepancy can be explained by forming of the metallic puddles whose the size and number increased by nucleation and percolation[1,2] during the electronic transition progress from 120 K to 180 K. The puddles have an insulating monoclinic structure before the structural phase transition at ∼185 K. These metallic puddles are induced by the MIT not related to the SPT (structure phase transition). (1. M. M. Qazilbash et al., Science 318, 1750 (2007); 2. B. J. Kim et al., Phys. Rev. B 77, 235401(2008))

1:15PM J17.00011 Interplay of chemical pressure and spin degrees of freedom on the magnetic properties of the $A\mathbf{Ag}_2M[\mathbf{VO}_4]_2$ type of compounds[1] , ANGELA MÖLLER, NGOZI AMUNEKE, PHILLIP DANIEL, DANA GHEORGHE, Department of Chemistry and Texas Center for Superconductivity, University of Houston, TX, USA, BERND LORENZ, Texas Center for Superconductivity and Department of Physics, University of Houston, TX, USA — A series of layered compounds of the $A\mathrm{Ag}_2M[\mathrm{VO}_4]_2$ type of structures, featuring the magnetic ions on a triangular lattice, have been synthesized by solid state reactions. Studies on the interplay of i) the chemical pressure induced by the differences in cation sizes (A^{II} = Sr, Ba) and ii) the spin system (M^{II} = Mn, Co, Ni, Cu) provide further insights into the structure-properties relationships which have been investigated by specific heat and magnetization measurements. Furthermore, spectroscopic methods have been employed to evaluate vibrational and electronic structural aspects in detail.

[1]We thank the Welch Foundation (Grant G099857) for support.

1:27PM J17.00012 Trimer Formation and Metal-Insulator Transition in Triangular-Lattice Systems $\mathbf{LiV}X_2$ (X=O,Se,S) , JUNKI YOSHITAKE, YUKITOSHI MOTOME, Dept. of Appl. Phys., Univ. of Tokyo — Geometrically-frustrated systems sometimes lift their degeneracy by spontaneous formation of multisite clusters via coupling to other degrees of freedom. A fascinating example is found in a triangular-lattice system $LiVO_2$, which exhibits a three-site trimer formation. The origin was argued to be an orbital ordering under strong electronic correlation [1], however, recent experiments on a series of $LiVX_2$ (X=O,Se,S) suggest that the system is intermediately correlated and rather close to a metal-insulator transition [2]. In this contribution,we revisit this problem within a multiorbital Hubbard model in a wide range of Coulomb interaction by strong-coupling perturbation and Hartree-Fock approximation. We find a new trimer state under substantial trigonal crystal-field splitting; it is located in the vicinity of a metal-insulator transition and not adiabatically connected to the trimer state previously proposed. We discuss the origin of this new trimerization and the relation to experimental results.

[1] H. F. Pen *et al.*, Phys. Rev. Lett. **78**, 1323 (1997).
[2] N. Katayama *et al.*, Phys. Rev. Lett. **103**, 146405 (2009).

1:39PM J17.00013 ABSTRACT WITHDRAWN –

1:51PM J17.00014 Electronic Excitations in Vanadates[1] , WILLIAM THORNTON, Unversity of Tennessee, ANTON KOZHEVNIKOV, ETH Institute for Theoretical Physics, ADOLFO EGUILUZ, University of Tennessee — Vanadates represent an electronic analogue to the cuprates, which have one hole in the 3d shell. There are many realizations of the vanadates, as the solid-state chemistry of the V-O system allows various coordination numbers. Here we probe the electronic structure of vanadates by studying neutral electronic excitations computed within a time-dependent density functional theory framework. We evaluate the dynamical electronic response in both a Bloch basis and a Wannier basis, for both large momentum transfers, and in the optical limit. We compare our results with available experimental data, and assess the importance of many-body (excitonic) interactions.

[1]This work was supported by NSF project OCI-0904972 and made use of resources at the Center for Computational Sciences at Oak Ridge National Laboratory under contract DE-AC05-00OR22725.

2:03PM J17.00015 A microscopic view on the Mott transition in chromium-doped V_2O_3 , G. SANGIOVANNI, Institute of Solid State Physics, Vienna University of Technology, Austria, S. LUPI, L. BALDASSARRE, D. NICOLETTI, M. MARSI, P. HANSMANN, N. PARRAGH, A. TOSCHI, T. SAHA-DASGUPTA, O.-K. ANDERSEN, K. HELD — V_2O_3 is the prototype system for the Mott transition, one of the most fundamental phenomena of electronic correlation. Temperature, doping or pressure induce a metal-to-insulator transition (MIT) between a paramagnetic metal (PM) and a paramagnetic insulator. This or related MITs have a high technological potential, among others, for intelligent windows and field effect transistors. However the spatial scale on which such transitions develop is not known in spite of their importance for research and applications. Here we unveil for the first time the MIT in Cr-doped V_2O_3 with submicron lateral resolution: with decreasing temperature, microscopic domains become metallic and coexist with an insulating background. This explains why the associated PM phase is actually a poor metal. The phase separation can be associated with a thermodynamic instability near the transition. This instability is reduced by pressure, that promotes a genuine Mott transition to an eventually homogeneous metallic state.

Nature Communications **1**, 105 (2010) doi: 10.1038/ncomms1109

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J18 GMAG DMP: Focus Session: Low D/Frustrated Magnetism - Molecular Magnets I D172

11:15AM J18.00001 Magnetic field-induced XY-AFM in 2D Heisenberg Antiferromagnet $[Cu(pyz)_2(pyO)_2](PF_6)$, YOSHIMITSU KOHAMA, NHMFL, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, MARCELO JAIME, NHMFL, Los Alamos National Laboratory, Los Alamos NM 87545, USA, JAMIE MANSON, Dept. of Chem. and Biochem., E. Washington Univ., Cheney, WA 99004, USA — Specific heat (C_p) and magnetic susceptibility (χ) measurements were performed on the two-dimensional spin-1/2 Heisenberg antiferromagnet $[Cu(pyz)_2(pyO)_2](PF_6)_2$ in DC and pulsed magnetic fields up to H = 15 T and 40 T, respectively [1]. We observe no long-range magnetic order down to 500 mK in zero applied magnetic field, suggesting that $[Cu(pyz)_2(pyO)_2](PF_6)_2$ is close to an ideal 2D AFM and instead undergoes a Berezinskii-Kosterlitz-Thouless (BKT) transition. However, the application of a finite magnetic field induces a clear anomaly in C_p, although not in χ. This behavior is known to be a remarkable signature of magnetic field induced XY-AFM [2]. In addition, C_p(H) measurements in pulsed fields, performed down to T = 1.5 K and up to H = 40 T, were used to map out the asymmetric Field-Temperature phase diagram which provides additional support for an ideal realization of field-induced XY-AFM in $[Cu(pyz)_2(pyO)_2](PF_6)_2$.
[1] Y. Kohama et al., *Rev. Sci. Instrum.* **81**, 104902 (2010).
[2] A. Cuccoli et al., *Phys. Rev.* **B68**, 060402(R) (2003).

11:27AM J18.00002 Pressure-induced Jahn-Teller axis switching in $Cu(pyz)F_2(H_2O)_2$? , J.L. MUSFELDT, University of Tennessee, Z. LIU, Carnegie Institute of Washington, S. LI, Virginia Commonwealth University, J. KANG, C. LEE, North Carolina State University, P. JENA, Virginia Commonwealth University, J.L. MANSON, Eastern Washington University, J.A. SCHLUETER, Argonne National Laboratory, G.L. CARR, Brookhaven National Laboratory, M.-H. WHANGBO, North Carolina State University — We employed infrared spectroscopy along with complementary lattice dynamics and spin density calculations to investigate local structure and magnetism through the series of pressure-driven transitions in $Cu(pyz)F_2(H_2O)_2$. Rather than frequency shifts that dovetail with the recently proposed pressure-induced Jahn-Teller switching model, we overall mode hardening, particularly in the Cu–OH_2 bending mode. We combine these findings with a reanalysis of the crystal structure to reveal the series of pressure-induced transitions as a combination of a-axis rotation, c-directed compression that acts to weaken O-H...F hydrogen bonds, and pyrazine ring buckling. The magnetic dimensionality crossover can be understood in terms of changes in magnetic orbital overlap.

11:39AM J18.00003 Lost and found: The missing diabolical points in the Fe_8 molecular magnet[1] , FEIFEI LI, ANUPAM GARG, Northwestern University — The tunneling spectrum of the single-molecule-magnet Fe_8 is known to have diabolical points (DP's). For magnetic fields along the hard axis, there are four such points for tunneling between the ground pair of levels, whereas the simplest model including only second-order anisotropy would predict ten DP's. The difference is due to a very weak fourth-order anisotropy, which in a semiclassical picture generates instantons with endpoint discontinuities, one of which dominates for large enough fields, and having no interfering partner, causes six of the underlying DP's to go away. However, as shown by Bruno, the six missing DP's do not truly disappear, but merely move off the hard axis into the hard-medium plane. In this talk, we report on a numerical search for these "missing" DP's. This search is nontrivial because the energy surface is like a smooth golf course, on which the DP's are extremely localized and deep holes. We therefore locate the DP's by following the lines of the Berry curvature which have monopole singulairities at the DP's. This exercise is performed for tunneling between excited pairs of levels also. An experimental observation of the rediscovered DP's would be an important test of the underlying spin Hamiltonian for Fe_8. (Submitted to the arxiv: Nov. 18, 2010.)

[1]Work supported by the NSF via grant no. PHY-0854896.

11:51AM J18.00004 Magnetic Superatoms[1] , J. ULISES REVELES, VICTOR M. MEDEL, A.C. REBER, S.N. KHANNA, Virginia Commonwealth University, V. CHAUHAN, P. SEN, Harish-Chandra Research Institute, DEPARTMENT OF PHYSICS, VIRGINIA COMMONWEALTH UNIVERSITY COLLABORATION, HARISH-CHANDRA RESEARCH INSTITUTE COLLABORATION — The electronic states in metal clusters are grouped in shells much in the same way as in atoms. Filling of the electronic shells leads to stable species called magic numbers. This has led to the preposition that selected stable metal clusters can mimic chemical properties of atoms on the periodic table and can be classified as superatoms. Here, we propose an extension of the superatom concept to magnetic species by invoking systems that hybridize localized and delocalized electronic states. Through first principles studies focusing on the electronic structure and magnetic moment, we show that $TMMg_n$ (TM = Sc, Ti, V, Cr, Mn, Fe, Co, and Ni) clusters exhibit a new class of magnetic superatoms stabilized by magnetic supershells. The talk will include possible applications of the new building blocks.

[1]We gratefully acknowledge support from U. S. Department of the Army through a MURI Grant #W911NF-06-1-0280.

12:03PM J18.00005 Tunnel-diode Resonator Spectroscopy of Quantum Levels in $Cr_{12}Ln_4$ (Ln=Y,Eu,Gd,Tb,Dy,Ho,Yb) Magnetic Molecules , STEVEN YENINAS, MARSHALL LUBAN, RUSLAN PROZOROV, Ames Laboratory, Ames, IA, 50011, WILLIAM A. CONIGLIO, CHARLES C. AGOSTA, Dept. of Physics, Clark University, Worcester, MA 01610, LARRY ENGELHARDT, Dept. of Physics and Astronomy, Francis Marion University, Florence, SC 29501, GRIGORE A. TIMCO, RICHARD E.P. WINNPENNY, School of Chemistry, University of Manchester, Manchester, UK — The differential magnetic susceptibility for a series of $Cr_{12}Ln_4$ (Ln=Y,Eu,Gd,Tb,Dy,Ho,Yb) magnetic molecules was measured in static (up to 16 T) and pulsed (up to 45 T) magnetic fields using a rf tunnel-diode resonator (TDR). At low temperatures, the behavior of these finite spin systems is governed by discrete energy spectra of the individual molecules. In magnetic field, low-energy quantum levels Zeeman-split, crossing at field values where magnetization exhibits a step corresponding to switching between different spin states. In high fields, we detect multiple level crossings which allow for a detailed mapping of the energy diagram. We then perform quantum Monte Carlo (QMC) using a Heisenberg Hamiltonian with three adjustable exchange constants whose values are chosen so as to optimize agreement with the experimental energy spectrum. The variations in results for the studied molecules are correlated to the magnetic properties of the lanthanide ions.

12:15PM J18.00006 Spin-electric coupling in Cu_3, V_{15} and other frustrated molecular magnet rings: a first principle study , M.F. ISLAM, J.F. NOSSA, C.M. CANALI, Linnaeus University, M.R. PEDERSON, Naval Research Laboratory — Frustrated triangular single-molecule magnets (SMMs) without inversion symmetry, such as Cu_3 and V_{15}, are characterized by a doubly degenerate S=1/2 ground-state (GS) with opposite chirality. Recently it has been proposed theoretically [1] and verified by ab-initio calculations [2] that an external electric field can couple these two chiral spin states, even in the absence of spin-orbit interaction (SOI). The efficiency of these coupling depends on the electric dipole moment between chiral states. In this talk we report on first-principle calculations of the coupling strength for the triangular SMMs Cu_3 and V_{15}. The spin-electric coupling is found to be considerably stronger in V_{15} than in Cu_3. We discuss the mechanism leading to an enhanced spin-electric coupling, which can be used as a convenient guide to synthesize SMMs that can respond more efficiently to an external electric field.

[1] M. Trif et.al. Phys. Rev. B 82, 045429 (2010). Mircea Trif et.al. Phys. Rev. Lett. 101, 217201 (2008)
[2] M.F. Islam et.al. Phys. Rev. B 82, 155446 (2010)

12:27PM J18.00007 ABSTRACT WITHDRAWN –

12:39PM J18.00008 Magnetic anisotropy and high-spin effects in single-molecule transistors , ALEXANDER ZYAZIN, TU Delft, JOHAN VAN DEN BERG, EDGAR OSORIO, NIKOS KONSTANTINIDIS, MARTIN LEIJNSE, FALK MAY, WALTER HOFSTETTER, CHIARA DANIELI, ANDREA CORNIA, MAARTEN WEGEWIJS, HERRE VAN DER ZANT — Fabrication of single-molecule transistors where electron transport occurs through an individual molecule has become possible due to the recent progress in molecular electronics. Three-terminal configuration allows charging molecules and performing transport spectroscopy in multiple redox states. Single-molecule magnets combining large spin with uniaxial anisotropy are of special interest as appealing candidates for high density memory applications and quantum information processing. We study single-molecule magnets Fe_4. Three-terminal junctions are fabricated using electromigration of gold nanowires followed by a self-breaking. High-spin Kondo effect and inelastic cotunneling excitations show up in transport measurements. Several excitations feature the energy close to the energy of zero-field splitting (ZFS) of a ground spin multiplet in bulk. This splitting is caused by the anisotropy and is a hallmark of single-molecule magnets. We observe nonlinear Zeeman effect due to a misalignment of an anisotropy axis and a magnetic field direction. The ZFS energy is increased in oxidized and reduced states of the molecule indicating enhancement of the anisotropy in these states.

12:51PM J18.00009 Magneto-optical spectroscopic studies of solid and solution-phase tetraphenyl porphyrin[1] , JACOB WAHLEN-STROTHMAN, ZHEN WEN PAN, LANE MANNING, MADALINA FURIS, KELVIN CHU, University of Vermont — Tetraphenylporphyrin (TPP) is a synthetic heterocyclic compound that serves as a model system for heme proteins and cytochromes. TPP can accomodate a metal ion in the center; D-shell ion porphyrin complexes with a crystalline solid phase are of interest for magnetic studies because of the possibility of macroscopic long range magnetic order of the ion spins. We have investigated the 5K magnetic properties of poly-crystalline thin films of the heme protoporphyrin IX analogue tetra-phenyl porphyrin, complexed with Zn and Mn, deposited through a capillary pen technique that produces 100um to 1 mm sized grains. Our novel experimental setup measures the UV/VIS, linear dichroism and magnetic circular dichorism simultaneously, incorporates a photoelastic modulator and a microscopy superconducting magnet for high-field (5T) measurements. We present solution and crystalline data on metal-complexed TPP; data are analyzed in terms of A and B-type MCD using a perimeter model. We find good agreement with previous solution data, and novel crystalline phase spectra that are correlated to the long range ordering.

[1]This work supported by NSF DMR-0821268, DUE-0942562 and EPS-0701410.

1:03PM J18.00010 Chiral molecule for spin filtering purposes: the study of L- and D-Alanine[1] , ESMERALDA YITAMBEN, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL 60439, RICHARD ROSENBERG, Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, NATHAN GUISINGER, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL 60439 — The field of molecular electronics has attracted scientists by the great opportunities and versatility it offers as a replacement for standard semiconductor electronics with organic materials, thus bringing down the cost, and opening endless possibilities for chemical synthesis, and scientific breakthrough. Of particular interest is the use of chiral molecules, such as alanine, for spin filtering studies in hope of creating highly spin-polarized charge carriers for spintronics applications. Preliminary studies of both L- and D-alanine on Cu(111) were conducted using scanning tunneling microscopy and spectroscopy, revealing the formation of a 2-dimensional phase at low coverage, a hexagonal "flower" pattern at intermediate coverage, and a chain and ring superstructures at high coverage. A model is proposed to explain the surface chemistry and bonding of the molecules on the metallic surface. Current studies of L- and D-alanine on Fe/W show promises in the intermediate coverage regime.

[1]This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

1:15PM J18.00011 DFT and STM studies of magnetism in single Co(TCNE) complexes on an ultrathin insulating film[1] , M. BADAL, T. CHOI, D. STROUD, J.A. GUPTA, Ohio State U. — We present results from large-scale ab initio DFT calculations for geometry and electronic structure of Co(TCNE) complexes on a c$(2 \times 2)$$Cu_2N$ substrate. The long-term aim is to study charge and spin transport in molecular systems. The work is done in concert with STM experiments. In particular, we perform calculations to help explain STM observations indicating that the electronic and magnetic properties of Co(TCNE) complexes vary with apparent molecular orientation. Using plane wave DFT with a GGA functional and spin polarization, we perform geometry optimization to identify the most commonly seen orientations of Co(TCNE). We further study the resulting electronic structure, using calculated LDOS and simulated STM images, to compare with observations. To study the strong in-plane magnetic anisotropy suggestd by spin-flip spectroscopy, we do noncollinear magnetic calculations on the relaxed structure, including spin-orbit coupling effects.

[1]Supported by NSF MRSEC, Grant No. DMR08-20414.

1:27PM J18.00012 Non-equilibrium transport through a single molecular Kondo impurity in a scanning tunneling microscope junction , UNGDON HAM, Department of Physics and Astronomy, University of California, Irvine, WILSON HO, Department of Physics and Astronomy and Department of Chemistry, University of California, Irvine — An unpaired spin from a single electron trapped in a molecular orbital in a double barrier scanning tunneling microscope (STM) junction at sub-Kelvin temperature and high magnetic field showed a non-equilibrium transport through a Kondo impurity. Hysteresis and switching in a conductance allows the spin and charge state of the molecule in the junction to be controlled. Mechanically tuning the coupling of the single spin to STM tip showed a gradual change from lowest order spin-flip inelastic tunneling spectroscopy (IETS) to the Kondo resonance. Using the imaging capability of STM, we observed clear sub-molecular node structures of the spin-flip IETS and the Kondo resonance.

1:39PM J18.00013 Electronic transport through single-molecule magnets by scanning tunneling spectroscopy , SIMRANJEET SINGH, Department of Physics, University of Central Florida, Orlando, Fl, JYOTI KATOCH, Department of Physics and NanoScience Technology Center, University of Central Florida, Orlando, Fl, TAKETO TAGUCHI, GEORGE CHRISTOU, Department of Chemistry, University of Florida, Gainesville, Fl, MASA ISHIGAMI, Department of Physics and NanoScience Technology Center, University of Central Florida, Orlando, Fl, ENRIQUE DEL BARCO, Department of Physics, University of Central Florida, Orlando, Fl — Atomic structure of molecules and electrodes are expected to sensitively influence the properties of molecular spintronics devices. We have studied the transport properties of individual Mn_4 single-molecule magnets bound to a surface using atomic force and scanning tunneling microscopy at cryogenic temperatures Unlike previous scanning probe microscopy experiments, we are able to continuously tune the density of states of individual molecules using novel device geometries in-situ We will discuss transport properties of single-molecule magnets as a function of their atomic structure, coupling to electrodes and the Fermi levels.

1:51PM J18.00014 Magnetic excitations from an S=1/2 antiferromagnetic tetramer system Cu_2PO_4OH , M. MATSUDA, D.L. ABERNATHY, Neutron Scattering Science Division, Oak Ridge National Laboratory, K. TOTSUKA, Yukawa Institute for Theoretical Physics, Kyoto University, Japan, A.A. BELIK, National Institute for Materials Science, Japan — Cu_2PO_4OH is a candidate material for the S=1/2 diamond-shaped antiferromagnetic tetramer system.[1] The magnetic susceptibility shows a spin-gap behavior and the exchange interaction J was estimated to be 138 K. Since there have not been so many experimental studies in the spin tetramer systems, it is important to clarify the magnetism in this compound. We have performed inelastic neutron scattering experiments on a powder sample of Cu_2PO_4OH on a chopper neutron spectrometer ARCS installed at SNS at ORNL in order to study the magnetic excitations from the tetramer spin system. We have clearly observed two magnetic excitations at ∼12 and ∼20 meV, whose widths in energy are broader than the instrumental resolution. It was found that the energy levels cannot be explained with the simple antiferromagnetic tetramer model with only nearest-neighbor interaction. We will discuss the results including further-neighbor interactions.

[1]A. A. Belik *et al.*, Inorg. Chem. 46, 8684 (2007).

2:03PM J18.00015 High-field EPR study of a $ReCl_4(CN)_2$ molecular magnet building block , JUNJIE LIU, Department of Physics, University of Florida, T. DAVID HARRIS, JEFFREY LONG, Department of Chemistry, University of Californian, Berkeley, STEPHEN HILL, NHMFL and Department of Physics, Florida State University — Slow magnetic relaxation has been observed in the single-chain magnet $(DMF)_4MReCl_4(CN)_2$ (M = Mn, Fe, Co, Ni) [D. Harris *et al.*, J. Am. Chem. Soc. **132**, 3980 (2010)]. The $ReCl_4(CN)_2$ **(1)** molecule has been synthesized in which the local environment of the Re^{IV} ion is same as in the single-chain magnet. Electron Paramagnetic Resonance (EPR) measurements have been performed on single crystal of complex **1** to determine the magnetic anisotropy of the Re^{IV} ions. Both intra and inter Kramer's doublet transitions are observed in high-field (up to 36T) EPR experiments. The data indicate a significant axial anisotropy of the easy-plane type ($D > 0$), with sizeable rhombic E term. In light of these findings, we are developing a theoretical model to account for the slow relaxation in the single-chain magnet.

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J19 GMAG DMP FIAP: Focus Session: Spin Transport & Magnetization Dynamics in Metals IV D170

11:15AM J19.00001 Vortex-Core Reversal Dynamics: Towards Vortex Random Access Memory , SANG-KOOG KIM, Seoul National University — An energy-efficient, ultrahigh-density, ultrafast, and nonvolatile solid-state universal memory is a long-held dream in the field of information-storage technology. The magnetic random access memory (MRAM) along with a spin-transfer-torque switching mechanism is a strong candidate-means of realizing that dream, given its nonvolatility, infinite endurance, and fast random access. Magnetic vortices in patterned soft magnetic dots promise ground-breaking applications in information-storage devices, owing to the very stable twofold ground states of either their upward or downward core magnetization orientation and plausible core switching by in-plane alternating magnetic fields or spin-polarized currents. However, two technologically most important but very challenging issues — low-power recording and reliable selection of each memory cell with already existing cross-point architectures — have not yet been resolved for the basic operations in information storage, that is, writing (recording) and readout. Here, we experimentally demonstrate a magnetic vortex random access memory (VRAM) in the basic cross-point architecture. This unique VRAM offers reliable cell selection and low-power-consumption control of switching of out-of-plane core magnetizations using specially designed rotating magnetic fields generated by two orthogonal and unipolar Gaussian-pulse currents along with optimized pulse width and time delay. Our achievement of a new device based on a new material, that is, a medium composed of patterned vortex-state disks, together with the new physics on ultrafast vortex-core switching dynamics, can stimulate further fruitful research on MRAMs that are based on vortex-state dot arrays.

11:51AM J19.00002 Dynamics of coupled vortices in spin-valve nanostructures , PAOLO BORTOLOTTI, N. LOCATELLI, V. CROS, J. GROLLIER, Unité Mixte de Physique CNRS/Thales, Palaiseau, France, V.V. NALETOV, G. DE LOUBENS, CEA-SPEC Saclay, Gif-sur-Yvette, France, C. ULYSSE, G. FAINI, CNRS Phynano team, Marcoussis, France, O. KLEIN, CEA-SPEC Saclay, Gif-sur-Yvette, France, A. FERT, Unité Mixte de Physique CNRS/Thales, Palaiseau, France — Recently, vortex dynamics driven by spin-transfer torque have been considered for new generation of nano-oscillators and memory devices. In this work we study the coupled vortex dynamics in FeNi(15nm)/Cu(10nm)/FeNi(4nm) samples where one single vortex state is favoured in both magnetic layers. Our experimental data are in good agreement with the corresponding simulations obtained through a 3D spin diffusion approach. Each vortex is characterized by a given chirality and polarity controllable separately by varying the external field (both in-plane and out-of-plane) and by applying a DC current perpendicular to the sample plane. The system modes are detected by static magneto-transport and microwave emissions analysis. In particular, it can be shown that vortex dynamics with large power appear only for configuration characterized by vortex cores pointing in opposite directions. The coupling of those two vortices allows to reach very narrow peak linewidth (down to 50 kHz), two order of magnitude smaller than in the uncoupled case.

12:03PM J19.00003 Statistical Behavior of Formation Process of Magnetic Vortex State in Permalloy Nanodisks[1] , MI-YOUNG IM, PETER FISCHER, cxro/lbnl, YAMADA KEISUKE, Kyoto Univ., SHINYA KASAI, nims — Magnetic vortices in magnetic nanodots, which are characterized by an in-plane (chirality) and an out-plane (polarity) magnetizations, have been intensively attracted because of their high potential for technological application to data storage scheme and their scientific interest for an understanding of fundamental physics in magnetic nanostructures. Complete understanding of the formation process of vortex state in magnetic vortex systems is very important issue in both technical and scientific points of view. In our work, we have statistically investigated the formation process of vortex state in permalloy ($Ni_{80}Fe_{20}$) nanodisks through the direct observation of vortex structure utilizing a magnetic transmission soft X-ray microscopy (MTXM) with a high spatial resolution down to 20 nm. We found a particular selectivity between the circulation sense of chirality and orientation sense of polarity for each other in the formation process of vortex state. Dzyaloshinskii-Moriya interaction inevitably generated in magnetic nanodisks is mainly responsible for the experimentally witnessed selectivity between chirality and polarity.

[1]This work was supported by the Director, Office of Science, Materials Sciences and Engineering Division, of the U.S. Department of Energy.

12:15PM J19.00004 Imaging Magnetic Normal Modes Driven by Spin Transfer Torque in Magnetic Nanopillars using Soft X-ray Microscopy[1] , YONG-TAO CUI, LIN XUE, Cornell University, PETER FISCHER, MI-YOUNG IM, Center for X-ray Optics, Lawrence Berkeley National Laboratory, R.A. BUHRMAN, D.C. RALPH, Cornell University — Motivated by the desire to understand the spatial structure of the high-frequency dynamical magnetic modes that can be excited by spin transfer from spin-polarized currents, we report measurements using X-ray microscopy to image magnetic normal modes in nanopillar devices resonantly excited by spin torque from a microwave frequency current. The frequency of the microwave current is phase locked to the incident X-ray pulses. We achieve 70 ps time resolution and 25 nm spatial resolution, enabling us to study the spatial configuration of the magnetization throughout the cycle of resonant magnetization dynamics. We will discuss the initial results of our measurements and comparisons with micromagnetic simulations.

[1]This work was supported by the U.S. Department of Energy under Contract No. DE-AC02-05-CH11231.

12:27PM J19.00005 Voltage-controlled Spin Wave Logic Device: Ring Interferometer[1] , TIANYU LIU, Department of Physics and Astronomy, GIOVANNI VIGNALE, Department of Physics and Astronomy, University of Missouri-Columbia — Spin wave logic circuitry transmits information by propagating spin waves along magnetically insulating wave guides. This is less power-consuming than ordinary circuits and is expected to work at THz frequency and room temperature. Logical operations are performed by modulating the interference of spin waves through a phase shifter. A great deal of effort has been devoted to the problem of controlling the phase of spin waves by means of a spatially varying magnetic field, either extrinsic or intrinsic (i.e., by passing the spin wave through a non-uniform magnetic texture). Here we introduce a new approach, which exploits the response of spin waves to an external *electric field* via the spin-orbit coupling of this electric field to the electrons that mediate the magnetic interaction. Based on the Heisenberg Hamiltonian modified by spin-orbit coupling, we show how a ring interferometer made of a magnetic insulator (e.g, YIG) can be used to implement NOT logic (and other logic functions) under voltage control.

[1]Work supported by ARO Grant No. W911NF-08-1-0317.

12:39PM J19.00006 Phenomenology of Current-Induced Dynamics in Antiferromagnets[1] , KJETIL M.D. HALS, Department of Physics, Norwegian University of Science and Technology, NO-7491, Trondheim, Norway, YAROSLAV TSERKOVNYAK, Department of Physics and Astronomy, University of California, Los Angeles, California 900095, USA, ARNE BRATAAS, Department of Physics, Norwegian University of Science and Technology, NO-7491, Trondheim, Norway — In antiferromagnets, an electric current can induce a torque on the staggered magnetization. We derive a novel phenomenology of current-induced dynamics in antiferromagnets. The theory includes effects of damping, external magnetic fields, and both adiabatic and non-adiabatic current-induced torques. We apply our theory to an antiferromagnetic domain wall system, and find an analytic solution for the domain wall motion in the low current density regime. In this regime, the domain wall velocity is proportional to the ratio between the non-adiabatic torque and the damping coefficient. In addition, the domain wall develops a net magnetic moment. This opens the route to an alternative way to observe current-induced effects in antiferromagnets.

[1]This work was partially supported by the European Union FP7 grant no. 251759 "MACALO."

12:51PM J19.00007 Temperature dependence of domain wall dynamics in Permalloy nanowires , JUSANG YANG, JAMES L. ERSKINE, Department of Physics, The University of Texas at Austin — Current-driven [1] and current-assisted field-driven [2] domain wall dynamics in ferromagnetic nanowires have the thermal effects resulting from Joule heating, which make difficult to separate the spin-torque effects on domain wall displacements. To understand the thermal effects on domain wall dynamics, temperature dependence of field-driven domain wall velocity was studied using high-bandwidth scanning Kerr polarimetry. Domain wall velocity curves of 20 nm thick Permalloy nanowires with various widths (from 400 nm to 1000 nm) were measured with increasing temperature from 300 K to 400 K. Walker critical fields decreased with increasing temperature, which can be attributed to thermal excitations, and temperature-induced stochastic dynamics mode changes were observed. The results will be discussed in relation to internal domain wall structures.

[1] M. Klaui et al., Phys. Rev. Lett. 95, 026601 (2005).
[2] G.S.D. Beach et al., Phys. Rev. Lett. 97, 057203 (2006).

1:03PM J19.00008 Voltage induced by domain wall motion in a ferromagnetic nanowire[1] , YANG LIU, OLEG TRETIAKOV, ARTEM ABANOV, Department of Physics, Texas A&M University — We study current-induced domain-wall motion in a narrow ferromagnetic wire. This motion is described by effective equations of motion which depend only on four parameters. These parameters are set by the magnetic Hamiltonian and the shape of the wire. We propose a new way to measure these parameters by measuring time dependent voltage generated by the domain wall motion.

[1] This work was supported by the NSF Grant No. 0757992 and Welch Foundation (A-1678).

1:15PM J19.00009 Discrete positioning of domain walls due to localized pinning sites in current driven motion along nanowires , XIN JIANG, LUC THOMAS, RAI MORIYA, STUART PARKIN, IBM ALMADEN RESEARCH CENTER, SAN JOSE, CA 95120, USA TEAM — Current driven domain wall motion is studied in spin-valve nanowires. The position of the domain wall after nanosecond long driving current pulses is determined with an accuracy of better than 50 nm by measuring the resistance of the nanowire. Although the domain wall displacement scales linearly with the current pulse length, its final position is discretized. This is attributed to relaxation of the domain wall into local pinning potential minima along the nanowire after the current pulse is turned off.

1:27PM J19.00010 Direct imaging of domain wall pinning in artificially created asymmetric potentials , D.E. READ, Imperial College London, L. O'BRIEN, University of Cambridge, S. LADAK, K. ZEISSLER, Imperial College London, T. TYLISZCZAK, Lawrence Berkeley National Lab, A.-V. JAUSOVEC, H.T. ZENG, E.R. LEWIS, J. SAMPAIO, Imperial College London, A. FERNANDEZ-PACHECO, D. PETIT, R.P. COWBURN, University of Cambridge, W.R. BRANFORD, Imperial College London — Domain walls (DWs) in ferromagnetic nanowires are ideal candidates for a wide variety of technological applications including high density data storage devices. To realise functional DW devices the processes associated with DW pinning must be understood and controlled. Magnetostatic pinning of DWs has already been observed experimentally using spatially resolved MOKE measurements. Using high resolution scanning transmission x-ray microscopy (STXM) we were able to directly image DWs in NiFe nanowires pinned in asymmetric potentials which were created by nano-patterning additional ferromagnetic wires perpendicular to the DW conduit. Tailoring the pinning potential in this way allows us to probe the rigidity of the DW in the region of the pinning site, increasing our understanding of DW deformation in magnetostatic traps and paving the way for future commercial applications.

1:39PM J19.00011 Spin-torque-driven ballistic switching with $<$ 50ps pulses , OUKJAE LEE, DAN RALPH, ROBERT BUHRMAN, Cornell University — Spin-torque-driven ballistic switching is a fast, energy-efficient, non-thermal operation in which the magnetization of a nanomagnet rotates from one equilibrium state to the other without any preceding small-angle precession. This reversal scheme can be implemented with a non-collinear structure in which the magnetic free layer is located between an out-of-plane spin polarizer and an in-plane polarizer. Both for achieving better fundamental understanding of magnetic dynamics and for realizing technological advances, it is desirable to demonstrate experimentally that the free layer can be reliably reversed with a current pulse as short as possible. Moreover it is necessary to achieve an asymmetrical response as the function of both the initial state and the pulse current polarity in order to obtain the desired final state with a simple unipolar pulse. We will discuss experimental results that show that the interval of pulse widths giving reliable switching is strongly dependent on the initial magnetic state and on the current. We will also discuss strategies to further improve ballistic switching operations.

1:51PM J19.00012 First-principles calculation of the photon-shortage mystery in femtosecond magnetism[1] , GUOPING ZHANG, Department of Physics, Indiana State University, MINGSU SI, Lanzhou University, YIHUA BAI, Indiana State University, T.F. GEORGE, University of Missouri-St. Louis — Laser-induced femtosecond magnetism needs photons to influence the magnetization in a sample, but there is a debate on whether the photon-shortage really exists [1]. Here we directly compute the number of photons used in ferromagnetic nickel, and we find that for nearly all the experiments, there are enough photons. The key is that one has to compute this number correctly using the surface instead of volume as a parameter [1,2]. Then we use the first-principles method to compute the magnetization for a fixed number of photons. Our results show that the number of photons is not a decisive factor, since for a fixed number, the laser amplitude and pulse duration can be changed systematically. We suggest that it is more appropriate to use the laser amplitude and pulse duration as two decisive parameters to characterize the role of photons, instead of the photon number. [1] M. S. Si and G. P. Zhang, J. Phys.: Cond. Matt. **22**, 076005 (2010). [2] G. P. Zhang, W. Hübner, G. Lefkidis, Y. H. Bai, and T. F. George, Nature Phys. **5**, 499 (2009).

[1]Supported by the U.S. DOE under Contract No. DE-FG02-06ER46304, NERSC and Argonne Leadership Computing Facility.

2:03PM J19.00013 *Ab initio* investigation of ultrafast spin-manipulation: Λ processes in charged two-magnetic-center nanostructures with bridging atoms[1] , CHUN LI, Northwestern Polytechnical University, WEI JIN, GEORGIOS LEFKIDIS, WOLFGANG HÜBNER, Kaiserslautern University of Technology — We present a fully *ab initio* investigation of ultrafast laser-induced magnetic switching mechanisms in charged two-magnetic-center nanostructures via Λ processes [1,2]. In order to improve the spin transferability between the magnetic centers and fulfill the energy-difference requirements for the Λ processes [3], a small number of nonmagnetic bridging atoms (O and Mg) is used to connect the magnetic centers. These bridging atoms influence the overlap between the magnetic centers. It is shown that both bridging atoms can redistribute the spin density on the structure by changing either the local spin density or even the total spin localization. Especially, the spin-transfer scenario achieved in [Fe-O(Mg)-Co]$^+$ confirms that using bridging atoms can significantly enhance the spin transferability between the magnetic centers.
[1] C. Li, T. Hartenstein, G. Lefkidis *et al*, PRB **79**, 180413(R) (2009).
[2] T. Hartenstein, C. Li, G. Lefkidis *et al*, JPD **41**, 164006 (2008).
[3] G. Lefkidis, G. P. Zhang, and W. Hübner, PRL **103**, 217401 (2009).

[1]Supported by the National NSF (No. 11002109) of China, Fundamental Research Fund (JC200935), and the Ao-Xiang Star Project at NWPU.

Tuesday, March 22, 2011 11:15AM - 2:15PM –
Session J20 FIAP: Optoelectronic Devices & Applications D168

11:15AM J20.00001 Scanning Ladar: Spatial Imaging Performance Through Turbulence , MAZEN NAIRAT, Physics Department, New Mexico State University, DAVID VOLEZ, SRINIVASU PUDI, Elecrical and Computer Engeering Department, New Mexico State University — The performance of scanning laser radar is studied for generating two-dimension spatial images at long ranges. Performance is described in terms of the Modulus Transfer Function (MTF). A simple analytic expression for the MTF associated with wave front tilt caused by propagation through atmospheric turbulence is explicitly derived. The derivation includes consideration of the influence of the Fresnel length. A physical optics simulation is employed to demonstrate the applicability of the MTF approach. The results are compatible with theoretical expressions that describe the image.

11:27AM J20.00002 Stimulated Terahertz Smith-Purcell Radiation in Planar Gunn Diodes , ALEXEY BELYANIN, DON D. SMITH, Department of Physics and Astronomy, Texas A&M University — We propose a room-temperature semiconductor source of coherent narrowband Smith-Purcell radiation (SPR) in the spectral range of 0.1-1.2 THz. Spontaneous SPR in semiconductors has been observed at low temperature with very low power. Practical vacuum SPR devices utilize a pre-bunched electron beam to achieve the stimulated mode of operation. However, electron bunches quickly dissipate in semiconductors. We propose to utilize the Gunn instability to form stable charge bunches (Gunn domains) that enable semiconductor sources of stimulated SPR. The device is a planar Gunn diode with a thin dielectric spacer layer and metallic grating deposited on the drift region. The SPR frequency is determined by the domain velocity and the grating period. In contrast to conventional Gunn diodes, the frequency is not limited by the transit time. Our calculations show that technologically relevant power density levels (1-100 nW per micrometer of device width) may be achieved by this method.

11:39AM J20.00003 Correlated photon fluctuations at the onset of first-order optical coherence , PATRICK FOLKES, Army Research Laboratory, Adelphi MD — We report the observation of correlated photon fluctuations over a narrow range of current at threshold of an interband cascade laser using single-detector photon noise measurements. The correlated photon noise is manifested by large fluctuations in the low-frequency photon noise spectral density at certain discrete frequencies which are sensitive to the laser gain characteristics. We observe the concurrent emergence and growth of the lasing mode over the same current range indicating that the correlated photon noise provides evidence of the occurrence of a change in the photon fluctuation statistics and the onset of first-order coherence in the laser emission.

11:51AM J20.00004 Self Generation of Chaos From Electrical Solitons , OZGUR YILDIRIM, DONHEE HAM, Harvard University — The nonlinear transmission line (NLTL) is a structure that can generate electrical solitons of subpicosecond duration. As an autonomous soliton generator utilizing the NLTL, thus far, only periodic electrical soliton oscillators have been reported. These circuits self generate a periodic train of solitons, where an amplifier with a saturable absorber prevents the generation of multiple solitons and hence their nonlinear collisions. However, if the amplifier encourages the generation of multiple solitons and their collisions, the system can attain chaos, because the position of the soliton modulates after each collision, disrupting the periodicity. In this work, for the first time, we experimentally demonstrate such a chaotic system. Our circuit self generates an aperiodic signal, which has a continuous spectral distribution. We confirm its chaotic behavior by calculating the largest Lyapunov exponent, and show that the dimensionality of the generated chaos is high (d>3) by performing a false-nearest-neighbors analysis. Moreover, we explicitly measure the route from periodic soliton oscillation to chaotic oscillation via decreasing the time constant of the saturable absorber, showing the effect of soliton collisions on period-doubling bifurcations and finally the creation of chaos.

12:03PM J20.00005 Harmonic Bloch and dipole oscillations and their transition in elliptical optical waveguide arrays[1] , YUN SAN CHAN, MING JIE ZHENG[2], KIN WAH YU, The Chinese University of Hong Kong — We have studied harmonic oscillations in an elliptical optical waveguide array in which the couplings between neighboring waveguides are varied in accord with a Kac matrix so that the propagation constant eigenvalues can take equally spaced values. As a result, the long-living optical Bloch oscillation (BO) and dipole oscillation (DO) are obtained. Moreover, when a linear gradient in the propagation constant is applied, we achieve a switching from DO to BO and vice versa by ramping up or down the gradient profile [1]. The various optical oscillations as well as their switching are investigated by field evolution analysis and confirmed by Hamiltonian optics. The equally spaced eigenvalues in the propagation constant allow viable applications in transmitting images, switching and routing of optical signals.

[1]. M. J. Zheng, Y. S. Chan and K. W. Yu, J. Opt. Soc. Am. B 27, 1299 (2010).

[1]Work supported by the General Research Fund of the Hong Kong SAR Government.
[2]Now in University of Wisconsin - Madison

12:15PM J20.00006 Bloch-dipole-Zener Oscillations in Binary Parabolic Optical Waveguide Arrays[1] , MING JIE ZHENG[2], YUN SAN CHAN, KIN WAH YU, The Chinese University of Hong Kong — We have studied the propagation and Zener tunneling of light in the binary parabolic optical waveguide arrays (BPOWA) consisting of two evanescently coupled dissimilar optical waveguides. BPOWA attains two minibands with a gap at the zone edge due to Bragg reflections. Various superposition of optical oscillations and Zener tunneling are identified for different parameters on the phase diagram. In particular, both Bloch-Zener oscillation [1] and Bloch-dipole-Zener oscillation are obtained in the BPOWA by the field-evolution analysis. The research results may have potential applications in optical splitting and waveguiding devices and shed light on the coherent phenomena in lattice structures [2].

[1] F. Dreisow, A. Szameit, M. Heinrich, T. Pertsch, S. Nolte, A. Tunnermann, and S. Longhi, "Bloch-Zener Oscillations in Binary Superlattices," Phys. Rev. Lett. 102, 076802 (2009).
[2] M. J. Zheng, G. Wang, and K. W. Yu, "Tunable Hybridization at Mid Zone and Anomalous Bloch-Zener Oscillations in Optical Waveguide Ladders," Opt. Lett. (in press).

[1]Work supported by the General Research Fund of the Hong Kong SAR Government.
[2]Now in University of Wisconsin - Madison

12:27PM J20.00007 Cavity phase matching for a high efficient sheet optical parametric oscillator , Z.D. XIE, X.J. LV, S.N. ZHU, Department of Physics, Nanjing University — Cavity phase matching (CPM) was first proposed in the early days in nonlinear optics by J. A. Armstrong, N. Bloembergen, J. Ducuing and P. S. Pershan in theory in 1962 as one of the three protocols to realize phase matching in nonlinear medium. The other two protocols have been developed into the well-known quasi-phase matching (QPM) technique. CPM has equivalent capability to compensate for the phase mismatching as QPM in principle and people has been attempting to achieve CPM in several kinds of semi-conductor materials. However, there is no convincing experimental realization up to date. In the work, we manufactured, for the first time, a CPM optical parametric oscillator (OPO) which consisted of a 217μm thick KTP crystal sheet whose two surfaces were optically coated for the resonance recirculation of signal and idler. The sheet OPO could emitted the near-frequency-degenerate signal and idler beams in near-infrared region with a quasi-continuously tunable frequency difference ranging from 0.35 to 26.1THz. This mini-device showed the high slope efficiency up to 22%, and as well the unique spectral and spatial features, like single-longitudinal-mode, single-spatial-mode, narrow linewidth, etc.

12:39PM J20.00008 Variation of Losses with Detuning in Bragg Gratings , SERGIY MOKHOV, DERREK DRACHENBERG, GEORGE VENUS, BORIS ZELDOVICH, LEONID GLEBOV, CREOL, The College of Optics and Photonics, UCF — The optical losses due to small scattering and absorption in Bragg gratings are proportional to the loss coefficient, and also depend on the integral of optical power over grating length. At different resonant conditions this integral of stored optical power inside a grating differs from the product of power by length for transmitted beams far from resonance. We have found an analytical expression for the relative value of this integral in the case of a uniform grating. If it equals unity for a beam propagating out of resonance, then for a grating in Bragg resonance with reflectance of 99% it equals 0.332 due to exponential decay of reflected and transmitted power inside the grating and grows up to 2.027 near the first zero of the reflection spectrum due to increased resonant capacity of the grating similar to a Fabry-Perot resonator. Also, we have found analytically that in the case of spatially modulated grating losses with Bragg period the odd-functional term will be present in the expression for relative losses in addition to the term for averaged losses. We have measured this variation of losses in volume Bragg grating at a small incidence angle, and in this case can resolve the incident and reflected beams and precisely measure the power balance in the experimental setup, and the results show good agreement with theory.

12:51PM J20.00009 Temperature dependence of polaritons in ZnO based hybrid micro-cavity , RYOKO SHIMADA, SANKAR DAVULURI, HADIS MARKOC, ARUP NEOGI — We have studied the temperature dependence of cavity polaritons in bulk ZnO-based hybrid microcavities. The bulk ZnO-based micro cavity is formed by 36 pairs of AlGaN/(Al)GaN distributed Bragg reflector at the bottom of (lambda)/4 thick ZnO cavity and eight pairs of SiO2/SiN DBR as top mirror. Shift in exciton resonances with temperature resulted in shift in the energy levels of upper and lower polariton modes. The magnitude of observed energy shifts in polariton modes is dependent on the angle at which photoluminescence is collected. It can be possible to obtain either a upper or lower polariton mode that is stable over a long range of temperature by selectively collecting the polaritons modes emitted at a particular angle. The temperature dependent carrier dynamics of the upper or lower polariton mode has been studied by time resolved spectroscopy.

1:03PM J20.00010 Study of the Coherent Phonon-Polariton effect on the Terahertz pulse generation in <110> ZnTe crystal[1] , CHIEN-MING TU, JENG-CHUNG CHEN, CHENG-CHUNG CHI, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan — We report a study of the wave form and spectrum of the THz radiation generated by illuminating <110> ZnTe crystal with femto-second optical pulses of 750 nm in wavelength. The co-linearly measured wave form consists of a main W-shaped THz pulse and a trailing quasi monochromatic damped oscillation (QMDO) with a duration of several tens of pico-seconds. In Fourier-transformed spectrum of the measured THz waveform, there are two peaks, one centered at 0.6 THz and the other one at 2.7 THz, which correspond to the main THz pulse and the QMDO respectively. Our calculation of the THz pulse generated by the optical pulse indicates that the QMDO is caused by the phase matching of the optical pulse and the coherent phonon-polariton in ZnTe. We observe that, by increasing the optical pulse width, the duration of the trailing QMDO shrinks in time domain, and the amplitude of the phase-matching component also reduces, both of which are consistent with our calculations. There remain some subtle differences between the experimental results and the theoretical calculations, the origin of which will be discussed.

[1]Supported by the NSC grant 99-2120-M-007-002.

1:15PM J20.00011 Accurate Formulation and Numerical Calculation of Faraday, Magnetic Circular Dichroism (MCD) and Kerr Effect of Light in Magnetized Cubic Crystal[1] , JIN T. WANG, SEAN HALL, YI ZHEN, DONG-SHENG GUO, Southern University, SUBR-P TEAM — Faraday, magnetic circular dichroism and Kerr effects are three important magneto-optic effects. They are significant in fundamental sciences and applications. Presently, scientists in this field believed that Faraday and Kerr effects are caused by the difference in real parts of the refractive indices of the magnetic crystal for left-and right-circularly polarized light and the magnetic circular dichroism is caused by the difference in the imaginary parts of the refractive index (absorption) of the magnetic crystal for left-and right-circularly polarized light. However, the derived equations for these effects are approximated only. In our paper we obtained accurate formulations for these effects and found that there are mistakes in the present conclusions with respect to the above mentioned these effects. The precise equations, conclusions from our derivation and the results of numerical calculation are presented.

[1]ONR Grant N00014-08-1-0785

1:27PM J20.00012 Quantum cascade laser with low threshold and high characteristic temperature $T_0 > 300K$ at ~ 14 μm[1] , XUE HUANG, WILLIAM CHARLES, CLAIRE GMACHL, Princeton University, MIRTHE TEAM — High-performance quantum cascade (QC) lasers with wavelength in $4 \sim 12$ μm range are widely used in trace gas sensing. However, lack of high performance for longer wavelength in the $12 \sim 16$ μm range, where exist the strongest absorption lines of BTEX (benzene, toluene, ethylbenzene, and xylenes) and Uranium Hexafluoride, prohibits QC laser applications in sensing these important gases. The QC laser emitting at ~ 14 μm we investigate here is based on a diagonal-transition design. The depletion of the lower laser state is achieved by a one-phonon-continuum scheme instead of the widely used "continuum" lower mini-bands in existing long-wavelength lasers. This scheme reduces LO scattering from the upper laser state, the leakage from the injector and thermal back-filling to the lower laser state, thus attaining population inversion efficiently. The laser shows low threshold (J_{th} =2.4 kA/cm^2 for a 1.97-mm-long laser at room temperature), and a high characteristic temperature T_0 =309K fitted from $J_{th}(T) = J_0 e^{T/T_0}$, which is comparable with the record highest characteristic temperature. The peak power is 1.4W at 80K and 0.25W at 300K.

[1]Work supported in part by MIRTHE (NSF-ERC).

1:39PM J20.00013 The effect of energy density on laser flyer velocity , H.R. BRIERLEY, Cavendish Laboratory, University of Cambridge, T.A. VINE, QinetiQ Ltd, Fort Halstead — Laser driven flyers are produced on the interaction of a laser pulse with a thin film of metal. When an Nd:YAG laser is focussed through a fused silica substrate onto a 5 micron layer of aluminium, a fraction of the metal is ablated. This causes the remaining aluminium to be punched from the film and launched as a discrete flyer. By varying the energy of the incident laser pulse, the velocity of the resulting flyer is changed. The Nd:YAG laser beam was spatially filtered to remove higher order modes. This improved the beam quality and reduced the focal spot diameter. The resulting higher energy densities led to faster flyer velocities for a given pulse energy.

1:51PM J20.00014 Spatially-sculpted aberrated optical tweezers for delivery of nanoparticles onto cells , SHIVARANJANI SHIVALINGAIAH, SUYASH CHHAJED, SAMARENDRA MOHANTY, UT Arlington — Nanoparticles (NP) are emerging as photochemical and photothermal agents for delivery of drugs and heat onto the targeted cells. Here, we report spatially-sculpting of transverse potential landscape by introducing aberration in the optical tweezers beam for delivery of therapeutic NP on to the prostate cancer PC3 cells. A tunable Ti-Sapphire laser beam was focused to a diffraction limited spot by use of a high numerical aperture microscope objective for optical trapping. A cylindrical lens was used to create the beam profile astigmatic, which led to spatially extended potential landscape. In order to facilitate transport of NP, Comatic potential was created by tilting of the astigmatic beam with respect to the optic axis. NPs were attracted towards the potential minima, transported along the major axis of the elliptic spot and ejected out along the direction having lower stiffness. The Carbon NPs as well as Poly Lactic-*co*-Glycolic Acid NPs were efficiently transported and concentrated near the PC3 cells *in-vitro*. The direction and the speed of transport of nano-particles could be reversed by change in tilt direction and angle. Further, by utilizing the scattering force with the asymmetric gradient force, three-dimensional transport of nanoparticles was achieved. The effect of laser beam power and size / refractive index of the nano-particles on the speed of transport will be presented.

2:03PM J20.00015 Mapping force of interaction between PLGA nanoparticle with cell membrane using optical tweezers , SUYASH CHHAJED, LING GU, HOMA HOMAYONI, KYTAI NGUYEN, SAMARENDRA MOHANTY, UT Arlington — Drug delivery using magnetic (Fe_3O_4) Poly Lactic-*co*-Glycolic Acid (PLGA) nanoparticles is finding increasing usage in therapeutic applications due to its biodegradability, biocompatibility and targeted localization. Since optical tweezers allow non-contact, highly sensitive force measurement, we utilized optical tweezers for studying interaction forces between the Fe_3O_4-PLGA nanoparticles with prostate cancer PC3 cells. Presence of Fe_3O_4 within the PLGA shell allowed efficient trapping of these nanoparticles in near-IR optical tweezers. The conglomerated PLGA nanoparticles could be dispersed by use of the optical tweezers. Calibration of trapping stiffness as a function of laser beam power was carried out using equipartition theorem method, where the mean square displacement was measured with high precision using time-lapse fluorescence imaging of the nanoparticles. After the trapped PLGA nanoparticle was brought in close vicinity of the PC3 cell membrane, displacement of the nanoparticle from trap center was measured as a function of time. In short time scale ($<$ 30sec), while the force of interaction was within 0.2 pN, the force increased beyond 1pN at longer time scales ($\sim$ 10 min). We will present the results of the time-varying force of interactions between PLGA nanoparticles with PC3 cells using optical tweezers.

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J21 DMP GIMS DCP: Focus Session: Imaging and Modifying Materials at the Limits of Space and Time Resolution I D161

11:15AM J21.00001 Transformation of carbon nanoparticles under laser microirradiation , NINAD INGLE, VIJAYALAKSHMI VARADARAJAN, ALI KOYMEN, SAMARENDRA MOHANTY, UT Arlington — Functional, mechanical, electrical and thermal properties of carbon nanoparticles (CNP) have been shown to change significantly with change in its shape and structure. Here, we show that shape of the CNPs can be transformed by exposure to tightly focused near-infrared Ti: Sapphire laser beam. The CNPs were prepared using electric plasma discharge generated in an ultrasonic cavitation field of liquid benzene. High resolution TEM image showed nanoparticles with average radius of $\sim$5nm with crystalline structure. A Nanonics Multiview Atomic Force Microscopy (AFM) was integrated on the laser micro-irradiation system to reveal the shape transformation of the CNPs before and after laser irradiation. Since near-IR laser irradiation can lead to significant heat generation in CNP in absence of aqueous solution (sink), the system is far from thermal equilibrium and can curve or bend graphitic layers by introducing topological defects. The photothermally-induced shape transformation can occur below laser power required for complete melting of CNP since surface melting can suffice the observed shape transformation. The results show significant reduction in the volume of irradiated CNP-clusters, which was attributed coalescing of melted CNPs. Raman spectroscopic measurements are being carried out to evaluate possibility of ultrastructural changes.

11:27AM J21.00002 The effect of Au condensation in laser desorption/ionization of organic materials , ANEESH PRABHAKARAN, ARNAUD DELCORTE, Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, Belgium — Matrix-assisted desorption/ionization (MALDI) mass spectrometry, where the analyte is mixed in a low molecular weight matrix, often constitutes a limitation for the analysis and imaging of real world samples. Herein, we investigate the influence of a thin layer of gold (1-15nm) deposited on the surface of different organic materials, in the laser ablation using 355nm wavelength light. We see a significant effect of the condensed metal nanoparticles in the laser ablation process. Compared to pristine samples, the metallized samples show a significant intensity of characteristic fragments as well as metal cationized molecules. Relatively soft desorption/ionization is indicated by the observation of characteristic molecular ions of the different analytes. The observed effects can be explained by the increased laser absorption by the gold nanoparticles in this wavelength range and the increased ionization by the gold. Hence the metallization improves the surface characterization using lasers and also proves to be a novel technique for chemical imaging of organic surfaces.

11:39AM J21.00003 Atomic-level simulations of structural transformations in layered Au-Cu and Ag-Cu metal targets irradiated by a femtosecond laser pulse[1] , CHENGPING WU, University of Virginia, DEREK THOMAS, University of Tokyo, Japan, ZHIBIN LIN, Colorado School of Mines, LEONID ZHIGILEI, University of Virginia — The structural transformations in Ag/Au film - Cu substrate systems irradiated by femtosecond laser pulses are investigated in simulations performed with a model that couples the molecular dynamics method with a continuum-level description of the laser excitation and subsequent relaxation of the excited electrons. The higher strength of the electron-phonon coupling in Cu compared to Ag and Au results in a preferential sub-surface heating and melting of the Cu substrate. The melting is followed by rapid cooling and resolidification. In the case of Cu-Ag system, the rapid resolidification results in a complex structure of the interfacial region, where the lattice-mismatched interface is separated from the Ag-Cu mixing region by an intermediate pseudomorphic bcc Cu layer that grows epitaxially on the (001) face of the fcc Ag film during the final stage of the resolidification process. The new lattice-mismatched interface consists of a periodic array of stacking fault pyramids outlined by stair-rod partial dislocations. The intermediate bcc layer and the stacking fault pyramid structure of the mismatched interface present a barrier for dislocation propagation, resulting in the effective hardening of the layered structure treated by laser irradiation.

[1]This work is supported by NSF (Grant No. DMR-0907247)

11:51AM J21.00004 Optical Antennas for Enhanced Light Absorption and Emission[1] , LUKAS NOVOTNY — The absence of optical antennas in technological applications is primarily associated with their small scale. Antennas have characteristic dimensions on the order of a wavelength, demanding fabrication accuracies better than 10nm for the optical frequency regime. The advent of nanoscience and nanotechnology provides access to this length scale but material challenges associated with optical antennas remain. For example, the penetration of radiation into metals can no longer be neglected. The electromagnetic response is then dictated by collective electron oscillations (plasmons) characteristic of a strongly coupled plasma. These collective excitations make a direct downscaling of traditional antenna designs impossible and demand the careful study of plasmon resonances in metal nanostructures. The introduction of the antenna concept into the optical, infrared and terahertz frequency regime holds promise for a wide range of novel technological applications. Optical antennas can be employed to enhance the eciency of photovoltaics, to release energy from nanoscale light-emitting devices, and to boost the eciency of photochemical or photophysical detectors. In this presentation, I will outline the physical properties of optical antennas, review relevant history and recent work.

[1]Supported by DOE and NSF

12:27PM J21.00005 In Situ 3D Coherent X-ray Diffraction Imaging of Shock Experiments: Possible? , JOHN BARBER, Los Alamos National Laboratory — In traditional coherent X-ray diffraction imaging (CXDI), a 2D or quasi-2D object is illuminated by a beam of coherent X-rays to produce a diffraction pattern, which is then manipulated via a process known as iterative phase retrieval to reconstruct an image of the original 2D sample. Recently, there have been dramatic advances in methods for performing fully 3D CXDI of a sample from a single diffraction pattern [Raines et al, Nature 463 214-7 (2010)], and these methods have been used to image samples tens of microns in size using soft X-rays. In this work, I explore the theoretical possibility of applying 3D CXDI techniques to the in situ imaging of the interaction between a shock front and a polycrystal, a far more stringent problem. A delicate trade-off is required between photon energy, spot size, imaging resolution, and the dimensions of the experimental setup. In this talk, I will outline the experimental and computational requirements for performing such an experiment, and I will present images and movies from simulations of one such hypothetical experiment, including both the time-resolved X-ray diffraction patterns and the time-resolved sample imagery.

12:39PM J21.00006 Lattice dynamics of laser excited self-assembly gold nanocrystals by time resolved X-ray diffraction , KOUHEI ICHIYANAGI, HIROSHI SEKIGUCHI, University of Tokyo, SHUNSUKE NOZAWA, TOKUSHI SATO, SHIN-ICHI ADACHI, High Energy Accelerator Research Organization, YUJI C. SASAKI, University of Tokyo — The self-assembled gold nanoparticle has attracted considerable interest from researchers as the new nanodevices and bio-sensors. Functional groups such as thiols and amines have assembled on the gold nanoparticles in solution. For using the functional optical nanomaterial, it is necessary to reveal the mechanism of interaction between the laser and the functional nanomaterial. In the present work, we observed the effect of photo-excited process of self-assembled gold nanocrystal in ethanol solution using picosecond time-resolved X-ray diffraction. Gold nanocrystals deposited on the NaCl (100) substrate. After isolation of gold nanocrystals from the substrate, these nanocrystals were assembled with 10-Carboxydecyl disulfide molecules in ethanol. The nanocrystals size was the diameter of about 60 – 120 nm. The X-ray energy, pulse width and repetition rate for probing the gold nanocrystals were 15 keV, 100 ps and 945 Hz, respectively. The excitation wavelength and the pulse width were 400 nm and 150 fs. The detailed results of the lattice dynamics inside gold nanocrystals will be presented in the presentation.

12:51PM J21.00007 Ultrafast Laser Matter Interaction and Pump-probe Imaging of Transient Electric Fields , JIAN-MIN ZUO, HYUK PARK, Materials Science and Engineering, University of Illinois — Ultrafast electron diffraction and microscopy use pulsed laser as pump to initiate dynamic processes in solids. Under irradiation of pulsed laser beam of picoseconds or less, electrons inside a solid can be heated to high temperatures for a short period of time (several picoseconds). A part of hot electrons can be emitted from the surface in a similar way of thermionic emission. The emitted electrons, travel at speeds, produce transient electric fields (TEFs) together with the positively charged surface [1]. However, the effect of photoemitted electrons and their electric fields on ultrafast electron diffraction and microscopy has been a subject of debate [2]. Here we report direct measurement of TEFs using time-resolved electron beam imaging techniques based on the pump-probe approach. Results obtained from Pt thin films, Cu and ZnO nanowires will be shown. We demonstrate that TEFs produced by ultrafast laser irradiation can lead to large beam deflections that depend on the electron beam distance to sample surface, laser fluence and laser wavelength. The work shows that there is clearly a critical need for better understanding of TEFs in the field of ultrafast electron microscopy. The work is supported by DOE DEFG02-01ER4592, DEFG02-91-ER45439 and DOE DEFG02-07ER46453. [1] H. Park and J. M. Zuo, Applied Physics Letters 94, 251103 (2009). [2] H. Park and J. M. Zuo, Physical Review Letters 105, 059603 (2010).

1:03PM J21.00008 Femtosecond Nanocrystallography with X-ray Free-Electron Lasers[1] , HENRY CHAPMAN, Center for Free-Electron Laser Science, DESY, and the University of Hamburg — The ultrafast pulses from X-ray free-electron lasers have opened up a new form of protein nanocrystallography. The X-ray pulses are of high enough intensity and of sufficiently short duration that individual single-shot diffraction patterns can be obtained from a sample before significant damage occurs. This "diffraction before destruction" method may enable the determination of structures of proteins that cannot be grown into large enough crystals or are too radiation sensitive for high- resolution crystallography. Ultrafast pump-probe studies of photoinduced dynamics can also be studied. We have carried out experiments in coherent diffraction from protein nanocrystals, including Photosystem I membrane protein, at the Linac Coherent Light Source (LCLS) at SLAC. The crystals are filtered to sizes less than 2 micron, and are delivered to the pulsed X-ray beam in a continuously flowing liquid jet. Millions of diffraction patterns were recorded at the LCLS repetition rate of 60 Hz. Tens of thousands of the single-shot diffraction patterns have been indexed, and combined into a single crystal diffraction pattern, which can be phased for structure determination and analysed for the effects of pulse duration and fluence. Experimental data collection was carried out as part of a large collaboration involving CFEL DESY, Arizona State University, Max Planck Institute for Medical Research, University of Uppsala, SLAC, LBNL, LLNL, using the CAMP apparatus which was designed and built by the Max Planck Advanced Study Group at CFEL.

[1]The LCLS is operated by Stanford University on behalf of the U.S. Department of Energy, Office of Basic Energy Sciences.

1:39PM J21.00009 Plans for an Upgrade of the Advanced Photon Source[1] , DENNIS MILLS, Argonne National Laboratory, APS-U PROJECT TEAM — We are presently developing plans for an upgrade of the Advanced Photon Source facility. Science has formally issued Critical Decision 0 and approved the Mission Need Statement in April of 2010, authorizing the APS to develop a conceptual design for the APS Upgrade (APS-U) project. The proposed upgrade will include enhancements to the accelerator, beamlines, and facility infrastructure. The high brilliance x-ray beams at high photon energy (e.g. $>$ 25 keV) provided by the APS Upgrade will have strong impact on research in energy, the environment, new or improved materials, and biological studies. High-energy x-rays can penetrate into a wide range of realistic and/or extreme environments and allow imaging of structures and processes in unprecedented detail on picosecond time scales and nanometer length scales. The presentation will include some of the essential goals of the APS-U and proposed strategies to attain those goals.

[1]The Advanced Photon Source at Argonne National Laboratory is supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

1:51PM J21.00010 The Jefferson Lab VUV-FEL at 10 eV and above[1] , GWYN WILLIAMS, Jefferson Lab, FEL TEAM — We will present details of the vacuum ultraviolet performance of the Jefferson Lab Free Electron Laser. The JLab FEL is oscillator-based [1] and uses a superconducting energy recovered linac for CW RF operation at up to 75 MHz. Lasing at a fundamental wavelength of 372 nm, the third harmonic is at 124 nm, corresponding to a photon energy of 10 eV. The energy per pulse in the fundamental is 20 microJoules, which at 9 MHz yields an average power of 180 Watts. The pulses have a FWHM of order 300 fs, which essentially determines the optical bandwidth. The third harmonic, which is a 0.1 - 1% fraction of this, is considerably brighter than any other source in the region. Further, being an FEL, there is a wide range of tunability in the 1 eV to 15 eV range. Additional reach is possible with increased electron beam energy, and some options will be discussed in the talk.

[1] S. Benson et al. Nucl. Instrum. Methods A582, 14-17 (2007).

[1]We acknowledge funding from ONR, AFRL and DOE-BES under contract AC05-060R23177.

2:03PM J21.00011 Ultrafast optical fiber microbeam for in-depth fabrication, trapping and fluorescence excitation , MERVYN PINTO, UT Arlington, YOGESHWAR MISHRA, CUSAT, NINAD INGLE, SAMARENDRA MOHANTY, UT Arlington — Micro-focused laser beam is finding widespread application in two-photon polymerization (TPP), microsurgery, two-photon fluorescence microscopy and optical trapping of microscale objects. However, limited by short working distance of the microscope objective, it is essential to develop fiber based laser microbeam for in-depth applications. While fiber-optic two-photon fluorescence excitation (TPE) has been explored in past for endoscopic imaging, only recently we demonstrated optical trapping and microsurgery using single fiber optical microbeam. Here, we present use of ultrafast laser coupled to microfabricated single mode optical fiber for in-depth fabrication of microstructures by TPP as well as TPE and manipulation of microscopic objects by fiber optical microbeam tweezers. The microfabrication of fiber optic axicon tip was optimized so as to perform all the four functions, namely fabrication, excitation, manipulation and collection of fluorescence from the trapped object. Owing to the propagation distance of Bessel-like beam emerging from the axicon-fiber tip, relatively longer streak of fluorescence was observed along the microsphere length. Stable trapping of the fluorescent objects was observed due to reduced scattering force as compared to axial gradient force. These results using multifunctional optical fiber will be presented.

Tuesday, March 22, 2011 11:15AM - 2:15PM –
Session J22 DCMP: Theory of Non Fermi Liquids D163

11:15AM J22.00001 Resistivity of a non-Galilean Fermi liquid near Pomeranchuk Quantum Criticality , DMITRII MASLOV, University of Florida, VLADIMIR YUDSON, Russian Academy of Sciences, ANDREY CHUBUKOV, University of Wisconsin-Madison — We analyze the effect of the electron-electron interaction on the resistivity of a metal near a Pomeranchuk quantum critical point (QCP). We show that Umklapp processes are not effective near a QCP, and one must consider the interplay between interaction and disorder. By power counting, the correction to the residual resistivity at low T scales as $AT^{(D+2)/3}$ at QCP ($T^{4/3}$ in 2D). We show, however, that that $A = 0$ for a simply connected and convex Fermi surface in 2D due to hidden integrability of the electron motion. We argue that $A > 0$ in a two-band ($s - d$) model with light and heavy carriers, and propose this model as an explanation for the observed $T^{(D+2)/3}$ behavior.

11:27AM J22.00002 Transport Properties near Quantum Critical Point in 2D Hubbard Model[1] , KUANG-SHING CHEN, SANDEEP PATHAK, SHUXIANG YANG, Louisiana State University, SHI-QUAN SU, Oak Ridge National Laboratory, DIMITRIS GALANAKIS, Nanyang Technological University, Singapore, KARLIS MIKELSONS, Georgetown University, JUANA MORENO, MARK JARRELL, Louisiana State University — We obtain high quality estimates of the self energy $\Sigma(K, \omega)$ by *direct* analytic continuation of $\Sigma(K, i\omega_n)$ obtained from Continuous-Time Quantum Monte Carlo. We use these results to investigate the transport properties near the quantum critical point found in the 2D Hubbard model at finite doping. Resistivity, thermal conductivity, Wiedemann-Franz Law, and thermopower are examined in the Fermi liquid, Marginal Fermi liquid (MFL), and pseudo-gap regions. $\Sigma''(k, \omega)$ with k along the nodal direction displays temperature-dependent scaling similar to that seen in the experiment. A next-nearest neighbor hopping $t' < 0$ increases the doping region where MFL character is found.

[1]NSF OISE-0730290

11:39AM J22.00003 Quantum Phase Transition in Interacting Quantum Wires[1] , MEHUL DIXIT, The Ohio State University, TOBIAS MENG, MARKUS GARST, ACHIM ROSCH, Institute for Theoretical Physics, University of Cologne, JULIA MEYER, SPSMS, CEA-INAC/UJF, Grenoble — We consider the quantum phase transition of interacting electrons in a quantum wire from a one-dimensional (1D) to a quasi-1D state as a function of an external gate voltage. At weak interactions, a Lifshitz transition occurs when electrons start filling the second subband of transverse quantization. The physics in the vicinity of the transition is characterized by pronounced correlations as interactions in the second subband are effectively strong due to the diverging density of states close to the band bottom. Inter-subband interactions lead to the formation of polarons, but the nature of the transition is unchanged, i.e., one finds a Lifshitz transition of impenetrable polarons. By contrast, strongly interacting electrons form a (quasi-)1D Wigner crystal, and the transition corresponds to the linear crystal splitting into a zigzag crystal. This Ising transition in the charge sector is decoupled from the spin excitations in the system.

[1]This work was supported in part by the U.S. DOE, Office of Science, under Contract No. DE-FG02-07ER46424.

11:51AM J22.00004 Conductance of Tomonaga-Luttinger liquid wires and junctions with resistances , DIPTIMAN SEN, ABHIRAM SOORI, Indian Institute of Science, Bangalore — We study the effect that resistive regions have on the conductance of a quantum wire with interacting electrons which is connected to Fermi liquid leads. Using the bosonization formalism and a Rayleigh dissipation function to model the power dissipation, we use Green's function techniques to derive the DC conductance. The resistive regions are generally found to lead to incoherent transport. For a single wire, we find that the resistance adds in series to the contact resistance of e^2/h for spinless electrons, and the total resistance is independent of the Luttinger parameter K_W of the wire. We numerically solve the bosonic equations to illustrate what happens when a charge density pulse is incident on the wire; the results depend on the parameters of the resistive and interaction regions in interesting ways. For a junction of Tomonaga-Luttinger liquid wires, we use a dissipationless current splitting matrix to model the junction. For a three-wire junction, there are two families of such matrices; we find that the conductance matrix depends on K_W for one family but is independent of K_W for the other family.

12:03PM J22.00005 Holographic metals and fractionalized Fermi liquids[1] , SUBIR SACHDEV, Harvard University — I show that there is a close correspondence between the physical properties of holographic metals near charged black holes in anti-de Sitter (AdS) space, and the fractionalized Fermi liquid phase of the lattice Anderson model. The latter phase has a "small" Fermi surface of conduction electrons, along with a spin liquid of local moments. This correspondence implies that certain mean-field gapless spin liquids are states of matter at non-zero density which realize the near-horizon, $AdS_2 \times R^2$ physics of Reissner-Nordstrom black holes. I will also go beyond this mean-field theory, and discuss connections between gauge theories of fractionalized Fermi liquids and holographic theories.

[1]Supported by DMR-0757145

12:15PM J22.00006 Dynamically Generated Gap from Holography: Mottness from a Black Hole[1] , KA-WAI LO, MOHAMMAD EDALATI, ROBERT LEIGH, PHILIP PHILLIPS, university of illinois — In the fermionic sector of top-down approaches to holographic systems, one generically finds that the fermions are coupled to gravity and gauge fields in a variety of ways, beyond minimal coupling. In this paper, we take one such interaction – a Pauli, or magnetic dipole, interaction – and study its effects on fermion correlators. We find that this interaction modifies the fermion spectral density in a remarkable way. As we change the strength of the interaction, we find that spectral weight is transferred between bands, and beyond a critical value, a hard gap emerges in the fermion density of states. A possible interpretation of this bulk interaction then is that it drives the dynamical formation of a (Mott) gap, in the absence of any symmetry breaking.

[1]NSF DMR-0940992

12:27PM J22.00007 Quantum phase transitions in the pseudogap Anderson Holstein model[1] , MENGXING CHENG, KEVIN INGERSENT, U. Florida — We study a pseudogap Anderson-Holstein model of a magnetic impurity level that (1) hybridizes with a conduction band whose density of states vanishes in power-law fashion at the Fermi energy, and (2) couples, via its charge, to a nondispersive bosonic mode (e.g., an optical phonon). The model exhibits quantum phase transitions (QPTs) of different types depending on the strength λ of the impurity-boson coupling. For small λ, the suppression of the density of states near the Fermi energy leads to QPTs between strong-coupling (Kondo) and local-moment phases. A sufficiently large λ, however, transforms the bare Coulomb repulsion between a pair of electrons in the impurity level into an effective attraction, leading to QPTs between strong-coupling (charge-Kondo) and local-charge phases. Critical exponents characterizing the response to a local magnetic field (for small λ) or electric potential (for large λ) suggest that the QPTs belong to the same universality class as the QPT of the previously studied pseudogap Anderson model. One specific case of the pseudogap Anderson-Holstein model may be realized in a double-quantum-dot device, where the QPTs manifest themselves in the finite- temperature linear electrical conductance.

[1]Supported by NSF grant DMR-0710540

12:39PM J22.00008 Statistical fluxes and the sodium cobaltate Curie-Weiss metal , KAI WU, ZHENG-YU WENG, Institute for Advanced Study, Tsinghua University, JAN ZAANEN, Instituut Lorentz for Theoretical Physics, Leiden University — A central pursuit in the study of quantum matter is whether non Fermi liquid states exist, as invoked in trying to explain e.g. high-T_c superconductivity. A quite different context is the search for thermodynamic materials in energy applications, which require at the same time a very large thermopower and a low resistivity. Here we predict a new state of matter that descends from a strongly interacting microscopy described by a t-J model on a triangular lattice. Due to the altered role of quantum statistics the spins are "localized" in statistical Landau orbits, while the charge carriers form a Bose metal that feels the spins through random gauge fields. In contrast to the Fermi-liquid state, this state naturally exhibits a Curie-Weiss susceptibility, large thermopower, and linear-temperature resistivity, explaining the physics of Na_xCoO_2 at $x > 0.5$. A "smoking gun" prediction for neutron scattering is presented.

12:51PM J22.00009 Spin-incoherent behavior in the ground state of strongly correlated systems[1] , GREGORY FIETE, Department of Physics, The University of Texas at Austin, Austin, Texas 78712, USA, ADRIAN FEIGUIN, Department of Physics and Astronomy, University of Wyoming, Laramie, Wyoming 82071, USA — It is commonly believed that strongly interacting one-dimensional Fermi systems with gapless excitations are effectively described by Luttinger liquid theory. However, when the temperature of the system is high compared to the spin energy, but small compared to the charge energy, the system becomes "spin-incoherent." We present numerical evidence showing that the one-dimensional "t-J-Kondo" lattice, consisting of a t-J chain interacting with localized spins, displays all the characteristic signatures of spin-incoherent physics, but in the ground state. We argue that similar physics may be present in a wide range of strongly interacting systems.

[1]We gratefully acknowledge funding from ARO grant W911NF-09-1-0527 and NSF Grants DMR-055778, DMR-0955707. A. E. Feiguin and G. A. Fiete, arXiv:1005:4707.

1:03PM J22.00010 DMRG study of the Phase Diagram of the Infinite U Hubbard Model , LI LIU, Stanford University, HONG YAO, UC Berkeley, EREZ BERG, Harvard University, STEVE WHITE, UC Irvine, STEVE KIVELSON, Stanford University, BRIAN MOLTZ COLLABORATION — Despite decades of discussion, the phase diagram of the paradigmatic Hubbard model in the strong coupling limit remains uncertain. Here, we study Hubbard ladders with infinite on site repulsion and electron density ranging from n=0 to n=1 per site. DMRG calculations shows that the phase diagrams of two, three and four-leg laddders share the following similarities: as a function of decreasing n a fully polarized (half metallic ferromagnetic phase is followed by a partially polarized ferromagnetic metallic state, and finally by a paramagnetic (unpolarized) phase for n less than a critical value of roughly n $\sim$ 0.5, but which differs somewhat depending on the number of legs. Unexpectedly, the ferromagnetic metal phase is reentrant in the sense that it is interrupted at a special commensurate density (n=0.75 for the two-leg and 4-leg ladders and n=0.8 for the three leg) by an incompressible commensurate density wave phase with zero net ferromagnetic moment. All results appear to extrapolate smoothly to the limit of infinite ladder length. We conclude with some speculations about the phase diagram of the 2D infinite U Hubbard model.

1:15PM J22.00011 Mobile impurities in ferromagnetic liquids[1] , ADRIAN KANTIAN, Universite de Geneve, ULRICH SCHOLLWOECK, Ludwigs-Maximillian Universitaet Munich, THIERRY GIAMARCHI, Universite de Geneve — Recent work has shown that mobile impurities in one dimensional interacting systems may exhibit behaviour that differs strongly from that predicted by standard Tomonaga-Luttinger liquid theory, with the appearance of power-law divergences in the spectral function signifying sublinear diffusion of the impurity. Using time-dependent matrix product states, we investigate a range of cases of mobile impurities in systems beyond the analytically accessible examples to assess the existence of a new universality class of low-energy physics in one-dimensional systems.
Correspondence: Adrian.Kantian@unige.ch

[1]This work was supported in part by the Swiss SNF under MaNEP and division II.

1:27PM J22.00012 ABSTRACT WITHDRAWN –

1:39PM J22.00013 Nonlinear Collective Field Theory for models with inverse square interaction and exchange , FABIO FRANCHINI, SISSA, Trieste (Italy), MANAS KULKARNI, Stony Brook University and Brookhaven National Laboratory, ALEXANDER ABANOV, Stony Brook University — We present fully nonlinear dynamics [1] in inverse square models such as spin-Calogero model and Haldane-Shastry model. Hydrodynamic equations of motion are written for these models in the regime where gradient corrections to the exact hydrodynamic formulation of the theory may be neglected. We then show how this collective field theory allows to calculate correlation functions [2] that cannot be considered with conventional bosonization. We will also present the case of including external harmonic confinement [3] and show that the Calogero family is strikingly similar to models with delta (short-ranged) interaction and can be used as a toy model for cold atom experiments. Including harmonic trap usually ends up destroying integrability. However, Calogero family is special in this regard and the system remains integrable. In addition, we will present results of collective field theory which include gradient corrections thereby enabling us to go beyond gradient catastrophe.

[1] M. Kulkarni, F. Franchini, A. G. Abanov, Phys. Rev. B 80, 165105 (2009)
[2] F. Franchini, M. Kulkarni, Nucl. Phys. B, 825, 320 (2010)
[3] M. Kulkarni, A. G. Abanov, arXiv:1006.0966

1:51PM J22.00014 Renyi entropy of gapless spin liquids , TARUN GROVER, YI ZHANG, ASHVIN VISHWANATH, UC Berkeley — Spin liquids are exotic quantum states that do not break any symmetry. Though much is known about gapped spin-liquids, critical spin-liquids with strongly interacting gapless excitations in two and three spatial dimensions are less understood. Candidate ground state wave-functions for such states however can be constructed using the Gutzwiller projection method. We use bipartite entanglement entropy, in particular the Renyi entropy S_2 to investigate the quantum structure of these wave-functions. Using the Variational Monte-Carlo technique, we calculate the Renyi entropy of a critical spin liquid - the projected Fermi sea state on the triangular lattice. We find a violation of the boundary law, with S_2 enhanced by a logarithmic factor, an unusual result for a bosonic wave-function reflecting the presence of emergent spinons that form a Fermi surface. The Renyi entropy for algebraic spin liquids is found to obey the area law, consistent with the presence of emergent Dirac fermions in the system. Projection is found to completely alter the entanglement properties of nested Fermi surface states. These results show that the Renyi entropy calculations could serve as a diagnostic for gapless fractionalized phases.

2:03PM J22.00015 Power-Law Behavior of Bond Energy Correlators in a Kitaev-type Model with a Parton Fermi Surface[1] , HSIN-HUA LAI, OLEXEI I. MOTRUNICH, California Institute of Technology — We study bond energy correlation functions in an exactly solvable quantum spin model of Kitaev type on the kagome lattice with stable Fermi surface of partons proposed recently by Chua *et al.*, Ref. [arXiv:1010.1035]. Even though any spin correlations are ultra-short ranged, we find that the bond energy correlations have power law behavior with a $1/r^3$ envelope and oscillations at incommensurate wavevectors. We determine the corresponding singular surfaces in momentum space, which provide a gauge-invariant characterization of this gapless spin liquid.

[1]National Science Foundation and A. P. Sloan Foundation

Tuesday, March 22, 2011 11:15AM - 1:51PM –
Session J23 DCMP: Superconductivity: Fluctuation Phenomena D165

11:15AM J23.00001 Systematic determination of the superconducting fluctuation regime in the cuprates with torque magnetometry , GUICHUAN YU, University of Minnesota, YUAN LI, RUIHUA HE, Stanford University, XUDONG ZHAO, Jilin University, China, MARTIN GREVEN, University of Minnesota — Among the most important temperature scales in the high-$T_c$cuprates are those associated with the normal state pseudogap and the superconducting (SC) gap. Early Nernst effect and torque magnetometry measurements appeared to suggest an onset of SC fluctuations well above T_c in $La_{2-x}Sr_xCuO_4$ (LSCO). Recently, stripe correlations were found to contribute to the observed large Nernst signal in LSCO, leading to a reinterpretation of the earlier Nernst data. We report a systematically torque magnetometry study of the SC fluctuation regime in the simple model compound $HgBa_2CuO_{4+\delta}$, which has the highest T_c (97 K) among all single-layer cuprates, as well as initial results for LSCO. We demonstrate that the SC fluctuation regime is narrow and that it closely tracks T_c, which implies that the higher temperature scale observed in LSCO does indeed not result from SC fluctuations.

11:27AM J23.00002 Superconducting fluctuation regime in $HgBa_2CuO4_{+\delta}$ revealed by microwave measurements , NEVEN BARISIC, University of Minnesota, USA, MIHAEL GRBIC, ANTONIJE DULCIC, University of Zagreb, Croatia, YUAN LI, Stanford University, USA, XUDONG ZHAO[1], Jilin University, PR China, GUICHUAN YU, MARTIN GREVEN, University of Minnesota, USA, MIROSLAV POZEK, University of Zagreb, Croatia — There have been many attempts to measure the fluctuations preceding the superconducting long-range order in the cuprates with various experimental techniques, yet the onset temperature of the fluctuation regime has proven difficult to determine. We used a novel approach to microwave conductivity measurements in order to elucidate the phase diagram of the cuprates. Initial measurements were performed on the single-layer material $HgBa_2CuO_{4+\delta}$. From c-axis data for a sample close to optimal doping, we clearly discern the opening of the pseudogap at T*=185 K, the appearance of the superconducting fluctuations at the much lower temperature T'=105 K, and the transition to the superconducting state at T_c=94.3 K. Our result implies that the superconducting fluctuations extend only to about 10 K above T_c. Using the same approach, a narrow fluctuation regime is also found in other cuprates.

[1]University of Minnesota, USA

11:39AM J23.00003 Superconducting phase diagram and fluctuations in $SmFeAsO_{0.85}F_{0.15}$ single crystals , U. WELP, C. CHAPARRO, W.-K. KWOK, Argonne National Laboratory, A. RYDH, University of Stockholm, Sweden, N.D. ZHIGADLO, J. KARPINSKI, ETH Zuerich, Switzerland, S. WEYENETH, University of Zuerich, Switzerland — We use micro-calorimetry to investigate the anisotropic phase diagram and effects of superconducting fluctuations in sub-micro-gram single crystals of $SmFeAsO_{0.85}F_{0.15}$. Our measurements reveal that $SmFeAsO_{0.85}F_{0.15}$ is characterized by a large anisotropy of $\Gamma \sim$8 and a short in-plane Ginzburg-Landau coherence length of $\xi_{ab}(0) \sim$ 1.3 nm. These materials parameters promote strong superconducting fluctuations which are seen in the zero-field specific heat as clear upwards curvature in C/T at temperatures below T_c = 49.5 K and long tails above T_c. The resulting anomaly is cusp-shaped with height of $\Delta C/T_c$ = 24 mJ/moleK^2, which can be fitted with 3D-Gaussian fluctuations. The transition shows pronounced broadening in magnetic fields applied along the c-axis. The field evolution in fields higher than 3 T is well described in the frame of 3D lowest-Landau-level scaling of fluctuations using an upper critical field slope of -4.4 T/K. We will compare these characteristics to the behavior of other members of the FeAs-family. This work was supported by DOE-BES under Contract No. DE-AC02-06CH11357.

11:51AM J23.00004 A dynamical study of phase fluctuations and their critical slowing down in amorphous superconducting films[1] , WEI LIU, Johns Hopkins University, MINSOO KIM, GANAPATHY SAMBANDAMURTHY , University at Buffalo-SUNY, PETER ARMITAGE, Johns Hopkins University — We report a comprehensive study of the complex AC conductance of amorphous superconducting InO_x thin films. Using a novel broadband microwave "Corbino" spectrometer we measure the explicit frequency dependency of the complex conductance and the phase stiffness over a range from 0.21 GHz to 15 GHz at temperatures down to 350 mK. Dynamic AC measurements are sensitive to the temporal correlations of the superconducting order parameter in the fluctuation range above T_c. Among other aspects, we explicitly demonstrate the critical slowing down of the characteristic fluctuation rate on the approach to the superconducting state and show that its behavior is consistent with vortex-like phase fluctuations and a phase ordering scenario of the transition.

[1]NSF DMR-0847652

12:03PM J23.00005 Superconducting fluctuations in high-Tc cuprate superconductors , BRIGITTE LERIDON, LPEM-UMR8213-CNRS — Experimental results on electrical transport in various high-Tc cuprate superconductors are shown (namely in $YBa_2Cu_3O_{6+x}$, $Bi_2Sr_2CaCu_2O_{8+d}$, $La_{1-x}Sr_xCuO_4$). The part of the conductivity associated to superconducting fluctuations in the vicinity of the transition – also named paraconductivity - is extracted using different techniques for evaluating the normal state conductivity. Whenever possible, the conductivity measured under high pulsed field (50T) is used for the analysis. The results are compared to other experimental probes such as the Nernst effect, and are discussed from one compound to the other. It is shown that some straightforward conclusions can be drawn from relatively simple observations.

12:15PM J23.00006 Pairing associated with a single quantum critical energy in superconducting electron-doped cuprates , KUI JIN, NICHOLAS BUTCH, KEVIN KIRSHENBAUM, PAUL BACH, JOHNPIERRE PAGLIONE, RICHARD GREENE, Center for Nanophysics & Advanced Materials and Department of Physics, University of Maryland, College Park, MD 20742, USA — Though a comprehensive study of magnetotransport on electron-doped $La_{2-x}Ce_xCuO_4$ thin films, we show that an envelope of spin fluctuations yielding non Fermi liquid behavior ($\rho = \rho_0 + AT$) surrounds the superconducting dome in the overdoped region (x =0.15 to 0.21). This behavior survives to zero temperature over a range of fields exceeding the upper critical field. For example, the resistivity of x = 0.15 is linear in temperature over three decades down to 20 mK at 7.5 T. We demonstrate that all of the relevant energy scales in this system: those determining superconducting pairing, spin correlations, and the Fermi liquid metallic state, emanate from one common critical point at the end of the superconducting dome. These observations suggest that the superconductivity pairing is associated with spin fluctuations and with a single quantum critical energy in electron-doped cuprates. This work was partially supported by NSF-DMR 0653535.

12:27PM J23.00007 Shot noise measurements in mesoscopic N-S-N structures[1] , MARTIN STEHNO, D.J. VAN HARLINGEN, University of Illinois at Urbana-Champaign — Nonlocal subgap transport in mesoscopic superconductor-hybrid devices has received attention as a possible route towards creating and detecting entangled electron pairs in solid state devices. We study local and nonlocal transport in multi-terminal Cu/Al structures with transparent interfaces and separation between contacts comparable to the coherence length in the superconductor. The current shot noise in the two branches of the device is measured simultaneously and compared to the shot noise in a single contact. We discuss cross-correlations expected from Crossed Andreev Reflection and Elastic Co-tunneling processes, non-equilibrium transport in the superconductor, and device heating.

[1]Work supported by the National Science Foundation grant DMR 06-05813

12:39PM J23.00008 Transport noise crossovers in disordered electron nematics , WAN-JU LI, BENJAMIN PHILLABAUM, ERICA CARLSON, Purdue University, KARIN DAHMEN, University of Illinois at Urbana Champaign — Recently, low-frequency transport noise in underdoped YBCO was shown to exhibit an enhancement below 250K, consistent with fluctuations associated with a symmetry-breaking collective electronic state [1]. We discuss these results in relation to crossovers associated with the development of local electronic nematic order. Using a mapping of disordered electron nematics to random anisotropic resistor networks, we predict the thermal evolution of the noise power in transport associated with the crossover to local electron nematic behavior.
[1] Caplan et al., Phys. Rev. Lett. **104**, 177001 (2010).

12:51PM J23.00009 Vortex Noise in Thin Nb Films on a Triangular Anti-Dot Lattice[1] , TANNER SCHULZ, Department of Physics and Astronomy, University of Minnesota, LIWEN TAN, BETH STADLER, Department of Electrical and Computer Engineering, University of Minnesota, E. DAN DAHLBERG, Department of Physics and Astronomy, University of Minnesota — Thin Nb films are deposited on a periodic, triangular, anti-dot lattice with a lattice constant of 100nm. The lattice serves as pinning sites where superconducting vortices are trapped. The vortex density is set by an external field. At a vortex density commensurate with the pinning lattice transport measurements show an increase in current density. Interstitial vortex pinning produces similar current features at integer multiples of the matching field. We examine the voltage noise spectra as the applied field and DC current bias are varied. Noise signals appear above a field dependent threshold current and show minima at the matching fields. The noise is due to vortex motion in a pinning potential that varies with vortex density and driving forces. We use our results to study vortex motion and compare our signals to existing vortex noise models.

[1]This work was supported primarily by the MRSEC Program of the National Science Foundation under Award Numbers DMR-0212302 and DMR-0819885

1:03PM J23.00010 Inelastic scattering effects in current noise for a one dimensional Landauer system[1] , MANOHAR KUMAR, ZHENG P. BAARDMAN, ROEL H.M. SMIT, JAN M. VAN RUITENBEEK, Kamerlingh Onnes laboratory, Leiden University, The Netherlands — Generally, current shot noise is measured at low bias currents, and it reflects the transmission probability of the electrons. Here we present the first measurement at bias currents above the phonon energy of the system, *i.e.* a chain of Au atoms. The onset of phonon emission processes is signaled by an abrupt jump in differential conductance which results from the change in the transmission probability of the electrons due to phonon excitation. One should expect a sign of this change to be visible in shot noise. Indeed, a distinct signature in the current shot noise signal is observed due to inelastic scattering as a linear deviation from the Levitov- Lesovik classical shot noise. Surprisingly, we have observed that the deviation of noise from the classical noise at the phonon frequency is either positive or negative, depending on whether the transmission is above or below 0.96G0. These observations agree with recent predictions of a sign change in the phonon-induced correction to the noise [1-3], but the point of cross-over is higher than predicted. References: *1. Federica Haupt et.al., PRL 103, 136601 (2009) 2. R. Avriller et. al., PRB 80 041309 (2009) 3. T.L.Schmidt et al., PRB 80 041307(R), (2009)*

[1]Authors are thankful for the grant from FOM(86), The Netherlands

1:15PM J23.00011 AC conductivity across the disorder driven superconductor insulator transition[1] , YEN LEE LOH, KARIM BOUADIM, NANDINI TRIVEDI, MOHIT RANDERIA, The Ohio State University — The superconductor-insulator transition (SIT) is defined, at the most fundamental level, in terms of electromagnetic response. The Mattis-Bardeen theory for conventional superconductors becomes inadequate near the disorder-tuned SIT, where phase fluctuations become important. We present AC conductivity results obtained using determinant quantum Monte Carlo simulations, which include both quantum and thermal phase fluctuations. We find unexpected low-energy weight in the AC conductivity especially near the SIT, and we identify possible sources of this weight. We comment on implications for experiments [1,2].

[1] R. Valdés Aguilar et al., Phys. Rev. B 82, 180514 (2010)
[2] I. Hetel et al., Nature Physics 3, 700-702 (2007)

[1]Acknowledgments: DOE DE-FG02-07ER46423 and Ohio Supercomputer Center

1:27PM J23.00012 Spectroscopic probes of the disorder-driven superconductor-insulator transition[1] , MOHIT RANDERIA, KARIM BOUADIM, YEN-LEE LOH, NANDINI TRIVEDI, The Ohio State University — In spite of decades of research, the mechanism of the disorder- driven superconductor- insulator transition (SIT) and the nature of the insulator are not understood. We use quantum Monte Carlo simulations that treat, on an equal footing, inhomogeneous amplitude variations and phase fluctuations, a major advance over previous theories. The energy gap in the density of states survives across the transition, but coherence peaks exist only in the superconductor. A characteristic pseudogap persists above the critical disorder and critical temperature, in contrast to conventional theories. Surprisingly, the insulator has a two-particle gap scale that vanishes at the SIT, despite a robust single-particle gap. Our predictions are testable with scanning probe experiments.

[1]We acknowledge support from grants DOE DE-FG02-07ER46423 and NSF-DMR 0706203 and computational support from Ohio Supercomputing Center.

1:39PM J23.00013 Fast vortices in the cuprates? A vortex plasma model analysis of the THz conductivity and diamagnetism in $La_{2-x}Sr_xCuO_4$[1] , LUCAS BILBRO, ROLANDO VALDES AGUILAR, Johns Hopkins University, GENNADY LOGVENOV, OSHRI PELLEG, IVAN BOZOVIC, Brookhaven National Labs, N.P. ARMITAGE, Johns Hopkins University — We present measurements of the fluctuation superconductivity in an underdoped thin film of$La_{1.905}Sr_{0.095}CuO_4$ using time-domain THz spectroscopy. We compare our results with the measurements of diamagnetism in a similarly doped crystal of $La_{2-x}Sr_xCuO_4$. Through a vortex-plasma model, we show that if the fluctuation diamagnetism originates in vortices, then we necessarily obtain an anomalously large vortex diffusion constant, more than 100 times larger than estimates from the Bardeen-Stephen model.

[1]JHU Institute for Quantum Matter DOE DE-FG02-08ER46544

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J24 DCOMP DMP: Focus Session: Multiscale Modeling: Structural Materials D167

11:15AM J24.00001 Origin of Plasticity Length-Scale Effects in Fracture and Deformation , WILLIAM CURTIN[1], Brown University — Engineering design of essentially all metallic components used in structural applications relies heavily on the framework of continuum plasticity. However, many experiments now show that the plastic flow stress in metals increases in micron-scale material volumes, i.e. "smaller is stronger". The failure of conventional plasticity is particularly manifest at a crack tip, where infinite toughness can be predicted. Phenomenological strain-gradient plasticity models and discrete-dislocation models have emerged to handle size effects but there is no clear physical identification of material length scales controlling size-dependence, in spite of wide speculation. Here, we use a new discrete-dislocation/cohesive-zone model to unambiguously demonstrate that the spacing between obstacles to dislocation motion is one dominant material length scale controlling the fracture toughness of plastically deforming metals. With this insight, we propose a new "stress gradient plasticity" concept based on the behavior of dislocations in a "pile-up" at an obstacle under a stress gradient, which (i) rationalizes our fracture results and (ii) predicts size-effects under other loading conditions (bending, torsion, indentation). Quantitative agreement between theory and experiments is then demonstrated in several cases.

[1]In collaboration with Srinath S. Chakravarthy, School of Engineering, Brown University.

11:51AM J24.00002 Chemistry and Deformation: First Principles Studies of Local Plasticity , CHRISTOPHER WOODWARD, Air Force Research Laboratory — In order to understand the how chemistry influences deformation, an adequate description of the strain field near the center of dislocations (i.e. the core) is required. Continuum level descriptions of deformation ignore this short-range coupling between dislocations and the local atomic lattice. Interactions at this scale are non-linear and can strongly influence plastic deformation in fcc and bcc metals. Here, density functional theory is used in conjunction with a flexible boundary condition method to calculate the equilibrium dislocation core structure in a variety of bcc and fcc metals. The problem is divided into two parts: a solution for the nonlinear dislocation-core region and a solution for the long-range elastic response. Solving these individual problems is straightforward and by iteratively coupling the two solutions we can efficiently solve for the strain field in all space. Chemical effects, in the form of local solute-dislocation interactions, can also be calculated using this method. Derived solute-dislocation interactions are used to inform new models of solution hardening (and softening) in bcc Mo-X (X=Re, Pt) and fcc Al-X (X=Mg, Cr, Si, Cu) alloys. Currently, solute dislocation interactions are being assessed in bcc Fe-H alloys using this first principles technique.

12:27PM J24.00003 Ab-initio Concurrent Multiscale Method to Address Defects in Metals , GEORG SCHUSTERITSCH, Harvard University, THOMAS KÜHNE, Johannes Gutenberg University of Mainz, EFTHIMIOS KAXIRAS, Harvard University — We present a concurrent multiscale method for metallic systems based on coupling a region calculated using Kohn-Sham Density-Functional-Theory (KS-DFT) to a macroscopic region employing the Embedded Atom Method (EAM). By construction, our method is particularly well suited for treating defects such as grain boundaries (GBs), dislocations and chemical impurities, where quantum mechanical interactions in a small region near the defect may affect the mechanical properties at the macroscopic scale. Results for two metals, Nickel and Copper, are presented in the context of chemical embrittlement. We study the effects of impurities near GBs and investigate the surrounding strain field. This gives us insights into the role defects play in the underlying physical mechanism of chemical embrittlement.

12:39PM J24.00004 Multiscale Modeling of Irradiation Induced Hardening in Ferritic-Martensitic Steels , HUSSEIN ZBIB, IOANNIS MASTORAKOS, Washington State University, MOHAMMAD KHALEEL, XIN SUN, Pacific Northwest National Laboratory — The development of structural materials for use in new generation nuclear reactors depends critically on predicting and understanding the underlying physical mechanisms responsible for microstructural evolution along with corresponding dimensional instabilities and mechanical property changes. As the phenomena involved are very complex and span in several length scales, a multiscale approach is necessary in order to fully understand the degradation of materials in irradiated environments. The purpose of this work is to study the mechanical behaviour of Fe systems (namely a-Fe, Fe-Cr and Fe-Ni) under irradiation using both Molecular Dynamics (MD) and Dislocation Dynamics (DD) simulations. Critical information is passed from the atomistic (MD) to the microscopic scale (DD) in order to study the degradation of the material under examination. In particular, information pertaining to the dislocation-defects (particularly voids, helium bubbles and prismatic loops) interaction is obtained from MD simulations. This information is used in large scale DD simulations to analyze systems with high dislocation and defect densities, predicting the dependence of strength and ductility on defect density.

12:51PM J24.00005 A QCDFT Study of Hydrogen embrittlement at Crack Tip , QING PENG, Rensselaer Polytechnic Institute — Study of hydrogen embrittlement is of great importance due to widespread availability of hydrogen in all environmentally influenced cracking phenomena. We used QCDFT: Density functional theory based Quasi-continuum method to study the system where hydrogen atoms are presented on crack tip surface in single aluminum crystal under mode-I loading. We found that the presence of 0.1% hydrogen atoms increases the energy for nucleation of dislocations and enhance the brittlement of aluminum by 5%. The presence of hydrogen atoms also makes the geometry of crack tip to be sharp. The bonding and electronic charge transfer between hydrogen atoms and aluminum atoms were studied and the mechanism of hydride-induced embrittlement will be discussed.

1:03PM J24.00006 Models of defects at bi-material interfaces , KIPTON BARROS, TURAB LOOKMAN, Los Alamos National Laboratory — Multi-phase composite materials with a high density of bi-material interfaces can exhibit striking strength and robustness in extreme conditions such as shock and radiation damage. Laminar composites of Ag-Cu, Cu-Nb, and Ag-Fe with submicron to nano-scale layer thicknesses have recently been fabricated, but theoretical models of such systems are lacking. The plastic deformation behavior of nano-scale composites is dominated by defects, such as dislocations and twins, that are controlled by the interfaces. We investigate the phenomenology of defect dynamics at bi-material interfaces using Landau theory based models that span atomic and mesoscales.

1:15PM J24.00007 First Principles Simulations of Beta to Omega Transformation in the Titanium-Molybdenum System , ARUN DEVARAJ, NIRAJ GUPTA, SOUMYU NAG, University of North Texas, HAMESH FRASER, Ohio State University, RAJ BANERJEE, SRINIVASAN SRIVILLIPUTHUR, University of North Texas — The omega phase precipitation in beta titanium (Ti) alloys influence the beta to alpha phase transformation, and ultimately the mechanical properties of these alloys. Molybdenum (Mo) and other alloying additions affect both the relative phase stability and the energy barrier of the transformation. In this work we perform first principle calculations using Nudeged Elastic Band Method(NEB) implemented in Vienna Ab initio Simulation Package (VASP) to determine the minimum energy path, and thereby the energy barrier in beta Ti-Mo alloys with up to 20wt.% Mo. We report the energetics of beta to omega transformation path, proposed by De. Fontaine et al (Acta Metallurgica, vol. 19, p 1153 (1971)). The atomic configurations along the minimum energy transformational path will be compared with our 3D atom probe tomography and probe corrected high-resolution scanning transmission electron microscopy results.

1:27PM J24.00008 Shock-induced Spallation Phenomena in Copper-Niobium Nanolayered Composites , NIRAJ GUPTA, University of North Texas, ALEXANDER STUKOWSKI, Lawrence Livermore National Laboratory, MICHAEL BASKES, Los Alamos National Lab, SRINIVASAN SRIVILLIPUTHUR, University of North Texas — Shock-induced spallation phenomena in Copper-Niobium nanolayered composites conforming to a Kurdjumov-Sach's orientation relation were simulated using molecular dynamics to determine both spallation strength and the nature of void formation. The target structures consisted of varying numbers of alternating copper and niobium layers with thicknesses varying from 1 nm to 22 nm. Flyer velocities ranged from 3.5 to 11.5 A/ps, corresponding to an approximate strain rate of 10^9 s^{-1}. Spallation occurs in the vicinity of the Cu-Nb interface, and always in the copper layer. The proposed factors contributing to spallation will be discussed, as well as what effect the layer morphology has on the strength of the target.

1:39PM J24.00009 A First-Principles Study of Structure and Stability of Nickel Carbides , JOSH GIBSON, JAMAL UDDIN, University of North Texas, NELLI BODIFORD, University of Texas at Arlington, THOMAS CUNDARI, ANGELA WILSON, University of North Texas — Computational studies of nickel carbides, particularly Ni2C, are scarce. A systematic density functional theory study is reported for Ni2C, along with NiC and Ni3C, to understand the stability and electronic structure of nickel carbides of varying stoichiometry. A comprehensive study was executed that involved 28 trial structures of varying space group symmetry for Ni2C. An analysis of the electronic structure, geometry and thermodynamics of Ni2C is performed, and compared with that for Ni3C and NiC as well as several defect structures of varying composition. It is found that the most stable ground state arrangement of Ni2C exists within a simple orthorhombic lattice and that it has metallic character. The calculated formation energies (kcal/mol) of NiC, Ni2C, and Ni3C are 48.6, 7.9 and 6.4, respectively.

1:51PM J24.00010 Atomistic Simulations of Deformation of Nanoscale FCC Materials , SHIVRAJ KAREWAR, NIRAJ GUPTA, University of North Texas, ALEX STUKOWSKI, Lawrence Livermore National Laboratory, MICHAEL BASKES, Los Alamos National Laboratory, SRINIVASAN SRIVILLIPUTHUR, University of North Texas — We compare the deformation behavior of gold single crystal nanospheres with ∼6-30 nm diameters with gold spherical shells of varying inner to outer diameter ratios. Gold nanospheres are modeled with an EAM potential and the indenter is described by a repulsive potential. Yield strength dependence on sample size, geometry and temperature was studied in these nanospheres. The deformation mechanism is aided by the continuous displacement burst accompanying dislocation escape from the nanospheres. Based on this, a dislocation starvation mechanism has been discussed. Extended dislocations are found to be the prominent defect type in both solid and hollow nanospheres. Flow stresses are lower in hollow nanoshells. Low flow stresses are accounted for the presence of additional surface area for dislocation nucleation and emergence at the inner surface of the hollow shell.

2:03PM J24.00011 First-principles investigation of migration barriers in bulk (Cr,Co)-doped Ni_3Al (γ) and Ni_3Al/Ni (γ'/γ) interface , PRIYA GOPAL, SRINIVASAN SRIVILLIPUTHUR, Department of Material Science, University of North Texas — Ni-based super-alloys possess desirable high-temperature properties including ductility, fracture toughness as well as resistance to creep and oxidation mainly due to the precipitation of ordered Ni_3Al γ' precipitates within a γ (Ni,Al) matrix. Various studies have shown that the mechanical properties can be improved by adding substitutional elements. It is thus very important to understand the electronic structure and diffusion kinetics of the substitutional elements and the role each one has on the overall microstructure. \pardthis work we present our results on the systematic study of the energetics and migration barriers of Cr and Co in bulk Ni_3Al and Ni_3Al/Ni (γ'/γ) interface. We did simulations of migration of vacancy and substitutional element in a complete set of migration paths and evaluated the barrier energies in both bulk Ni_3Al and Ni_3Al/Ni (γ'/γ) interface using density functional theory methods. We will briefly discuss our results on the effect of migration barriers on the partitioning behavior of Cr and Co between the and ' phases in Ni-based super-alloy.

Tuesday, March 22, 2011 11:15AM - 2:03PM –

Session J26 DMP DCOMP: Focus Session: Iron Based Superconductors – Vortices & High Fields D162/164

11:15AM J26.00001 Anomalous High-Field Meissner Effect in Pnictide Superconductors , RUSLAN PROZOROV, MAKARIY A. TANATAR, SERGEY L. BUD'KO, PAUL C. CANFIELD, Ames Laboratory, Ames, IA 50011, USA, BING SHEN, PENG CHENG, HAI-HU WEN, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — The Meissner effect has been studied in $Ba(Fe_{0.926}Co_{0.074})_2As_2$ and $Ba_{0.6}K_{0.4}Fe_2As_2$ single crystals and compared to well known, type-II superconductors $LuNi_2B_2C$ and V_3Si. Whereas flux penetration is mostly determined by the bulk pinning (and, perhaps, surface barrier) resulting in a large negative magnetization, the flux expulsion upon cooling in a magnetic field is very small, which could also be due to pinning and/or surface barrier effects. However, in stark contrast with the expected behavior, the amount of the expelled flux increases almost linearly with the applied magnetic field, at least up to our maximum field of 5.5 T, which far exceeds the upper limit for the surface barrier. One interpretation of the observed behavior is that there is a field-driven suppression of magnetic pair-breaking.

11:27AM J26.00002 Flux Creep associated with Strong Pinning in Isovalently Doped Iron-Based Superconductors , M. KONCZYKOWSKI, SULTAN DEMIRDIS, C.J. VAN DER BEEK, Laboratoire des Solides Irradies, Ecole Polytechnique, CNRS UMR 7642 & CEA/DSM/IRAMIS, 91128 PALAISEAU, France, R. PROZOROV, M. TANATAR, P.C. CANFIELD, Ames Laboratory, Ames, IA 50011, U.S.A., S. KASAHARA, T. SHIBAUCHI, YUJI MATSUDA, Department of Physics, Kyoto University, Kyoto 606-8502, Japan — Strong pinning in Iron-Based Superconductors leads to the ubiquitous central peak of the irreversible magnetization. Notably, isovalently doped materials such as $BaFe_2(As_{1-x}P_x)_2$ and $Ba(Fe_{1-x}Ru_x)_2As_2$ offer a paradigm for the study of strong pinning because it is the only contribution to the critical current density j_c. We have studied flux creep rates as function of field and temperature in the low- and high field regimes in which j_c is limited by the line tension of a single pinned vortex, and by vortex interactions, respectively. For $T < \frac{1}{2}T_c$, screening currents j are of the order of 10^9 Am^{-2}, in spite of a creep rate $d\ln j/d\ln t \sim 0.02$. Creep is initially Anderson Kim-like, *i.e.* , creep barriers U depend on j as $U \propto (1 - j/j_c)$ over an order of magnitude in j, before crossing over to a nonlinear behavior. j_c is easily extracted from the high-current, short-time part of the magnetic relaxation. The results cast doubt on the range of applicability of the often-used "interpolation formula" $j \propto [1 + (k_BT/U_c)\ln(t + t_0/\tau)]^{-1/\mu}$ for weak collective pinning.

11:39AM J26.00003 Strong Pinning and Nonlinear Creep Barriers in Iron-Pnictide Superconductors , S. DEMIRDIS, M. KONCZYKOWSKI, C.J. VAN DER BEEK, Laboratoire des Solides Irradies, Ecole Polytechnique, CNRS UMR 7642 & CEA/DSM/IRAMIS, 91128 PALAISEAU, France, R. PROZOROV, Ames Laboratory, Ames, IA 50011, U.S.A., S. KASAHARA, T. SHIBAUCHI, YUJI MATSUDA, Department of Physics, Kyoto University, Kyoto 606-8502, Japan — The irreversible magnetization of Iron-Based Superconductors is characterized by the presence of an ubiquitous peak of the critical current density j_c, centered around zero field. Closer examination shows that the field-dependence of j_c corresponds, in all cases, to a low-field plateau, followed by a power-law decrease, $j_c \propto B^{-\alpha}$ (with $\alpha \sim \frac{5}{8}$) above a cross-over field B^*. This strongly suggests that vortex pinning at low magnetic field is due to strong pinning by nanometer-scale defects. In isovalently doped materials such as $BaFe_2(As_{1-x}P_x)_2$, strong pinning is the only contribution to the critical current. The analysis of j_c allows one to extract, without a priori assumptions, the elementary pinning force and the defect density. In $BaFe_2(As_{1-x}P_x)_2$, the latter quantity is in qualitative agreement with that obtained by H. Shishido *et al.*[Phys. Rev. Lett. **104**, 057008 (2010)]. The temperature dependence of the screening current above B^* is strongly affected by flux creep. The current decays as $j \sim [(k_BT/U)\ln(t+t_0/\tau)]^{-1/\mu}$, with $\mu \sim 1.6$, showing that nonlinear creep barriers are not an exclusive feature of weak collective pinning.

11:51AM J26.00004 Model of vortex states in hole-doped iron-pnictide superconductors , YI GAO, HUAI-XIANG HUANG, CHUN CHEN, C.S. TING, WU-PEI SU — Based on a phenomenological model with competing spin-density- wave (SDW) and extended $s-$wave superconductivity, the vortex states in $Ba_{1-x}K_xFe_2As_2$ are investigated by solving Bogoliubov-de Gennes equations. Our result for the optimally doped compound without induced SDW is in qualitative agreement with recent scanning tunneling microscopy experiment. We also propose that the main effect of the SDW on the vortex states is to reduce the intensity of the in-gap peak in the local density of states and transfer the spectral weight to form additional peaks outside the gap.

12:03PM J26.00005 Angular dependence of the critical current and vortex phase diagram in Co-doped BaFe2As2 films with strong pinning , B. MAIOROV, Los Alamos National Laboratory, NM 87544, T. KATASE, H. HIRAMATSU, H. HOSONO, Tokyo Institute of Technology, Yokohama, Japan, L. CIVALE, Los Alamos National Laboratory, NM 87544 — Studying the angular dependence of the critical current density (Jc) as a function of temperature in superconductors with complex pinning landscapes is very important both from the technical and fundamental points of view. The low anisotropy found in the Ba122 family tightened with strong naturally grown pinning make Ba122 films very attractive. It is also interesting to understand the different factors affecting vortex pinning in different regimes of temperature (T) and magnetic field (H). We present results on iron-arsenide superconducting films with varied pinning landscapes composed of columnar defects and nanoparticles. We analyze different field and angular regimes. We find that the naturally grown correlated defects found in Co-doped BaFe2As2 films are effective up to very high fields (m0H=15T) affecting a very wide region o the angular phase diagram. We also investigate the effects of film's thickness and the addition of defects produced by irradiation

12:15PM J26.00006 Comparative study of flux pinning characteristics of $Ba(Fe_{1-x}Co_x)_2As_2$ and $BaFe_2(As_{1-x}P_x)_2$ single crystals[1]

, NORIKO CHIKUMOTO, Superconductivity RSCH LAB, ISTEC, WATARU HIRATA, SHIGEKI MIYASAKA, SETSUKO TAJIMA, Osaka Univ., KEIICHI TANABE, Superconductivity RSCH LAB, ISTEC — We have studied the magnetization behavior of iron-pnictide superconductor, $Ba(Fe_{1-x}Co_x)_2As_2$ (Co-doped Fe122) with various Co doping and $BaFe_2(As_{0.65}P_{0.35})_2$ (P-doped Fe122) single crystals. All of the Co-doped Fe122 crystals showed a very pronounced "peak effect" in all the temperature range, irrespective of doping state. It is important to mention that a similar peak effect was previously reported for $REBa_2Cu_3O_y$. In order to get further insight into the pinning mechanism of the present system, we analyzed the pinning force density $F_p = J_cB$. A good scaling of the F_p versus the reduced field, $b = B/B_{irr}$, was established for all the Co-doped Fe122 crystals and the scaling curves were well fitted with the function given by $F_p/F_{p,max} = Ab^p(1-b)^q$, where A is a numerical parameter, p and q are describing the actual pinning mechanism. It was found that p value monotonically increases with x, while q value decreases with x. On the other hand, P-doped Fe122 did not show "peak effect". We will discuss about the possible pinning mechanism causing the peak effect.

[1]This work was supported by JSPS through FIRST Program.

12:27PM J26.00007 Dynamics of Vortices in Heavy-ion Irradiated Co-doped $BaFe_2As_2$[1]

, TSUYOSHI TAMEGAI, TOSHIHIRO TAEN, HIDENORI YAGYUDA, TOMOTAKA TANIGUCHI, SHYAM MOHAN, YASUYUKI NAKAJIMA, Dep. of Appl. Phys., The Univ. of Tokyo, SATORU OKAYASU, Advanced Science Research Center, Japan Atomic Energy Agency, MASATO SASASE, The Wakasa-wan Energy Research Center, Research & Development Group, HISASHI KITAMURA, TAKESHI MURAKAMI, National Institute of Radiological Sciences, TADASHI KAMBARA, Nishina Center for Accelerator Based Science, RIKEN, YASUYUKI KANAI, IThe Institute of Physical and Chemical Research, RIKEN — Effects of heavy-ion irradiation on the critical current density, J_c, and vortex dynamics are investigated in $Ba(Fe_{1-x}Co_x)_2As_2$ irradiated by heavy- ions of various kinds. Irradiations induce a large enhancement of J_c in the case of 200 MeV Au creating nearly continuous columnar tracks. On the other hand, in the case of 800 MeV Xe irradiation, despite the enhancement of J_c, clear columnar defects are not observed. In the case of 2.6 GeV U irradiation, new types of structure appears in the M-H loop at high matching field. We also discuss the behavior of vortex dynamics in the irradiated $Ba(Fe_{1-x}Co_x)_2As_2$.

[1]This work is partly supported by JST, Transformative Research-Proiect on Iron Pnictides (TRIP)

12:39PM J26.00008 High critical current density in $BaAs_2(Fe,Co)_2$ thin films up to 35 T

, J. JIANG, National High Magnetic Field Laboratory, FSU, Tallahassee, Florida, C. TARANTINI, J.D. WEISS, J. JAROSZYNSKY, E.E. HELLSTROM, D.C. LARBALESTIER, S. LEE, C.W. BARK, H.W. JANG, C.M. FOLKMAN, S.H. BAEK, J.W. PARK, C.B. EOM, Y. ZHANG, C.T. NELSON, X.Q. PAN — In the Co-doped $BaFe_2As_2$ thin films we intensively investigated field and angular dependences of J_c down 4.2 K in high field. We found a strong correlated c-axis pinning and Jc for field along the c-axis exceeds J_c for H//ab plane up to ∼20T, inverting the expectation of the Hc2 anisotropy. As a consequence the angular dependence is very weak and J_c is still over 10^5 A/cm^2 at 20T. Moreover the maximum pinning force F_p(4.2K) reaches 35-40 GN/m^3 at 15-20T depending on the field configuration, indicative of strong high-field vortex pinning. High resolution transmission electron microscopy reveals that the strong vortex pinning is due to a high density of non-superconducting Ba-Fe-O nanocolumnar defects whose diameter is $\sim 2\xi$, perfect conditions for a strong pinning.

12:51PM J26.00009 Critical current in disordered iron-pnictide superconducting wires[1]

, DUSHKO KUZMANOVSKI, MAXIM VAVILOV, University of Wisconsin - Madison, ANTON VORONTSOV, Montana State University — We evaluate the critical current in narrow wires of disordered iron-based pnictide superconductors. We present the Eilenberger and Usadel equations for a two-band model of a pnictide superconductor which take into account both inter and intra-band scattering events. The intra-band scattering events are responsible for the momentum relaxation of charged excitations, but do not suppress the homogeneous superconducting state. On the contrary, the inter-band scattering acts as the depairing mechanism. We apply the Usadel equation to analyze the dependence of the critical current on the strength of disorder in narrow iron-pnictide wires.

[1]Supported by NSF Grant No. DMR-0955500

1:03PM J26.00010 Upper critical field measured up to 85T in different iron-based compounds

, C. TARANTINI, National High Magnetic Field Laboratory, FSU, Tallahassee, Florida, J. JAROSZYNSKY, A. GUREVICH, D.C. LARBALESTIER, F. BALAKIREV, H.H. WEN, E. BELLINGERI, I. PALLECCHI, C. FERDEGHINI — We report magneto-transport measurements of H_{c2}(T) at very high dc and pulsed magnetic field up to 85T on different families of iron-based single crystals and thin film superconductors with different doping levels and stress. Some of these materials show high H_{c2} extrapolating to ∼100T and extremely high slopes up to 20 T/K for H//c and over 200 T/K for H//ab, indicating significant Pauli pair breaking and a possibility of the Fulde-Ferrel-Larkin-Ovchinnikov state. The superconducting transitions remain sharp also at the highest field showing an irreversibility field close to H_{c2}.

1:15PM J26.00011 Flux Pinning and Quasi-particle Scattering in Charge- Doped Iron-Based Superconductors

, KEES VAN DER BEEK, S. DEMIRDIS, M. KONCZYKOWSKI, Laboratoire des Solides Irradies, Ecole Polytechnique, CNRS UMR 7642 & CEA/DSM/IRAMIS, 91128 PALAISEAU, France, S. KASAHARA, T. TERASHIMA, Research Center for Low Temperature and Materials Sciences, Kyoto University, Sakyo-ku, Kyoto 606-8501, Japan, R. OKAZAKI, T. SHIBAUCHI, YUJI MATSUDA, Department of Physics, Kyoto University, Sakyo-ku, Kyoto 606-8502, Japan — Whereas isovalently doped iron-based superconductors, such as $BaFe_2(As_{1-x}P_x)_2$ and $Ba(Fe_{1-x}Ru_x)_2As_2$ show only strong, "individual-defect" vortex pinning due to nanometer-sized defects, charge-doped iron-pnictide superconductors show a low-field, field-independent contribution to the critical current density j_c that is well described by the collective pinning theory. Quantitative analysis of the magnitude, temperature, and field-dependence of j_c in the $PrFeAsO_{1-y}$ compound shows that the behavior of j_c can be fully explained, if one assumes the oxygen vacancies in this material to be responsible for quasi-particle scattering in the vortex cores. Analysis of j_c of this and other charge-doped compounds such as NdFeAs(O,F), (Ba,K)Fe_2As_2, and $Ba(Fe,Co)_2As_2$ yields estimates for the transport scattering cross-section of the dopant impurities in all these materials. We find scattering to be in the Born limit, with a scattering phase angle δ_0 such that $\sin\delta_0 \sim 0.2 - 0.3$.

1:27PM J26.00012 Nearly Isotropic Critical Currents in SmFeAs(O,F) in High Magnetic Fields

, BERTRAM BATLOGG, Solid State Physics, ETH Zurich, PHILIP MOLL, Solid State Physics, ETH Zurich, Switzerland, ROMAN PUZNIAK, Institute of Physics, Polish Academy of Sciences Warsaw, Poland, FEDOR BALAKIREV, NHMFL, LANL, Los Alamos, NM, LUIS BALICAS, NHMFL, Tallahassee, FL, JANUSZ KARPINSKI, NIKOLAI ZHIGADLO, Solid State Physics, ETH Zurich, Switzerland — The layered structure of SmFeAs(O,F) naturally raises questions about the electronic anisotropy of this 55K superconductor. To investigate the transport anisotropy, we performed electric 4-probe measurements on Focused Ion Beam (FIB) cut single crystals with sub-μm^2 cross-section, with current along and perpendicular to the FeAs layers. The normal state resistivity is indeed anisotropic ($\rho_c/\rho_{ab} \approx 2$ at RT, ≈ 10 at 50K) and consistent with the calculated Fermi velocity anisotropy. In contrast, the dissipation in high fields below T_c is more isotropic. The critical current densities at 4K are nearly isotropic and very high ($> 2\ 10^6$ A/cm^2), and up to 14 T, they are almost independent of the field orientation and strength. These values agree well with magnetization measurements. Additional measurements to much higher fields are presented.

1:39PM J26.00013 Low-energy muons and polarized neutrons for studying superconductivity[1] , VLADIMIR KOZHEVNIKOV, Tulsa Community College, KRISTIAAN TEMST, Katholieke Universiteit Leuven, ANDREAS SUTER, Paul Scherrer Institute, TIMOTHY CHARLTON, Rutherford Appleton Laboratory, HELMUT FRITZSCHE, Chalk River Laboratories, THOMAS PROKSCHA, ELVEZIO MORENZONI, Paul Scherrer Intitut, MARGRIET VAN BAEL, CHRISTIAN VAN HAESENDONCK, JOSEPH INDEKEU, Katholieke Universiteit Leuven — The penetration of the magnetic field into superconductors (SC) in the Meissner state is one of the major resources for studying SC. The merit of this resource will be greatly enhanced by quantitative measurements of the field distribution over the penetration layer, which, in particular, may lead to new insights for unconventional SC. We will report on measurements of the magnetic field profile in In and Sn using low-energy muons (LE-mSR) and polarized neutrons (PNR). The results solidly demonstrate nonexponential decay of the magnetic induction in accord with the Pippard and BCS theories. However, in contrast to In, results on which were reported last year, the data for Sn show significant differences in the values of the London penetration depth and the Pippard coherent length with those known from the literature.

[1]Supported by NSF

1:51PM J26.00014 Incoherent Interplane Response of $FeTe_{0.55}Se_{0.45}$, S.J. MOON, Department of Physics, University of California, San Diego, La Jolla, California 92093, USA, C.C. HOMES, A. AKRAP, Z.J. XU, J.S. WEN, Z.W. LIN, Q. LI, G.D. GU, Condensed Matter Physics and Material Science Department, Brookhaven National Laboratory, Upton, New York 11973, USA, D.N. BASOV, Department of Physics, University of California, San Diego, La Jolla, California 92093, USA — We investigated the interplane c axis electronic response of iron-chalcogenide superconductor $FeTe_{0.55}Se_{0.45}$ using infrared spectroscopy. We found that the normal-state c axis electronic response of $FeTe_{0.55}Se_{0.45}$ is incoherent. The c axis optical conductivity does not display well-defined Drude response and it becomes further suppressed with decreasing temperature. This normal-state c axis optical response is remarkably similar to that of the mildly underdoped cuprates but is in sharp contrast to the coherent c axis response of $Ba_{1-x}K_xFe_2As_2$. From the analyses on the electronic anisotropy of various layered superconductors, we found a close correlation between the degree of the coherence in the c axis transport and the strength of the dissipation in the *ab* plane response.

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J27 GQI: Focus Session: Quantum Optics with Superconducting Circuits II C155

11:15AM J27.00001 Tomography and Correlation Function Measurements of Itinerant Microwave Photons[1] , ANDREAS WALLRAFF, ETH Zurich — At optical frequencies the radiation produced by a source, such as a laser, a black body or a single-photon emitter, is frequently characterized by analysing the temporal correlations of emitted photons using single-photon counters. At microwave frequencies, however, there are no efficient single-photon counters yet. Instead, well-developed linear amplifiers allow for efficient measurement of the amplitude of an electromagnetic field. Here, we demonstrate first- and second-order correlation function measurements of a pulsed microwave-frequency single-photon source integrated on the same chip with a 50/50 beam splitter followed by linear amplifiers and quadrature amplitude detectors [1]. We clearly observe single-photon coherence in first-order and photon antibunching in second-order correlation function measurements of the propagating fields [2]. We also present first measurements in which we reconstruct the Wigner function of itinerant single photon Fock states and their superposition with the vacuum. To perform these measurements we have developed efficient methods to separate the detected single photon signal from the noise added by the amplifier by analyzing the moments of the measured amplitude distribution up to 4th order. The techniques and methods demonstrated in this work may find application in quantum optics and quantum information processing experiments at microwave frequencies.

[1] M. P. da Silva, D. Bozyigit, A. Wallraff, and A. Blais, Phys. Rev. A 82, 043804 (2010)
[2] D. Bozyigit, C. Lang, L. Steffen, J. M. Fink, C. Eichler, M. Baur, R. Bianchetti, P. J. Leek, S. Filipp, M. P. da Silva, A. Blais, and A. Wallraff, Nat. Phys. in print (2010), also arXiv:1002.3738

[1]Work done in collaboration with D. Bozyigit, C. Lang, C. Eichler, M. P. da Silva, A. Blais, and members of the Quantum Device Lab at ETH Zurich and supported in part by the EU through an ERC starting grant.

11:51AM J27.00002 An integrated circuit for generating distributable and unconditional entanglement at microwave frequencies , HSIANG-SHENG KU, University of Colorado at Boulder, FRANCOIS MALLET, JILA, WILLIAM F. KINDEL, University of Colorado at Boulder, KONRAD W. LEHNERT, JILA and NIST, KENT D. IRWIN, GENE C. HILTON, LEILA R. VALE, EMANUEL KNILL, SCOTT C. GLANCY, NIST, JILA TEAM, NIST TEAM — Entanglement, the unique feature of quantum mechanics, is the central resource of quantum information. In the strategy of continuous-variables quantum information processing, unconditional and distributable entanglement can be obtained by combining two squeezed states on a balanced beam splitter. Our group has recently demonstrated the generation of squeezed microwave states using a Josephson Parametric Amplifier [1] and implemented on-chip balanced beam splitters [2]. This talk will present a device that combines all these components on a single chip. The design requirements for such an "on-chip entangler" of the electromagnetic field modes will be discussed.

[1] M. A. Castellanos-Beltran et al, Nature Physics, 4, 929 (2008).
[2] Hsiang-Sheng Ku et al, arXiv:1010.3232v1

12:03PM J27.00003 Measuring on-chip distributable and unconditional entanglement at microwave frequencies , FRANCOIS MALLET, HSIANG-SHENG KU, JILA, WILL KINDEL, SCOTT GLANCY, EMANUEL KNILL, KENT D. IRWIN, GENE C. HILTON, LEILA R. VALE, NIST, KONRAD W. LEHNERT, JILA — A squeezed mode of the light field exhibits reduced fluctuations, below the vacuum level, along one of its quadratures and conversely amplified fluctuations along the conjugate quadrature. In that sense, it is the electromagnetic analog of the particle states used by Einstein-Podolsky-Rosen to derive their famous paradox. Indeed, by combining two such squeezed modes on a balanced beam splitter, entanglement can be generated, in an unconditional and distributable way. Such experiments have been performed for some years at optical frequencies. This talk will present an experimental attempt to generate and characterize entanglement with squeezed light at microwaves frequencies, using superconducting electrical circuits. We will discuss the achieved degree of entanglement from the perspective of implementing quantum teleportation protocols at microwave frequencies.

12:15PM J27.00004 Observation of photon blockade in circuit QED using second-order correlation function measurements , C. LANG, D. BOZYIGIT, C. EICHLER, L. STEFFEN, J.M. FINK, A.A. ABDUMALIKOV JR., M. BAUR, S. FILIPP, A. WALLRAFF, ETH Zurich — Circuit quantum electrodynamics (QED) provides an attractive platform to effectively study photon-photon interactions mediated by their strong and resonant coupling to a superconducting qubit embedded into a transmission line resonator. Driving the coupled system with a coherent microwave frequency tone the anharmonicity of the Jaynes-Cummings ladder blocks the transmission of more than a single photon through the resonator at a time. Using on-chip microwave beam splitters, linear amplifiers, and quadrature amplitude detectors we observe fluorescence and Rayleigh scattering in Mollow-triplet-like spectra. We investigate the phenomenon of photon blockade in second-order correlation function measurements which show antibunching and signatures of Rabi oscillations induced by the continuous drive coupling the ground and first excited states of the Jaynes-Cummings ladder.

12:27PM J27.00005 Generation and reconstruction of two mode squeezed states in the microwave domain

, CHRISTOPHER EICHLER, DENIZ BOZYIGIT, CHRISTIAN LANG, MATTHIAS BAUR, LARS STEFFEN, JOHANNES FINK, STEFAN FILIPP, ANDREAS WALLRAFF, ETH Zurich — Squeezing between two radiation field modes at optical frequencies has already been used to realize various quantum information processing tasks such as teleportation and quantum key distribution. Here we present measurements at microwave frequencies in which we generate and reconstruct a two mode squeezed state in a circuit QED setup. We prepare the desired state with a Josephson parametric amplifier and detect all four quadrature components simultaneously in a two channel heterodyne setup using amplitude detectors. Recording two dimensional phase space histograms for all possible pairs of quadratures allows for the reconstruction of the full covariance matrix and the four dimensional Wigner function of the squeezed state which shows strong correlations between the quadrature noise in the two modes. Combining parametric amplifier devices in networks with beamsplitters and superconducting qubits could allow for future linear optics quantum computation with propagating microwave photons.

12:39PM J27.00006 Using Superconducting Qubit Circuits to Engineer Exotic Lattice Systems

, DIMITRIS TSOMOKOS[1], Royal Holloway University of London, SAHEL ASHHAB[2], FRANCO NORI[3], Institute of Physical and Chemical Research (RIKEN) Japan and Physics Department, University of Michigan — We propose an architecture based on superconducting qubits and resonators for the implementation of a variety of exotic lattice systems, such as spin and Hubbard models in higher or fractal dimensions and higher-genus topologies. Spin systems are realized naturally using qubits, while superconducting resonators can be used for the realization of Bose-Hubbard models. Fundamental requirements for these designs, such as controllable interactions between arbitrary qubit pairs, have recently been implemented in the laboratory, rendering our proposals feasible with current technology.

[1]Member of Institute of Physics, UK
[2]APS member
[3]APS member

12:51PM J27.00007 Microwave Cavity Lattices for Simulating Condensed Matter Systems

, DEVIN UNDERWOOD, ARTHUR SAFIRA, SRIKANTH SRINIVASAN, ANTHONY HOFFMAN, Princeton University, JENS KOCH, Northwestern University, ANDREW HOUCK, Princeton University — Recently, quantum phase transitions of light have been the focus of much theoretical attention. One possible experimental realization relies upon the circuit quantum electrodynamics architecture (cQED); however, in order for this to be successful, coupled arrays of superconducting resonators must first be realized with low disorder. Here we fabricate and characterize an array with low disorder consisting of 12 niobium resonators on a sapphire substrate in a honeycomb pattern with the photonic lattice sites forming a Kagome star. The structure is characterized by measuring transmission through different input-output port pairs and by varying the hopping rate between resonators. A family of resonant peaks corresponding to the various modes of the coupled array is identifiable and agrees well with both a tight-binding Hamiltonian and simulations from a commercial microwave software package. These experiments are an important step in realizing strongly correlated interactions in cQED.

1:03PM J27.00008 Synthetic gauge fields in Jaynes-Cummings-Hubbard ring lattices

, ANDREAS NUNNENKAMP, Yale University, JENS KOCH, Northwestern University, STEVEN GIRVIN, Yale University — Recently there has been much interest in many-body physics with photons in circuit-QED arrays. Here we explore the physics of a Jaynes-Cummings-Hubbard ring lattice subject to a synthetic gauge field, i.e. where the hopping terms carry a complex phase factor due to Josephson couplers between the resonators. There are critical phase twists at which the single-particle spectrum is degenerate so that even weak interactions can give rise to strong correlations. We compare to ultracold bosons in rotating ring lattices and study the out-of-equilibrium physics as relevant for current experiments.

1:15PM J27.00009 Multi-Resonator Circuit QED Part I: The Photon Shell[1]

, MATTEO MARIANTONI, H. WANG, RADOSLAW C. BIALCZAK, M. LENANDER, ERIK LUCERO, M. NEELEY, A.D. O'CONNELL, D. SANK, M. WEIDES, J. WENNER, T. YAMAMOTO, Y. YIN, J. ZHAO, JOHN M. MARTINIS, A.N. CLELAND, Department of Physics, UC Santa Barbara — The generation and control of quantum states of light constitute fundamental tasks in cavity quantum electrodynamics (QED). The superconducting realization of cavity QED, circuit QED, enables on-chip microwave photonics, where superconducting qubits control and measure individual photon states. A long-standing issue in cavity QED is the coherent transfer of photons between two or more resonators. Here, we use circuit QED to implement a three-resonator architecture on a single chip, where the resonators are interconnected by two superconducting phase qubits. We use this circuit to shuffle one- and two-photon Fock states between the three resonators, and demonstrate qubit-mediated vacuum Rabi swaps between two resonators. This illustrates the potential for using multi-resonator circuits as photon quantum registries and for creating multipartite entanglement between delocalized bosonic modes.

[1]This work was supported by IARPA under ARO award W911NF-08-1-0336 and under ARO award W911NF-09-1-0375. M. M. acknowledges support from an Elings Postdoctoral Fellowship. Devices were made at the UC Santa Barbara Nanofabrication Facility

1:27PM J27.00010 Multi-resonator circuit QED - Part 2: Generation and detection of NOON states[1]

, FRANK WILHELM, fwilhelm@iqc.ca, SETH MERKEL, University of Waterloo — NOON states, states between two modes of light of the form $|N,0\rangle + e^{i\phi}|0,N\rangle$ allow for super-resolution interformetry. We show how NOON states can be efficiently produced in circuit quntum electrodynamics using superconducting phase qubits and resonators. We propose a protocol where only one interaction between the two modes is required, creating all the necessary entanglement at the start of the procedure. This protocol makes active use of the first three states of the phase qubits. Additionally, we show how to efficiently verify the success of such an experiment, even for large NOON states, using randomly sampled measurements and semidefinite programming technique. This is more efficient that the full tomography implemented to-date, allowing to reliably verify higher NOON-states. Based on New J. Phys. **12**, 093036 (2010).

[1]Supported by IARPA through the MQCO program and NSERC

1:39PM J27.00011 Multi-Resonator Circuit QED Part III: Two-Resonator Entanglement

, HAOHUA WANG, MATTEO MARIANTONI, RADOSLAW C. BIALCZAK, M. LENANDER, ERIK LUCERO, M. NEELEY, A.D. O'CONNELL, D. SANK, M. WEIDES, J. WENNER, Y. YIN, J. ZHAO, JOHN M. MARTINIS, A.N. CLELAND, Department of Physics, UC Santa Barbara, T. YAMAMOTO, Green Innovation Research Laboratories, NEC, Japan — Quantum entanglement, a defining feature of quantum mechanics, has been demonstrated in a variety of nonlinear spin-like systems. Quantum entanglement in linear systems has proven significantly more challenging, as the intrinsic energy level degeneracy associated with linearity makes quantum control more difficult. Here we demonstrate the quantum entanglement of photon states in two independent linear microwave resonators utilizing two superconducting phase qubits coupled through a band-pass resonator. After entangling two qubits into a Bell state, we demonstrate the controlled sequential photon amplification and transferring procedures, creating N quanta excitations distributed in two resonators. We completely characterize the two-resonator states with bipartite Wigner tomography and prove the existence of entanglement.

1:51PM J27.00012 Observation of Collective Strong Coupling between a Superconducting Resonator and Bismuth Dopants in Silicon , NATANIA ANTLER, R. VIJAY, UC Berkeley, CHRISTOPH WEIS, Lawrence Berkeley National Laboratory, ELI LEVENSON-FALK, UC Berkeley, THOMAS SCHENKEL, Lawrence Berkeley National Laboratory, IRFAN SIDDIQI, UC Berkeley — All electrical readout and control of spin systems with superconducting circuitry is an attractive route for implementing hybrid quantum information processing. Isolated spins, in general, have much longer coherence times than present day superconducting qubits, and thus could be utilized as memory elements. Species with a zero-field splitting (ZFS), such as bismuth doped silicon or NV centers in diamond, are particularly attractive as the absence of a strong magnetic bias field facilitates compatibility with low loss superconducting circuitry. We present results on the interaction of a tunable superconducting resonator and an ensemble of Bi spins implanted in an epitaxial layer of 28Si. As the resonator tunes through the ZFS, we observe an avoided crossing indicative of collective strong coupling. We discuss coherence properties as a function of spin density as well as progress on the detection of a small number of spins using a dispersive nanoSQUID magnetometer.

2:03PM J27.00013 Qubit-oscillator systems in the ultrastrong-coupling regime and their potential for preparing nonclassical states[1] , FRANCO NORI, SAHEL ASHHAB, RIKEN and University of Michigan — We consider a system composed of a two-level system (i.e. a qubit) and a harmonic oscillator in the ultrastrong-coupling regime, where the coupling strength is comparable to the qubit and oscillator energy scales. We explore the possibility of preparing nonclassical states in this system, especially in the ground state of the combined system. The nonclassical states that we consider include squeezed states, Schrodinger-cat states and entangled states. We also analyze the nature of the change in the ground state as the coupling strength is increased, going from a separable ground state in the absence of coupling to a highly entangled ground state in the case of very strong coupling. Reference: S. Ashhab and F. Nori, Phys. Rev. A 81, 042311 (2010).

[1]We thank support from DARPA, AFOSR, NSA, LPS, ARO, NSF, MEXT, JSPS, FIRST, and JST

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J28 DCOMP DMP: Focus Session: Computational Materials Design - Data-Driven

C156

11:15AM J28.00001 Distributed Strategies for Materials Development , STEFANO CURTAROLO, Duke University — Through appropriate combinations of "ab-initio," "data-mining-high-throughput," "cluster expansion," "vibrational," and "electronic structure" techniques, we have parameterized the whole set of transition-metal binary intermetallics (435 alloys) and a list of ∼10,000 inorganic crystals. The presentation will introduce the method, the tools, the standards, and the approach for automatic discovery of trends in material development. We will analyze rules for miscibility in metallic catalytic materials, electronic structure correlations in scintillators, and high-throughput search of thermoelectric materials and topological insulator through the distributed network of data, accessible to the scientific community. The presentation will also extend the hybrid method to study phenomena at the nanoscale, like size-induced viscosity effects on the catalytic rate, self-consistent variational approaches to the shape of nano-catalysts and size-dependent Wulff plots for tailoring catalysts compositions and size (Sponsors: ONR, NSF, DHS, Teragrid).

11:51AM J28.00002 A database survey to search for new candidate *p*-type TCOs[1] , GIANCARLO TRIMARCHI, K. POEPPELMEIER, A. J. FREEMAN, Northwestern U., Evanston, IL — New *p*-type TCOs are often produced by reacting the prototype binary *p*-type oxides, i.e., Ag_2O and Cu_2O, with binary oxides of other transition metals or main-series elements. Yet, so far only a small part of all the multi-cation Cu and, in particular, Ag oxides have been assessed as candidate *p*-type TCOs. Furthermore, numerous multi-species Cu and Ag oxide systems are poorly characterized, which leaves ample scope for discovery of yet unknown compounds belonging to them, and, likely, of unsuspected new TCOs, too. Here, we survey a *complete* database of known multicomponent Ag and Cu oxides, without restrictions on element composition, to search for new candidate TCOs. We indexed all the compounds in this database by applying selected crystal structure descriptors as structure type, stoichiometry, and coordination environment of the Cu and Ag cations. Chemical insight points to a significant likelihood that 2- and 4-fold coordination of the noble metal cations yield band structure properties suitable for the transparency and hole conductivity needed in TCOs. We scanned the indexed database to find compounds that could match these requirements and identified a set of materials that could be interesting candidate *p*-type TCOs.

[1]Supported by the U.S. DOE EFRC for Inverse-Band Design.

12:03PM J28.00003 Ab-Initio Prediction of Phase Diagrams Using a Genetic Algorithm , WILL TIPTON, Cornell University, RICHARD HENNIG — The computational design and prediction of materials' properties is a goal on which much progress has been made. However, it is generally necessary to first determine a material's crystal structure, and this remains a difficult problem. Previously, genetic algorithms have been successful in searching for stable crystal structures at particular compositions. However, when approaching a new material system, it is often unknown at which compositions stable structures might form. In order to search all of composition space simultaneously, Trimarchi and Zunger have recently suggested a modification to the traditional GA approach. In this method candidate structures are evaluated according to their formation energies with repect to structure found previously. We have implemented this technique in our genetic algorithm code and are investigating the practical details of its use. We have predicted previously-unknown phases in the Li-Be and elemental Eu systems under high pressure.

12:15PM J28.00004 The Harvard Clean Energy Project. Large-scale computational screening and design of molecular motifs for organic photovoltaics on the World Community Grid , JOHANNES HACHMANN, ROBERTO OLIVARES-AMAYA, SULE ATAHAN-EVRENK, Harvard University, CARLOS AMADOR-BEDOLLA, UNAM Mexico, ALAN ASPURU-GUZIK, Harvard University — Organic solar cells are one of the promising approaches to ubiquitously establishing renewable energy sources; alas the necessary 10% energy conversion efficiency remains elusive. We present the Harvard Clean Energy Project (CEP, http://cleanenergy.harvard.edu) which is concerned with the screening and design of organic photovoltaics (and organic electronics in general) by means of first-principles computational quantum chemistry. We use modern DFT to assess the quality of candidate structures and systematically improve upon these based on the gathered understanding of structure-property relations. The CEP is a high-throughput investigation which utilizes the massive computational resource of the IBM World Community Grid, which allows us to characterize millions molecules of interest in the course of the next year. We address the combinatorial generation of our molecular library, our database, workflow organization and automation, data calibration and cheminformatics analysis, and the closure of the development cycle provided by our experimental collaborators.

12:27PM J28.00005 Computational design of new A2BX4 materials[1] , VLADAN STEVANOVIC, NREL, Golden CO — The A2BX4 family of ternary compounds represents an important class of materials. Members of this group, in addition to being among the earth most abundant materials, also span a significant range of physical properties including ferromagnetism, coexistence of transparency and p-type conductivity, ferroelectricity, etc. Today we know for about 800 A2BX4 compounds that have been characterized experimentally. This is only a portion of nearly 5000 A2BX4 combinations that could be constructed throughout the periodic table. In this talk I will present a systematic theoretical approach, based on ab initio calculations, for predicting new A2BX4 compounds. For a given new A2BX4 combination we find the candidate crystal structures from the classification of the existing A2BX4 in terms of the atomic orbital radii of the constituent A and B atoms (Zhang and Zunger, Adv. Funct. Mat. 20, 1944, 2010). This step is followed by the set of high-throughput ab initio calculations which are used to sort out the ground-state structure and compute the corresponding heat of formation. The stability of a given A2BX4 with respect to decomposition into competing phases is then tested against all possible combinations of known compounds involving the same elements. This is done by comparing the heat of formation of the new ternary and the heats of formation of the competing (existing) binary and ternary compounds. I will also discuss the algorithms for searching the chemical space of ternary compounds in order to find the materials with target properties.

[1]The work has been performed in collaboration with X. Zhang, M. d'Avezac, S. Lany and A. Zunger and is supported through the Center for Inverse Design, an EFRC funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences

1:03PM J28.00006 Discovering potentially overlooked Filled Tetrahedral Structure compounds by high-throughput first-principles calculation[1] , XIUWEN ZHANG, ALEX ZUNGER, National Renewable Energy Lab, SOLID STATE THEORY GROUP TEAM — Filled Tetrahedral Structures (FTS) such as LiZnP are derived from the binary zincblende family by splitting a cation such as Ga in GaP into two lower-valent cations Li+Zn, placing one on the original cation site and the other on one of the empty interstitial sites. Generalizing this process, it is possible to generate a few hundred of ABX compounds. Depending on the position of A, B, and X in the periodic table, the structure of such ABX can deviate from the parent tetrahedral framework. Using high-throughput total-energy calculation in GGA+U we have examined the stable structures and possible metastable structures of a few hundred ABX compounds, establishing the basic regularities relating structure to chemical identity. Their thermodynamical stability has been checked by taking into account the competing binary and ternary phases. We identify dozens of ABX compounds likely to have large band gaps, potentially suitable as solar absorbers and transparent conductors.

[1]This work was supported through the Center for Inverse Design, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

1:15PM J28.00007 GW band gap of Filled Tetrahedral Structuctures: absorbers and topological insulators ?[1] , JULIEN VIDAL, XIUWEN ZHANG, JUN-WEI LUO, ALEX ZUNGER, National Renewable Energy Laboratory, Golden, CO 80401, USA — Filled Tetrahedral Structures (FTS) such as LiZnP are derived from the binary zincblende material such as GaP by splitting a cation such as Ga into two lower-valent cations Li+Zn, placing one on the original cation site and the other on one of the empty interstitial sites. Generalizing this process, it is possible to generate a few hundred of ABX compounds. Their electronic structure has been previously calculated by bandgap-underestimating DFT assuming a zincblende-derived crystal structure. We use instead GW to establish (i) which ABX materials are potentially suitable as absorbers in solar cells and (ii) which of the ABX materials previously proposed as topological insulators based on DFT may not be so in a better approximation such as GW.

[1]This work was supported through the Center for Inverse Design, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

1:27PM J28.00008 Quantum Monte Carlo for Materials Design , TIM MUELLER, LUCAS WAGNER, JEFFREY GROSSMAN, Massachusetts Institute of Technology — When designing new materials it is important to have an accurate measure of the material's formation energy to assess thermodynamic stability and chemical activity. Computational materials science holds the potential to accurately predict formation energies, but widely-used methods such as density functional theory often yield large errors when calculating energy differences between compounds with significantly different electronic structures. More accurate quantum chemical methods tend to scale poorly with system size, making it infeasible to apply them to many materials. One exception is quantum Monte Carlo (QMC), which effectively scales linearly or better with system size when calculating formation energy per atom. QMC scales perfectly with the number of processors, making it ideally positioned to take advantage of the rapidly growing core count in central and graphics processing units. It has been shown that quantum Monte Carlo can successfully predict formation energies for some solid state materials, but a broad assessment has been lacking. We have run QMC calculations on a variety of different materials for which high-quality experimental data exists. We present data on the cost and accuracy of QMC, providing insight into the role QMC will play in materials design.

1:39PM J28.00009 Off-lattice self-learning kinetic Monte Carlo: application to 3D island decay on fcc(100) surface[1] , GIRIDHAR NANDIPATI, ABDELKADER KARA, SYED ISLAMUDDIN SHAH, TALAT S. RAHMAN, University of Central Florida — We report the development of an off-lattice kinetic Monte Carlo (KMC) method with a new three-dimensional (3D) pattern recognition scheme to better identify the local environment and processes involving 3D motion which was not possible in the earlier approach [1]. In the present scheme, to uniquely identify the 3D neighborhood around the central atom or leading atom we split it into 3D rectangular boxes whose dimensions dictate the accuracy with which the motion of the diffusing entity to be accounted. This technique combines the idea of self-learning KMC (SLKMC) [2] method with the new pattern-recognition scheme fitted to an off-lattice model. We present application of this off-lattice SLKMC to 3D island decay on fcc (100) surface and compare the results and computational efficiency to that available in the literature.

[1] A. Kara et al, J. Phys.: Condens. Matter, 21 (2009)
[2] O. Trushin et al, Phys. Rev. B, 72, 115401 (2005)

[1]Supported by NSF-ITR 0840389.

1:51PM J28.00010 Density-functional study of U-Mo alloys , ALEXANDER LANDA, PER SODERLIND, PATRICE E.A. TURCHI, Lawrence Livermore National Laboratory, Livermore, USA — The U-Mo and U-Zr alloys proved to be very promising fuels for advanced fast nuclear reactors. According to numerous experiments, the main advantages of U-Mo fuels over U-Zr fuels lies in a much lower constituent redistribution due to the existence a single γ-U-Mo phase with body-centered cubic structure over typical fuel operation temperatures. Density-functional theory (EMTO-CPA technique) previously used to describe phase equilibria in U-Zr alloys [A. Landa, P. Söderlind, P. E. A. Turchi, Journal of Alloys and Compounds, 478 (2009) 103] is extended to investigate the ground-state properties of U-Mo solid solutions. Calculated heats of formation of bcc U-Zr and U-Mo alloys are compared with CALPHAD assessments. We discuss how the heat of formation in both alloys correlates with the charge transfer between the alloy components, and how the specific behavior of the density of states in the vicinity of the Fermi level promotes the stabilization of the U_2Mo compound. Our calculations prove that, due to the existence of a single γ-phase over the typical fuel operation temperatures, γ-U-Mo alloys should indeed have much lower constituent redistribution than γ-U-Zr alloys for which binodal decomposition causes a high degree of constituent redistribution. This work was performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

2:03PM J28.00011 Inverse band design of SiGe superlattices with direct band-gaps[1] , MAYEUL D'AVEZAC, NREL, JUN-WEI LUO, ALEX ZUNGER, NREL, Golden, Co, THOMAS CHANIER, University of Iowa — Integrating optoelectronic functionalities directly into the mature Silicon-Germanium technology base would prove invaluable for many applications. Unfortunately, both Si and Ge display indirect band-gaps unsuitable for optical applications. It was previously shown (Zachai *et al.* PRL **64** (1990)) that epitaxially grown $[(\mathrm{Si})_n(\mathrm{Ge})_m]_p$ (i. e. a single repeat unit) grown on Si can form direc-gap heterostructures with weak optical transitions as a result of zone folding and quantum confinement. The much richer space of *multiple-period* superlattices $[(\mathrm{Si})_{n_1}(\mathrm{Ge})_{n_2}(\mathrm{Si})_{n_3}(\mathrm{Ge})_{n_4}\ldots Ge_{n_N}]_p$ has not been considered. If $M = \sum n_i$ is the total number of monolayers, then there are, roughly, 2^M different possible superlattices. To explore this large space, we combine a (i) genetic algorithm for effective configurational search with (ii) empirical pseudopotential designed to accurately reproduce the inter-valley and spin-orbit splittings, as well as hydrostatic and biaxial strains. We will present multiple-period SiGe superlattices with large electric dipole moments and direct gaps at Γ yielded by this search.

[1]This work is supported through the Center for Inverse Design, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J29 GQI: Focus Session: Quantum Information for Quantum Foundations - Structures in Hilbert Space C148

11:15AM J29.00001 Proofs of the Kochen-Specker theorem based on two qubits , MORDECAI WAEGELL, P.K. ARAVIND, Worcester Polytechnic Institute — The observables for a pair of qubits yield a system of 60 rays and 105 bases in a complex Hilbert space of four dimensions that contains over a hundred million parity proofs of the Kochen-Specker theorem. An overview of these proofs is given and they are compared with those in other 4-d systems, such as the 600-cell. The significance of the results is discussed.

11:27AM J29.00002 Proofs of the Kochen-Specker theorem based on the 600-cell , P.K. ARAVIND, MORDECAI WAEGELL, Worcester Polytechnic Institute, NORMAN MEGILL, Boston Information Group, MLADEN PAVICIC, ITAMP, Harvard University — It is shown that the system of 60 rays and 75 bases derived from the vertices of a 600-cell (a regular polytope in four dimensions) contains over a hundred million parity proofs of the Kochen-Specker theorem. An overview of the proofs is given, some examples of them are presented and the significance of the results is discussed.

11:39AM J29.00003 MUB Entanglement Patterns by Transformations in Phase Space , JAY LAWRENCE[1], Dartmouth College, Hanover, NH 03755 — All possible MUB entanglement patterns for systems of N prime-state particles are obtained from standard ones by unitary transformations in the Hilbert space, thus preserving the relationships between the generalized Pauli operators, the phase point operators, and the MUB projectors. The transformations are described geometrically in discrete phase space. Illustrative examples show the invariance of the total entanglement content and the connection of entanglement with Galois fields. Different field representations for the same dimension may produce inequivalent MUB sets. This work provides alternative constructions and generalizes previous work on qubit systems [1,2].

[1] J L Romero, G Bjork A B Klimov, and L L Sanchez-Soto, Phys. Rev. A **72**, 062310 (2005).
[2] A B Klimov, J L Romero, G Bjork, and L L Sanchez-Soto, Ann. Phys. **324**, 53 (2009).

[1]current address: University of Chicago, Chicago, IL 60637

11:51AM J29.00004 Entanglement in Mutually Unbiased Bases[1] , MARCIN WIESNIAK, University of Vienna, TOMASZ PATEREK, CQT Singapore, ANTON ZEILINGER, University of Vienna — Higher-dimensional Hilbert spaces are still not fully explored. One issue concerns mutually unbiased bases (MUBs). For primes [1] and their powers (e.g. [2]), full sets of MUBs are known. The question of existence of all MUBs in composite dimensions is still open. We show that for all full sets of MUBs of a given dimension a certain entanglement measure of the bases is constant. This fact could be an argument either for or against the existence of full sets of MUBs in some dimensions and tells us that almost all MUBs are maximally entangled for high-dimensional composite systems, whereas this is not the case for prime dimensions. We present a new construction of MUBs in squared prime dimensions. We use only one entangling operation, which simplifies possible experiments. The construction gives only product states and maximally entangled states.

[1] I. D. Ivanović, J. Phys. A 14, 3241 (1981).
[2] W. K. Wootters and B. D. Fields, Ann. Phys. (N.Y.) 191, 363 (1989).

[1]Research supported by ERC Advanced Grant QIT4QAD and FWF SFB-grant F4007 of the Austrian Science Fund.

12:03PM J29.00005 Qutrits under a microscope[1] , GELO NOEL TABIA, University of Waterloo, Perimeter Institute for Theoretical Physics, Institute for Quantum Computing — Gleason's theorem states that the set of quantum states is complete, in the sense that density operators specify the unique probability measure definable on the lattice of Hilbert space of projection operators according to the Born Rule. Particularly, Gleason showed that the theorem holds in all finite dimensions if and only if it holds in dimension 3. This suggests that the essential features defining the probability structure of quantum theory can already be found in 3-dimensional quantum systems. Hence, we establish key geometric properties of qutrit state space as they are expressed in terms of symmetric, informationally-complete (SIC) measurements. We provide a variety of important results, which include an elegant formula for describing pure qutrits, affine plane symmetries and the Hesse configuration in qutrit SICs derived from algebraic structure constants for $\mathrm{GL}(3, C)$, and a comparison of the SIC and generalized Bloch representations by analyzing plane cross-sections of qutrit state space. In addition, we present a new way of implementing SIC-POVMs using multi-port devices built from waveguide-based micro-optics, in particular, by proposing experimental circuits for qubits and qutrits.

[1]This work was supported in part by the U. S. Office of Naval Research (Grant No. N00014-09-1-0247).

12:15PM J29.00006 A Linear Dependency Structure Arising from Weyl-Heisenberg Symmetry[1] , HOAN BUI DANG, Perimeter Institute and University of Waterloo, MARCUS APPLEBY, Perimeter Institute, INGEMAR BENGTSSON, KATE BLANCHFIELD, Stockholm University, ASA ERICSSON, CHRISTOPHER FUCHS, Perimeter Institute, MATTHEW GRAYDON, GELO TABIA, Perimeter Institute and University of Waterloo — The Weyl-Heisenberg (WH) group was used by Hermann Weyl to construct finite-dimensional quantum mechanics in the earliest days of the theory and, through its ubiquitous use in quantum information theory, is even more important today. While investigating properties of symmetric informationally-complete (SIC) measurements, we found a linear dependency structure in a class of Weyl-Heisenberg covariant sets when certain conditions on the dimensionality of the Hilbert space are met. This result reveals more structure in WH symmetry than previously noted and helps us gain a better understanding of quantum state space. For example in the Quantum Bayesian framework of Fuchs and collaborators, the number of zeros of a quantum state in a SIC representation is directly related to this linear dependency.

[1]This work was supported in part by the U. S. Office of Naval Research (Grant No. N00014-09-1-0247).

12:27PM J29.00007 Regrouping phenomena of SIC POVMs covariant with respect to the Heisenberg–Weyl group[1] , HUANGJUN ZHU, Centre for Quantum Technologies, National University of Singapore — Symmetric informationally complete positive operator valued measures (SIC POVMs) covariant with respect to the Heisenberg–Weyl (HW) group form disjoint orbits under the action of the normalizer of the HW group—the (extended) Clifford group. Additional SIC POVMs can be obtained by a suitable regrouping of the fiducial vectors on certain orbits, for example, in Hilbert spaces of dimension three, four, eight and twelve. To understand these SIC POVM regrouping phenomena, we need to go beyond the Clifford group and consider a larger group, in particular the normalizer of the Clifford group. We prove that, when the dimension of the Hilbert space is not a multiple of four, the HW group is a characteristic subgroup of the Clifford group, and the normalizer of the Clifford group is itself; when the dimension is a multiple of four, there are exactly two normal subgroups in the Clifford group that are isomorphic to the HW group, which are conjugated to each other in the normalizer of the Clifford group. Based on this observation, we provide a unified framework for understanding the regrouping phenomena mentioned above and those potential candidates.

[1]This work is supported by the National Research Foundation and the Ministry of Education, Singapore.

12:39PM J29.00008 Quantum Computational Geodesic Derivative , HOWARD BRANDT, U.S. Army Reseaarch Laboratory — In recent developments in the differential geometry of quantum computation, the quantum evolution is described in terms of the special unitary group of n-qubit unitary operators with unit determinant. The group manifold is taken to be Riemannian. In the present work the geodesic derivative is clarified. This is applicable to investigations of conjugate points and the global characteristics of geodesic paths in the group manifold, and the determination of optimal quantum circuits for carrying out a quantum computation.

12:51PM J29.00009 Affine Maps of the Polarization Vector for Quantum Systems of Arbitrary Dimension[1] , MARK BYRD, Southern Illinois University, C. ALLEN BISHOP, YONG-CHENG OU, Physics Department, Southern Illinois University — The operator-sum decomposition (OS) of a mapping from one density matrix to another has many applications in quantum information science. To this mapping there corresponds an affine map which provides a geometric description of the density matrix in terms of the polarization vector representation. This has been thoroughly explored for qubits since the components of the polarization vector are measurable quantities (corresponding to expectation values of Hermitian operators) and also because it enables the description of map domains geometrically. Here we extend the OS-affine map correspondence to qudits, briefly discuss general properties of the map, the form for particular important cases, and provide several explicit results for qutrit maps. We use the affine map and a singular-value-like decomposition, to find positivity constraints that provide a symmetry for small polarization vector magnitudes (states which are closer to the maximally mixed state) which is broken as the polarization vector increases in magnitude (a state becomes more pure). The dependence of this symmetry on the magnitude of the polarization vector implies the polar decomposition of the map can not be used as it can for the qubit case. However, it still leads us to a connection between positivity and purity for general d-state systems.

[1]This material is based upon work supported by NSF-Grant No. 0545798 to MSB.

1:03PM J29.00010 Pseudo-unitary freedom in the operator-sum representation , YONG CHENG OU, Department of Chemistry, Texas Tech University, Lubbock, Texas 79409, MARK S. BYRD, Department of Physics and Department of Computer Science, Southern Illinois University, Carbondale, Illinois 62901 — A general dynamical map can be written in an operator-sum representation (OSR) by using a spectral decomposition, which needs not be completely positive. The OSR is not unique; there is freedom to choose a different set of operators in the OSR, yet still obtain the same map. We will show that, whereas the freedom for completely positive maps is unitary, the freedom for not completely positive maps is pseudo-unitary.

1:15PM J29.00011 Long-range spin-coupled interactions: a *Gedankenexperiment* on the nature of spin , IAN DURHAM, Saint Anselm College — What is intrinsic spin? It is at the heart of the quantum information revolution and yet it defies many of the efforts to better understand it, even to the point of pushing particle physics beyond the Standard Model. Long assumed to require the relativistic theory of Dirac, in 1967 Lévy-Lablond demonstrated that this was not the case: it is not necessarily a relativistic effect. In this article, we apply the Lévy-Lablond model to a simple *Gedankenexperiment* that suggests the existence of a quasi-fundamental long-range spin-coupled interaction. Calculations of the eigenfunctions of a test particle and the coupling constant of the force gives insight into the behavior of the potential that gives rise to this interaction. For large separation distances the potential looks like a simple potential well while for very small separation distances it exhibits a more complex nature. This, in turn, sheds additional light on the nature of intrinsic spin and a suggests a path for future research.

1:27PM J29.00012 Quantum simulation of time-dependent Hamiltonians and the convenient illusion of Hilbert space[1] , ROLANDO SOMMA, Los Alamos National Laboratory, DAVID POULIN, University of Sherbrooke, ANGIE QARRY, FRANK VERSTRAETE, University of Vienna — We consider the manifold of all quantum many-body states that can be generated by arbitrary time-dependent local Hamiltonians in a time that scales polynomially in the system size, and show that it occupies an exponentially small volume in Hilbert space. This implies that the overwhelming majority of states in Hilbert space are not physical as they can only be produced after an exponentially long time. We establish this fact by making use of a time-dependent generalization of the Suzuki-Trotter expansion, followed by a counting argument. This also demonstrates that a computational model based on arbitrarily rapidly changing Hamiltonians is no more powerful than the standard quantum circuit model.

[1]We acknowledge support from NSF, NSERC, and FQRNT

1:39PM J29.00013 Mathematical Constraint on Realistic Theories , JAMES FRANSON, University of Maryland at Baltimore County — We consider realistic theories in which some physical property f(r,t) is assumed to exist regardless of whether or not we measure it. It is shown that the value of f(r,t) at position r and time t is completely determined by its value at all other locations r′ and earlier times t′ < t provided that f(r,t) has continuous second partial derivatives [1]. Mathematical functions of this kind are sufficiently general to describe many situations of physical interest. These results are based on a mathematical identity that is similar in some respects to Cauchy's integral theorem and it can be viewed as a generalization of Green's third identity. The physical implications of weak determinism of this kind will be discussed and it will be contrasted with the properties of quantum systems.

[1] J.D. Franson, arXiv: 1007.1941.

1:51PM J29.00014 Construction of optimal witness for unknown two-qubit entanglement , S.-S.B. LEE, Department of Physics, Korea Advanced Institute of Science and Technology, H.S. PARK, H. KIM, S.-K. CHOI, Korea Research Institute of Standards and Science, H.-S. SIM, Department of Physics, Korea Advanced Institute of Science and Technology — Whether entanglement in a state can be detected, distilled, and quantified without full state reconstruction is a fundamental open problem. We demonstrate a new scheme encompassing these three tasks for arbitrary two-qubit entanglement, by constructing the optimal entanglement witness for polarization-entangled mixed-state photon pairs without full state reconstruction. With better efficiency than quantum state tomography, the entanglement is maximally distilled by newly developed tunable polarization filters, and quantified by the expectation value of the witness, which equals the concurrence. This scheme is extendible to multiqubit Greenberger-Horne-Zeilinger entanglement. This work is to appear in Physical Review Letters.

2:03PM J29.00015 ABSTRACT WITHDRAWN –

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J30 DCMP: Nanowires & Nanotubes: Electronic Properties C147/154

11:15AM J30.00001 Interplay between structural and electronic properties of bundled $Mo_6S_{9-x}I_x$ nanowires: an *ab initio* study , SEOUNG-HUN KANG, YOUNG-KYUN KWON, Kyung Hee University, DAVID TOMANEK, Michigan State University — We use first principles density functional theory to investigate the structural, electronic and magnetic properties of isolated and bundled $Mo_6S_{9-x}I_x$ nanowires with $x = 3, 4.5$, and 6. The skeleton of these nanowires consists of linear arrays of Mo_6 octahedra decorated with S and I atoms that are connected by flexible S_3 linkages. Due to the bi-stability of each sulfur linkage, free-standing and bundled nanowires are capable of stretching or compressing axially at almost no energy cost, giving rise to many structural minima. We explore the structural stability, elastic behavior and electronic structure at all these minima for different compositions. We find that axial strain and inter-wire interaction in bundles modify significantly the electronic structure. Most intriguing changes occur in nanowires with $x = 4.5$ and 6, which change from metal to semiconductor or undergo a magnetic transition upon axially stretching or compressing the nanowires or upon changing the inter-wire separation.

11:27AM J30.00002 A Hybrid Density Functional Study of Capped Silicon Carbide Nanotubes[1] , KAPIL ADHIKARI, ASOK RAY, Department of Physics, University of Texas at Arlington — A systematic study of fullerene hemisphere capped finite SiC nanotubes of type 1 using cluster approximation is presented. Nanotubes (3,3) and (5,0) are capped by C_{20}-fullerene hemisphere(C_{10}) and (5,5) and (9,0) are capped by C_{60}-fullerene hemisphere (C_{30}). Geometries of the tubes have been spin optimized using the functional B3LYP, 3-21G* basis set and the GAUSSIAN 03 software. The study indicates that fullerene capping of a SiC nanotube changes the electronic and geometric structure properties of SiC nanotubes. For example, the binding energy per atom for infinite nanotube (5,5) is 4.993eV whereas the same nanotube with C- and Si-caps has the binding energy per atom of 5.989eV and 4.812eV, respectively. C-capped nanotubes are energetically more preferable compared to Si-capped. The HOMO-LUMO gaps of the capped nanotubes are significantly lower compared to those of infinite nanotubes.

[1]This work is supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525).

11:39AM J30.00003 Low-energy spectral weights of the 1D Hubbard chain , STEFAN SOEFFING, Dept. of Physics and Research Center OPTIMAS, Univ. of Kaiserslautern, Germany, IMKE SCHNEIDER, Univ. of Dresden, Germany, ALEXANDER STRUCK, SEBASTIAN EGGERT, Dept. of Physics and Research Center OPTIMAS, Univ. of Kaiserslautern, Germany — We investigate the low-energy spectral weights of the 1D Hubbard chain by means of Density Matrix Renormalization Group (DMRG) calculations in comparison with Bosonization results. We identify the bosonic excitations of the underlying Luttinger liquid and analyze their evolution upon increasing the interaction strength in terms of their density of states (DOS). Comparing analytical and numerical results we point out the competition of spin/charge degrees of freedom vs. non-interacting spin up and down particles, which here become important due to the lattice nature of the model and higher order operators. Furthermore, we discuss the spatially resolved (local) DOS that can be calculated analytically by a recursive formula vs. numerically using DMRG.

11:51AM J30.00004 Implications of time-reversal symmetry for band structure of single-wall carbon nanotubes , SERGUEI GOUPALOV[1], Jackson State University — When electron states in carbon nanotubes are characterized by two-dimensional wave vectors with the components K_1 and K_2 along the nanotube circumference and cylindrical axis, respectively, then two such vectors symmetric about a $\mathbf{M}$-point in the reciprocal space of graphene are shown to be related by the time-reversal operation. To each nanotube there correspond five relevant $\mathbf{M}$-points with the following coördinates: $K_1^{(1)} = \mathcal{N}/2R$, $K_2^{(1)} = 0$; $K_1^{(2)} = \mathcal{M}/2R$, $K_2^{(2)} = -\pi/T$; $K_1^{(3)} = (2\mathcal{N}-\mathcal{M})/2R$, $K_2^{(3)} = \pi/T$; $K_1^{(4)} = (\mathcal{M}+\mathcal{N})/2R$, $K_2^{(4)} = -\pi/T$, and $K_1^{(5)} = (\mathcal{N}-\mathcal{M})/2R$, $K_2^{(5)} = \pi/T$, where $\mathcal{N}$ and $\mathcal{M}$ are the integers relating the chiral, $\mathbf{C}_h$, symmetry, $\mathbf{R}$, and translational, $\mathbf{T}$, vectors of the nanotube by $\mathcal{N}\,\mathbf{R} = \mathbf{C}_h + \mathcal{M}\,\mathbf{T}$, $T = |\mathbf{T}|$, and R is the nanotube radius. We show that the states at the edges of the one-dimensional Brillouin zone which are symmetric about the $\mathbf{M}$-points with $K_2 = \pm\pi/T$ are degenerate due to the time-reversal symmetry. Explicit expressions are obtained for the coördinates of the $\mathbf{K}$-points in the reciprocal space of graphene relevant to a given nanotube.

[1]also with Ioffe Institute, Russian Academy of Sciences

12:03PM J30.00005 Ab initio simulations of the eletronic and transport properties of nanotube bundles used as gas sensors , ALEXANDRE ROCHA, RODRIGO AMORIM, Universidade Federal do ABC, Brazil, ADALBERTO FAZZIO, ANTÔNIO J.R. DA SILVA, Instituto de Física, Universidade de São Paulo, Brazil — Carbon nanotubes (CNT) have exceptional mechanical and - particularly - electronic properties that make this material of great potential interest for applications in different areas of materials science. One of the possibilities which raises the highest hopes is the area of nanotube-based gas sensors. From the fabrication point of view, one is probably going to use bundles of CNTs instead of a single tube. In this work we initially use density functional theory (DFT) calculations to determine the electronic structure properties of different molecules interstitially positioned between the nanotubes in a bundle. From the most stable structures we couple the DFT calculations to a recursive Green's function method to simulate. The electronic transport properties of a disordered nanotube bundle containing a large number of molecules randomly distributed along the different tubes forming the ropes. This way one is able to simulate a realistic sensor based on three-dimensional nanotube bundles taking into consideration the effects of disorder.

12:15PM J30.00006 Theoretical studies of the electronic and transportation properties of Gd disilicide nanowires on Si(001)[1] , WENJIE OUYANG, YANNING ZHANG, University of California, Irvine, SHENGYONG QIN, ANPING LI, Oak Ridge National Lab, RUQIAN WU, University of California, Irvine — The scanning tunneling microscopy data demonstrate the successful growth of isolated $GdSi_2$ nanowires and wire bundles on Si (100) surface and the nano transport measurement shows the isolated nanowires exhibit a metal-insulator transition (MIT) upon cooling while the wire bundles maintain a metallic state. We investigate the structural and electronic properties of isolated $GdSi_2$ nanowires and wire bundles surface through extensive density functional calculations. A 8aSi-wide supercell was used to mimic the environment of a single nanowire, and a 5aSi-wide supercell was used for wire bundles. Interestingly, we found that the bundle structures frustrate the Perils-type structural transition that occurs easily in single nanowires. This can be regarded as the reason for the observed MIT. We also explored the effect of Si adatoms on top of wires and wire bundles. The electrical transport behaviors of $GdSi_2$ nanowires are further explained using the calculated local electronic density of states and band structures. The special magnetic ordering and its effect on other properties of nanowires will also be discussed.

[1]Work was supported by DOE, Basic Energy Science, and NERSC.

12:27PM J30.00007 Structural and Electronic properties of a bismuth nanowire encapsulated inside a boron nitride nanotube[1] , CHI-HSUAN LEE, CHIH-KAI YANG, Graduate Institute of Applied Physics, National Chengchi University, Taipei, Taiwan, ROC — The structural and electronic properties of a bismuth nanowire (BiNW) encapulated inside the boron nitride nanotube (BNNT) are investigated by first principles calculation. The results show that they depend both on the configuration of BiNW and the diameter of the BNNT. The interaction between the two constituents induces hybridization of energy bands from each subsystem, causing unexpected variation of dispersion and splitting of energy bands near the Fermi level. The role of spin-orbit interaction is especially decisive in the later outcome. It enhances the stability of the hybrid structure and produces more band-edge states. These results should be observable with the tool of scanning tunneling spectroscopy.

[1]Supported by the National Science Council of the Republic of China.

12:39PM J30.00008 Jastrow-Correlated Wavefunctions for Flat-Band Lattices , HAO WANG, V.W. SCAROLA, Department of Physics and Astronomy, Virginia Tech — The electronic band structure of many compounds, e.g., carbon-based nanostructures, can exhibit essentially no dispersion. Models of electrons in such flat-band lattices define non-perturbative strongly correlated problems by default. We construct a set of Jastrow-correlated ansatz wavefunctions to capture the low energy physics of interacting particles in flat bands. We test the ansatz in an example honeycomb ribbon. The model Hamiltonian is projected on a flat band of the ribbon, thus containing only the Coulomb interaction term. The properties of the ground states are studied using numerical diagonalization. We find that the ansatz wavefunction accurately captures the ground state in a transition from a crystal to a uniform quantum liquid.

12:51PM J30.00009 Electronic structures of potassium-doped C_{60} encapsulated in BN nanotubes , TAKASHI KORETSUNE, SUSUMU SAITO, Department of Physics, Tokyo Institute of Technology, JESSE NOFFSINGER, MARVIN L. COHEN, Department of Physics, University of California, Berkeley — Boron-nitride nanotubes have large band gap independent of chirality and are promising candidates for nanostructure control. Here, we investigate the electronic structure of potassium-doped C_{60} encapsulated in boron-nitride nanotubes using first-principles methods based on the density functional theory. We demonstrate that the material is one-dimensional metal where conducting electrons are only in the C_{60} chain. Interestingly, the material can have a large Fermi-level density of states, which indicates the possibility of various phase transitions including superconductivity as in the case of fcc K_3C_{60}. We therefore discuss the electron-phonon couplings as well as the pressure dependence of the electronic structures of this material.

1:03PM J30.00010 Effect of atomic defects and interwire coupling on the electronic properties of one-dimensional Gd silicide nanowires , SHENGYONG QIN, TAE-HWAN KIM, ARTHUR P. BADDORF, AN-PING LI, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, HANNO H. WEITERING, Department of Physics and Astronomy, The University of Tennessee, Knoxville, CHIH-KANG SHIH, Department of Physics, The University of Texas at Austin, WENJIE OUYANG, YANNING ZHANG, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine — Metallic nanowires have attracted great interest for understanding the electronic interactions and conductivity in one dimension. Electron transport is often dictated by quantum instabilities and strong localization at low temperature. Well-ordered and uniformly oriented GdSi2 nanowires are self-assembled on Si(100) in the form of either isolated nanowires or wire bundles with atomic interwire spacing. The effects of interwire coupling and atomic defects in these quasi-one-dimensional systems are studied by correlating the 4-probe STM electrical transport with STM local density of states of individual nanowires. While the isolated nanowires exhibit a metal-insulator transition associated with atomic defects, the wire bundles remain metallic at low temperature which we believe the interwire coupling suppress the lattice disorder and stabilize a robust metallic conductance. This research at ORNL's CNMS was sponsored by the Scientific User Facilities Division, Office of BES, U.S. DOE.

1:15PM J30.00011 Negative curvature energy in magnesium-boride nanotubes , HUI TANG, SOHRAB ISMAIL-BEIGI, Department of Applied Physics, Yale University — Mg-boride nano-materials have attracted much attention due to constant quest for novel superconducting materials on nanoscale. A recent experiment on Mg borides nanostructures has hinted at a possible superconducting temperature as high as 80K. More generally, studying the physics of pure and metal-doped boron nanosystems enhances understanding of novel properties that emerge in reduced dimensions. Here, based on first principles calculations, we describe an unusual nanoscale curvature effect in Mg-boride nanotubes and discuss its origin. We show that a number of 2D Mg-boride sheets prefer to spontaneously curve themselves into small diameter nanotubes and thus have negative curvature energies. This is rather unique when compared to other nanotubular materials: usually, curving the parent 2D sheet to create a nanotube imposes an energy cost. We explain the reason for the negative curvature energy by analyzing the charge state of the Mg atoms, its relation to the type of boron sublattice present in the nanostructure, and its consequences for the Mg-Mg interactions and hence the energetics.

1:27PM J30.00012 Quantum Size Effect and Electronic Stability of Freestanding Metal Atom Wires[1] , HAIPING LAN, PING CUI, U. of Sci. & Tech. of China, JUN-HYUNG CHO, Hanyang U., QIAN NIU, U. of Texas at Austin, JINLONG YANG, U. of Sci. & Tech. of China, ZHENYU ZHANG, Oak Ridge Nat. Lab, U. of Tennessee, U. of Sci. & Tech. of China — Using DFT calculations, we present a thorough study of the quantum size effects on the stability of freestanding metal atom wires. Our systems include Na, Ag, Au, In, Ga and Pb atom wires, i.e. s, sd, and sp electron prototypes. We found that the total energy always oscillates with the wire length, which clearly indicates the existence of preferred lengths. Increasing the length, the s-system exhibits even-odd oscillations following a 1/x decay law in the stability, which can be attributed to electron band filling and quantum confinement along the wire. The sd-system exhibits a similar oscillation pattern, even in the presence of sd hybridization. In sp-system, the energy oscillations are beyond the simple even-odd nature, likely due to unpaired p orbitals and the corresponding nontrival band filling. Our findings clearly demonstrate that electronic contribution is quite critical to the stability of freestanding wires, and this stability may be important even when wires are deposited on substrates or strained. This study sheds light on the underlying formation mechanism of metal atom wires.

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

1:39PM J30.00013 Gate controlled donor activation in silicon nanowires , ADAM GALI, Research Institute for Solid State Physics and Optics of the Hungarian Academy of Sciences, BINGHAI YAN, THOMAS FRAUENHEIM, Bremen University — Due to the proximity to an embedding medium with low dielectric constant (e.g., oxides), semiconductor nanowires have higher impurity ionization energy than their bulk counterparts, resulting lower free carrier density. Using ab initio calculations within density functional theory, we propose a way to reduce the ionization energy in nanowires by fabricating a special cross section with appropriate engineering of doping and an applied gate voltage. We demonstrate on a phosphorus-doped silicon nanowire that the ionization energy can be effectively tuned and the impurity backscattering can also be reduced. For instance, the free carrier density may increase by 40% in a silicon nanowire with 15 nm diameter and special cross section without special engineering of doping. Our proposal has profound implications to fabricate nanowire devices with high carrier density. Our proposed Si NW device realizes a fine manipulation of the interaction between electron and nuclear spins by using an external electric field which is a fundamental step to a silicon-based nuclear spin quantum computer. Moreover, with a negative voltage the ionization energy of P-donors can be increased even in larger silicon nanowires which opens up the possibility to manipulate the donor electron spin at room temperature [1]. [1] B. Yan, Th. Frauenheim and A. Gali, *Nano Lett.*, 2010, 10, 3791

1:51PM J30.00014 Non-Collinear Ferromagnetic Luttinger Liquids , NICHOLAS SEDLMAYR, SEBASTIAN EGGERT, JESKO SIRKER, TU Kaiserslautern — In the now classic Tomonaga-Luttinger model the presence of the electron-electron interaction in one dimension is shown to profoundly change the properties of the system. We consider here the magnetic and electronic properties of a *ferromagnetic* Luttinger liquid when it has a region of non-collinearity present, i.e. a domain wall. Spin-charge separation does not survive in this system, and the absence of both spin-charge separation and coherent spin-charge excitations has consequences for the spin-transfer-torque effects which cause domain wall motion. Furthermore the presence of the domain wall introduces a spin dependent scatterer into the problem, which will alter both the transport, and the static electronic, properties of the system. Finally we show how the magnetization dynamics of the domain wall will be modified for a Luttinger liquid.

2:03PM J30.00015 How to Extract Luttinger Liquid Velocity from Carbon Nanotubes , DARRYL H. NGAI, Cornell University, CHANG-YU HOU, Universiteit Leiden, EUN-AH KIM, Cornell University — We propose direct detection of Luttinger Liquid velocity of the charge collective mode in carbon nanotubes using optical conductivity and Coulomb blockade effect. We note that detection of such fractionalized excitation needs to exploit the energy or frequency scale tied to the finite length of the nanotube. This is why previous experimental attempts have been unsuccessful.[1] We will discuss features in the optical conductivity sensitive to the velocity of the collective mode which would be observable in the high temperature limit. In the low temperature limit, spacing between the Coulomb blockade peaks in the conductance as a function of gate voltage will be a sensitive probe.

[1]Z. Zhong *et al.*, Nature Nanotechnology **3**, 201 (2008)

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J31 DMP GSCCM DCOMP: Focus Session: Materials at High Pressure II: Elements

C145

11:15AM J31.00001 Multi-Scale Shock Compression Simulations of Metals and Metallic Phase Transitions[1] , NIR GOLDMAN, LARRY FRIED, Lawrence Livermore National Laboratory — We present a straightforward method for efficient molecular dynamics (MD) simulation of shock compression of materials that experience thermal electronic excitations at high pressure and temperature. Previous studies have shown that exclusion of the electronic temperature at extreme conditions can result in incorrect computation of dynamic and equation of state properties. The Multi-Scale Shock Technique (MSST) is a simulation methodology based on the Navier–Stokes equations for compressible flow that enables MD simulation of a shock wave with relatively small computational cost. We extend MSST to allow for changes in the electronic entropy during shock compression while conserving Hugoniot conditions. This allows for simulation of significantly higher shock velocities than previously possibly with MSST. We have used our simulation methodology in density functional tight binding simulations of shock compressed silicon. We observe that at high shock velocities inclusion of a non-zero electron temperature results in lower computed shock Hugoniot temperatures and pressures. Our methodology is well suited for shock compression simulations of any material that experiences changes in its electronic entropy under extreme thermodynamic conditions.

[1]Prepared by LLNL under Contract DE-AC52-07NA27344.

11:27AM J31.00002 Large-Scale Molecular Dynamics Simulations of Shock-Induced Plasticity in Tantalum Single Crystals[1] , R. RAVELO[2], University of Texas-El Paso, QI AN, California Institute of Technology, T.C. GERMANN, B.L. HOLIAN, Los Alamos National Laboratory — We report on large-scale non-equilibrium molecular dynamics (NEMD) simulations of shock wave compression in Ta single crystals. The atomic interactions are modeled via a recently developed and optimized embedded-atom method (EAM) potential for Ta, which reproduces the equation of state up to 200 GPa. We examined the elastic-plastic transition and shock wave structure for wave propagation along the low index directions: (100), (110) and (111). Shock waves along (100) and (111) exhibit an elastic precursor followed by a plastic wave for particle velocities below 1.1 km/s for (100) and 1.4 km/s for (111). The nature of the plastic deformation along (110) is dominated by twinning for pressures above 40 GPa.

[1]Part of this work was supported by the U.S. Department of Energy under contract DE-AC5206NA25396.

[2]Computational Physics Division, Los Alamos National Laboratory

11:39AM J31.00003 Transport of particulate matter from a shocked interface[1]

W.T. BUTTLER, J.E. HAMMERBERG, D. ORO, C. MORRIS, F. MARIAM, C. ROUSCULP, Los Alamos National Laboratory — We have performed a series of shock experiments to measure the evolution and transport of micron and sub-micron Tungsten particles from a 40 micron thick layer deposited on an Aluminum substrate. Densities and velocity distributions were measured using proton radiography at the Los Alamos Neutron Science Center for vacuum conditions and with contained Argon and Xenon gas atmospheres at initial pressures of 9.5 bar and room temperature. A common shock drive resulted in free surface velocities of 1.25 km/s. An analysis of the time dependence of Lithium Niobate piezo-electric pin pressure profiles is given in terms of solutions to the particulate drag equations and the evolution equation for the particulate distribution function. The spatial and temporal fore-shortening in the shocked gas can be accounted for using reasonable values for the compressed gas shear viscosities and the vacuum distributions. The detailed form of the pin pressure data for Xenon indicates particulate breakup in the hot compressed gas.

[1]This work supported by the U.S. Department of Energy under contract DE-AC52-06NA25396.

11:51AM J31.00004 Thermal Emission Determination of Argon under Extreme Pressure and Temperature

D. ALLEN DALTON, MICHAEL WONG, ALEXANDER F. GONCHAROV, JULIUS OJWANG, VIKTOR V. STRUZHKIN, Geophysical Laboratory, Carnegie Institution of Washington, ZUZANA KONOPKOVA, PETER LAZOR, Department of Earth Sciences, Uppsala University — Argon is a common pressure-transmitting medium in diamond anvil cell (DAC) experiments, and is often used as thermal insulation in the laser heated DAC. A more thorough understanding of the thermal properties of argon under extreme conditions is essential for measuring thermal properties of materials under similar conditions. A transient heating technique was applied to a symmetric DAC up to 50 GPa and 2500 K. A 1 μm thick iridium foil positioned within a recessed gasket hole filled with argon served as a laser absorber to pump thermal energy into the sample. Pump pulses of 6 μs temporal width were provided from an electronically modulated Yb-based fiber laser. We determined the temperature of the coupler with 500 ns time resolution by applying a Planckian fit to the thermal emission spectrum. Finite element calculations were also used to simulate thermal diffusion in the DAC cavity. The experimental results show slightly larger thermal conductivity with theory, but the results converge in the limit of high temperature. This work is supported by NSF EAR 1015239, NSF-REU, Carnegie Institution of Washington, and DOE-NNSA (CDAC).

12:03PM J31.00005 Thermal diffusivity of metals at high pressure[1]

BRUCE BAER, WILLIAM EVANS, Lawrence Livermore National Laboratory — Very few measurements of thermal diffusivity have been taken at high pressure. This is especially true of metals above 2 GPa. In earlier experiments, the Angstrom method has been employed for these types of measurements. However, this method is limited for high pressure because it requires a relatively large sample. We will discuss the use of sinusoidally modulated laser heating to measure thermal diffusivity in the diamond-anvil-cell.

[1]This work was performed under the auspices of the US DOE by LLNL under Contract DE-AC52-07NA27344.

12:15PM J31.00006 Pressure-Induced Structure Transitions in Europium Metal to 92 GPa[1]

W. BI, J. SCHILLING, Department of Physics, Washington University in Saint Louis, Y. MENG, HPCAT, Carnegie Institution of Washington, Argonne National Laboratory, R. KUMAR, A. CORNELIUS, Y. ZHANG, C. CHEN, HiPSEC and Department of Physics, University of Nevada, Las Vegas, R. HENNIG, Department of Materials Science and Engineering, Cornell University — Motivated by the recent discovery of pressure-induced superconductivity in Eu for pressures above 80 GPa [1], we have carried out high pressure angle-dispersive synchrotron x-ray diffraction measurements on Eu metal in a diamond anvil cell to 92 GPa. Our experiments confirm the bcc-to-hcp transition at 12 GPa reported in previous studies and identify two further phase transitions. The predictions of two independent density functional theory calculations are compared to the experimental results.

[1] M. Debessai, T. Matsuoka, J. J. Hamlin, J. S. Schilling, and K. Shimizu, Phys. Rev. Lett. **102**, 197002 (2009).

[1]This research is supported by NSF grant DMR-0703896 and by the Carnegie/DOE Alliance Center (CDAC) through NNSA/DOE grant number DE-FC52-08NA28554.

12:27PM J31.00007 Electronic structure and dynamics of elements at high pressures[1]

HO-KWANG MAO, Carnegie Institution of Washington — Electronic structure and dynamics information of materials under high pressure has been very scarce due to the experimental difficulties. The standard electronic probes using electron energy loss spectroscopy (EELS) is limited to vacuum pressures. The optical probes that can reach high-pressure samples through the diamond windows, on the other hand, are limited by the energy accessibility ($<$ 5 eV) and near-zero momentum transfer, $q = (4\pi/\lambda_0)\sin\theta$. These problems can be overcome by the newly advanced, two-photon, inelastic, xray, scattering (IXS) spectroscopy which uses high energy xrays ($\sim 10^4$ eV) to provide the atomic-level momentum transfer and to enter (with energy E) and exit (with energy E_0) the pressure vessel. The electronic spectra are revealed by analyzing the xray energy loss between the two photons, $\hbar\omega = E - E_0$. Using IXS facilities at third-generation synchrotron source, we studied electronic structure and dynamics of two elements at high pressures in a diamond-anvil cell: i.e., He, the widest-gap insulator, and Na, the archetypal free-electron metal. At 11.9-17.9 GPa in a single crystal ^{4}He, we observed rich electron excitation spectra, including a cut-off edge above 23 eV, a sharp exciton peak showing linear volume dependence, and a series of excitations and continuum at 26 to 45 eV. We determined electronic dispersion along the 100 direction over two Brillouin zones, and provided a quantitative picture of the helium exciton beyond the simplified Wannier-Frenkel description. At 1.6-4.39 GPa in a polycrystalline Na sample, we observed the sharp plasmon peak at low q and its dispersion beyond the critical q_c. The plasmon shifts to higher energy under compression and drastic reduction of r_s. *Ab-initio* theoretical calculations are conducted for interpretation of the experimental results.

[1]The speaker would like to acknowledge collaborating researchers: R. Ahuja, Y. Cai, P. Chow, Y. Ding, P. Eng, R.J. Hemley, C.C. Kao, S. Lebegue, W.L. Mao, E.L. Shirley, J. Shu, & Y. Xiao.

1:03PM J31.00008 Diffusion Monte Carlo calculations of Xenon melting under pressure[1]

L. SHULENBURGER, T.R. MATTSSON, Sandia National Laboratories — The slope of the melting temperature as a function of pressure yields, via the Clausius-Clapeyron equation, important information regarding the changes in density, energy, and entropy. It is therefore crucial to resolve the long-standing differences in melt lines under pressure between Diamond Anvil Cell data (low/flat melt line) and other methods, including density functional theory (DFT) simulations[1] (high/steep melt line). The disagreement for Ta was recently resolved[2] and although a similar situation exists in the literature on Xe,[3] the resolution may be quite different. For example, DFT with its lack of van der Waals forces is a prima facie less credible simulation method for Xe, although excellent agreement has been obtained between calculations of the Hugoniot of Xe and experiments.[4] We investigate whether this theoretical shortcoming is significant for the melting transition by applying diffusion Monte Carlo. The energy differences obtained in this way are compared to the DFT results in order to address any systematic errors that may be present near the melting transition. [1] Taioli et al. PRB **75**, 214103 (2007); [2] Dewaele et al. PRL **104**, 255701 (2010); [3] Belonoshko el al. PRB **74**, 054114 (2006); [4] Root et al. PRL **105**, 085501 (2010)

[1]Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corp. for the US Dep. of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

1:15PM J31.00009 Lattice dynamics at ultra-high pressures using high-resolution inelastic x-ray scattering , DANIEL FARBER, Lawrence Livermore National Laboratory — While our understanding of many physical properties is enhanced by the large body of neutron, the restrictions on sample size imposed by the technique relegated the achievable information to low or at most, moderate pressures (∼10 GPa) and to materials readily available in reasonable large quantities. The advent of third generation synchrotron sources and the construction of beamlines dedicated for inelastic x-ray scattering experiments (IXS), these limitations have to a great degree been overcome. Over the past few years our group has focused a large experimental and theoretical effort on quantifying the vibrational energies in metals at high-pressures and high-temperatures. Most recently, we have determined the phonon dispersions across the isostructural gamma- to alpha-cerium transition. Our new data place important thermodynamical and theoretical constraints on the underlying physics of this important transition.

1:27PM J31.00010 High-pressure phases of calcium[1] , AMANUEL TEWELDEBERHAN, JONATHAN DOBOIS, Lawrence Livermore National Laboratory, STANIMIR BONEV, Lawrence Livermore National Laboratory and Dalhousie University — The high-pressure phases of calcium have been investigated using a combination of density functional theory and diffusion quantum Monte Carlo calculations. Finite-temperature Gibbs free energies of several competing structures are computed at pressures near 50 GPa. The discrepancy between theory and experiment both at low and room temperature is resolved with input from diffusion quantum Monte Carlo. Furthermore, diffusion quantum Monte Carlo calculations are performed on 0 K crystalline structures up to 150 GPa. The resulting structures differ from those obtained with density functional theory.

[1]Work supported by LLNL, ACEnet, NSERC, and CFI. Prepared by LLNL under Contract DE-AC52-07NA27344.

1:39PM J31.00011 Lifshitz transition in *cI*16 Li at high pressures: Unfolding first-principles Fermi surfaces , CHIA-HUI LIN, TOM BERLIJN, WEI KU, Brookhaven National Laboratory/ Stony Brook University — The Fermi surface topology of *cI*16 Li is investigated using the recently developed first-principles band structure unfolding method [1]. The resulting unfolded Fermi surfaces display a clear Lifshitz transition at 47 GPa, explaining the anomalous change of superconducting transition temperature [2]. The unfolded Fermi surfaces also reveals a more complete picture of the driving force of the *cI*16 phase starting at 39 GPa [3]. In addition to the previously proposed "nesting" effect [3] along $[1\frac{1}{2}\frac{1}{2}]$, both [100] and $[\frac{1}{2}\frac{1}{2}0]$ wavevectors are found to contribute significantly to the structural instability as well, due to their large phase space, a more effective effect in 3D. We expect a wide range of applications of this Fermi surface unfolding method to the study of high pressure electronic structure.

[1] Wei Ku et al, Phys. Rev. Lett. **104**, 216401 (2010)
[2] S. Deemyad and J. S. Schilling, Phys. Rev. Lett. **91**, 167001 (2003)
[3] M. Hanfland et al, Nature **408**, 174 (1998)

1:51PM J31.00012 On the role of quantum ion dynamics for the anomalous melting of lithium[1] , SABRI ELATRESH, Department of Physics, Dalhousie University, Halifax, NS, B3H 3J5, Canada, STANIMIR BONEV, Lawrence Livermore National Laboratory, Livermore, California 94550 — Lithium has attracted a lot of interest in relation to a number of counterintuitive electronic and structural changes that it exhibits under pressure. One of the most remarkable properties of dense lithium is its anomalous melting. This behavior was first predicted theoretically based on first-principles molecular dynamics (FPMD) simulations, which treated the ions classically [1]. The lowest melting temperature was determined to be about 275 K at 65 GPa. Recent experiments measured a melting temperature about 100 K lower at the same pressure. In this talk, we will present FPMD calculations of solid and liquid lithium free energies up to 100 GPa that take into account ion quantum dynamics. We examine the significance of the quantum effects for the finite-temperature phase boundaries of lithium and, in particular, its melting curve.

[1] I. Tamblyn, J-Y. Raty, and S. A. Bonev, Phys. Rev. Lett. 101, 075703 (2008).
[2] E. Gregoryanz et al, Nature, in press.

[1]Work supported by NSERC, Acenet, and LLNL under Contract DE-AC52-07NA27344.

2:03PM J31.00013 Graphite under high pressure , YUEJIAN WANG, Yale University — As one of the longest-known forms of carbon, graphite has been extensively studied for several decades. However, its phase diagram under high pressures is still poorly understood. Here we use both in-situ high-pressure Raman spectroscopy and synchrotron x-ray diffraction, collected on both compression and decompression, to elucidate the high-pressure behavior of highly-ordered pyrolitic graphite (HOPG) at room temperature. The Raman spectra show that G band (1580 cm^{-1} at ambient pressure) of HOPG shifts to higher frequency with increased pressure, which has been attributed to pressure-induced in-plane lattice contraction. Above 19 GPa the broadening of this Raman peak indicates a reordering of the atomic structure, and is consistent with synchrotron x-ray diffraction measurements that also show a slight change in symmetry.

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J32 DMP: Focus Session: Electron, Ion, and Exciton Transport in Nanostructures: Nanowires C144

11:15AM J32.00001 Finite Size Effects in Electrical Transport in Nanowires and Nanowire-like Devices. , ALEC TALIN, NIST — Semiconductor nanowires posses many unique qualities including high crystallinity, simple growth techniques compatible with variety of low cost substrates, increased ability to accommodate strain, and nanoscale dimensions not easily accessible by 'top-down' lithographic means. These and other interesting characteristics have made nanowires an attractive topic for fundamental research, as well as for potential applications in nanoelectronics, photonics, sensors, and more recently energy conversion and storage. Most of these applications rely on charge transport, which can be profoundly affected by the high aspect ratio, high surface to volume ratio and nanoscale diameter typical of semiconductor nanowires. Properly identifying the factors that influence electrical transport characteristics is important for device design but also because extraction of material parameters such as the mobility relies on analysis with specific models. In my talk I will discuss several specific examples where nanoscale dimensions and geometry profoundly affect transport and device characteristics, including GaN and GaN/III-N core/shell nanowires; Si radial pn-junction photovoltaics; and all-nanowire Li-ion batteries..

11:51AM J32.00002 Photocurrent Spectroscopy of single ZB, WZ InP Nanowire devices , K. PEMASIRI, S. PERERA, A. WADE, H.E. JACKSON, L.M. SMITH, University of Cincinnati, Cincinnati, OH, J.M. YARRISON-RICE, Miami University, Oxford, OH, S. PAIMAN, Q. GAO, H.H. TAN, C. JAGADISH, Australian National University, Canberra, Australia — Photocurrent spectroscopy was performed on single InP nanowire devices having either zinc-blende (ZB) or wurtzite (WZ) crystal structures at 300 K and 10 K. Photolithography was used to fabricate Ohmic Ti/Al metal contact pads separated by 5 μm. Using a monochromatic white light set up or a tunable (1.30 to 1.55 eV) CW laser, the photocurrent is measured as a function of bias voltage and excitation energy. At room temperature, the lowest energy band of In WZ (1.408 eV) is found to be 70 meV above the ZB band gap (1.338 eV), consistent with previous photoluminescence measurements. At low temperatures (10 K), the ZB device shows strong evidence for a broadened excitonic resonance peak at 1.432 eV and the WZ device shows three excitonic peaks at 1.504 eV, 1.56 eV, and 1.65 eV corresponding to the A,B and C valence band energies, respectively, which coincide with recent photoluminescence excitation measurements. Support for this work was provided by the NSF (#0701703, #0806700 and #0806572) and the Australian Research Council.

12:03PM J32.00003 Photoresponse of solution-synthesized PbSe nanowire devices , TODD BRINTLINGER, EDWARD E. FOOS, JOSEPH G. TISCHLER, JANICE E. BOERCKER, THOMAS J. ZEGA, RHONDA M. STROUD, STEVE C. ERWIN, U.S. Naval Research Laboratory — PbSe nanowires are of interest for photovoltaic applications due to their variable band gap in the near infrared and potential for efficient multiexciton generation. Contributing to this effort, we present our ongoing studies of the photoresponse of PbSe nanowire devices. These materials are synthesized in solution by reaction of Pb and Se precursors in the presence of stabilizing organic ligands, and possess 10-20 nm diameters with lengths >1 μm. The nanowires are then dispersed on transparent silicon nitride membranes, allowing for both transmission electron microscopy and optical spectroscopy of individual devices. Devices show up to two-fold increases in current under illumination, with current density in the $\sim$1x10^9 A/m^2 range. Electrical transport and characterization of nanowires will be presented.

12:15PM J32.00004 Energy and Spatially Resolved Measurements of Plasmonically Enhanced Photocurrent in a Single Si Nanowire with Au Nanoparticles , JEROME HYUN, LINCOLN LAUHON, Department of Materials Science and Engineering, Northwestern University — Hybrid assemblies of nanowires and metallic particles have attracted great interest because of their potential as light harvesting systems. Optoelectronic measurements of the most basic light absorbing unit in such systems, consisting of a single nanowire and plasmonic particles, would provide further guidance for performance optimization schemes. Here, we present spatially and energy resolved photocurrent measurements across the visible spectrum on a Si nanowire device with Au nanoparticles using a confocal scanning microscope and a tunable wavelength laser source. A 50 nm diameter nanowire was used due to its monotonic optical response in the wavelength range of interest, and 50 nm size Au nanoparticles were selected in order to neglect the effects of Mie scattering. The photocurrent is shown to depend on the azimuthal location of the nanoparticles on the nanowire. Nanoparticles resting on the substrate adjacent to the nanowire can significantly modify the absorption with a strong polarization-dependent plasmonic response while nanoparticles resting directly in the line of sight between the nanowire and light source show minimal contribution to the photocurrent.

12:27PM J32.00005 Charge injection and transport in nanowires , FRANCOIS LEONARD, Sandia National Laboratories — Semiconductor nanowires show promise in electronic, optoelectronic, and sensing devices. To realize this promise, a fundamental understanding of charge injection and electronic transport in these novel nanomaterials is necessary. In this presentation, I will discuss recent work that couples experiment and theory to address this topic. For example, in GaN and InAs nanowires, we achieve efficient charge injection and find that space-charge-limited currents are unusually strong. In contrast, charge transport across individual Au-nanoparticle/Ge-nanowire interfaces is injection-limited, and surprisingly, the conductance increases with decreasing nanowire diameter due to a dominance of electron-hole recombination. Furthermore, we find that transport in GaAs nanowires is governed by charge traps, which can be activated to reveal the nature of the charge injection at the contacts. More generally, our results indicate that a broad range of electronic transport regimes can be observed in semiconducting nanowires depending on the particular material system and growth process.

1:03PM J32.00006 Photocurrent spectroscopy of CdS nanosheets , P. KUMAR, A. WADE, H.E. JACKSON, L.M. SMITH, University of Cincinnati, J. YARRISON RICE, Miami University, Y.-J. CHOI, J.-G. PARK, Korea Institute of Science and Technology, Seoul — We study the photocurrent from photoexcited charge carriers in CdS nanosheet (NS) structures. Metal-semiconductor-metal nanodevices are made with both Schottky and Ohmic contacts using photolithography followed by Ti/Al (20nm/200nm) metal evaporation and lift-off. Ohmic contacts are formed by Ar ion bombardment before the metal deposition to create donor sulfur vacancies which increases the electron concentration. Photocurrent spectra using a white light source filtered by a monochrometer show excitonic resonances at low temperatures corresponding to each of the A, B, and C hole bands. The photocurrent increases linearly with power for above gap excitation, and nonlinearly (quadratic) with laser power for below gap excitation, consistent with two-photon absorption with a nonlinear coefficient of $\beta = 2$ cm/GW. A wavelength dependence of the photocurrent with sub-band gap excitation to find the resonances and hence band structure is in progress. We acknowledge the financial support of the National Science Foundation through grants DMR-0806700, 0806572 and ECCS-0701703, and the KIST institutional research program 2E21060R.

1:15PM J32.00007 Electronic Devices with Dichalcogenide Nanolayers[1] , ANDRAS KIS, BRANIMIR RADISAVLJEVIC, MOHAMED BENAMEUR, JACOPO BRIVIO, EPF Lausanne — We have exfoliated single, two-dimensional layers 6.5 Angstrom thick from a number of dichalcogenide materials such as MoS2, using the micromechanical cleavage technique commonly used for the production of graphene. Optical microscopy together with AFM was used to characterize the nanolayers and establish optimal conditions for rapid identification of monolayers using optical methods. Our nanolayers are mechanically and chemically stable under ambient conditions. We have electrically contacted nanolayers using electron-beam lithography and fabricated field-effect transistors. Electrical transport measurements show that our devices have high on/off ratios and high mobilities. Our results indicate that two-dimensional dichalcogenide nanolayers could be interesting building blocks for nanoelectronic applications.

[1]Supported by a grant from ERC, no. 240076

1:27PM J32.00008 Electric Field Dependent Photocurrent Decay Length in Single Lead Sulfide Nanowire Field Effect Transistors , DONG YU, RION GRAHAM, CHRIS MILLER, U.C. Davis, EUNSOON OH, Chungnam National University, Korea — We determined the minority carrier diffusion length to be $\sim$1 μm in single PbS nanowire field effect transistors by scanning photocurrent microscopy. PbS nanowires grown by the vapor-liquid-solid method were p-type with hole mobilities up to 49 cm^2/Vs. We measured a photo-response time faster than 14 μs with near-unity charge separation efficiency at the contacts. For the first time, we also observed a field dependent photocurrent decay length, indicating a drift dominant carrier transport at high bias.

1:39PM J32.00009 Exciton Diffusion Measurements in III/V Nanowires using Spatially and Time Resolved Photoluminescence[1] , M.A. FICKENSCHER, L.M. SMITH, H.E. JACKSON, University of Cincinnati, J.M. YARRISON-RICE, Miami University, J.H. KANG, Q. GAO, H.H. TAN, C. JAGADISH, Australian National University — We present an optical investigation of transport in GaAs/AlGaAs core shell nanowires utilizing low temperature spatial and time resolved photoluminescence (PL). We use a solid immersion lens (SIL) to achieve a laser spot size and image resolution of 600 nm. With the laser spot fixed on the nanowire, the image of the wire is scanned across the entrance slit of the spectrometer taking time-decays at each point. Thus, we measure the spatial profiles of the exciton distribution in the wire as a function of time. We then extract the diffusion constant from the width squared of each spatial distribution as a function of time. The measured exciton diffusion constants are of the order of 100 cm^2s^{-1}, equivalent to a mobility of 100,000 $cm^2\ V^{-1}s^{-1}$ by using the Einstein relation. These values are comparable to the best hole mobilities seen in modulation doped two dimensional GaAs/AlGaAs heterostructures.

[1]Support for this work was provided by the NSF (0701703, 0806700 and 0806572) and the Australian Research Council.

1:51PM J32.00010 Electron transport in coupled InGaAs quantum wires[1] , VASYL KUNETS, SERGEY PROSANDEEV, SABINA KOUKOURINKOVA, VITALIY DOROGAN, YURIY MAZUR, MARCIO TEODORO, MORGAN WARE, MOURAD BENAMARA, PETER LYTVYN, GREGORY SALAMO, University of Arkansas, Physics Department, Fayetteville, AR 72701 — Remotely doped InGaAs/GaAs heterostructures were grown by molecular beam epitaxy on the (311)A plane of GaAs. Applying strain driven epitaxy on the (311)A GaAs surface, two-dimensional quantum wells (QW) and quasi-one-dimensional quantum wires (QWr) were formed by varying InGaAs coverage between 6 and 11 monolayers. Polarization dependent photoluminescence and electrical conductivity experiments revealed a remarkable anisotropy in the QWr samples, which was insignificant in the QWs, the dimensionality of which was confirmed by atomic force and cross-sectional transmission electron microscopies. The resulting complex behavior of the electric current anisotropy as function of InGaAs coverage, doping and temperature is explained through a multi-band conductivity model, which is supported by magneto-transport measurements at low and high magnetic fields along with the Hall effect theory in anisotropic media with multi-band conduction.

[1]This work was supported by the NSF under Grant No. DMR 0520550

2:03PM J32.00011 Probing charge density wave transition at the nanoscale in $NbSe_2$using NEMS resonators , SHAMASHIS SENGUPTA, HARI SOLANKI, VIBHOR SINGH, SAJAL DHARA, MANDAR DESHMUKH, Tata Institute, Mumbai, India — We study nanoelectromechanical (NEMS) resonators fabricated from suspended flakes of $NbSe_2$ (thickness $\sim$ 30–50 nm) to probe charge density wave (CDW) physics at nanoscale. Variation in elastic and electronic properties accompanying the CDW phase transition (around 30 K) are investigated simultaneously using the devices as self-sensing heterodyne mixers. Elastic modulus is observed to change by 10%, an amount significantly larger than what had been reported earlier in the case of bulk crystals. We also study the modulation of conductance by electric field effect, and examine its relation to the order parameter and the CDW energy gap at the Fermi surface.

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J33 DMP DCOMP: Focus Session: Dielectric, Ferroelectric, and Piezoelectric Oxides: Multiferroics & Magnetoelectrics II C143/149

11:15AM J33.00001 Correlation between magnetocapacitance effect and polarization flop direction in a slanted magnetic field in $Tb_{1-x}Dy_xMnO_3$, NOBUYUKI ABE, HAJIME SAGAYAMA, HIROSHI UMETSU, TAKA-HISA ARIMA, IMRAM, Tohoku University, KOUJI TANIGUCHI, Department of Advanced Materials Science, The University of Tokyo — Recent extensive studies show that the cycloidal spin system can possess electric polarization through the spin-orbit coupling. The magnetoelectric coupling in multiferroics is enhanced by the clamping of helimagnetic and ferroelectric domain walls. For example, $DyMnO_3$ shows a gigantic magnetocapacitance effect caused by the microscopic motion of multiferroic domain walls at a magnetic field induced **P**-flop transition. In contrast, the enhancement of capacitance at the **P**-flop transition is much smaller in $TbMnO_3$. Here, we show the systematic control of magnetocapacitance effect in helimagetic ferroelectric $Tb_{1-x}Dy_xMnO_3$ as a function of the composition ratio x and the intensity of the applied magnetic field. It has been also found that the rotation direction of **P** in a slanted magnetic field changes with x and H. The crossover between small and large enhancement in magnetocapacitance corresponds to the switch in the **P**-flop direction. The correlation can be explained by assuming the mobility of domain wall would be dominated by the thickness of domain walls in a helical magnet.

11:27AM J33.00002 Giant Magnetoelectric Effect in Antiferromagnetic $BaMnO_{3-\delta}$ and Its Derivatives[1] , M. GE, O.B. KORNETA, T.F. QI, S. PARKIN, L.E. DELONG, G. CAO, University of Kentucky, P. SCHLOTTMANN, Florida State University — Hexagonal perovskite 15R-$BaMnO_{2.99}$ with a ratio of cubic to hexagonal layers of 1/5 in the unit cell is an antiferromagnetic insulator that orders at a Néel temperature T_N= 220 K. Here we report structural, magnetic, dielectric and thermal properties of single crystal $BaMnO_{2.99}$ and its derivatives $BaMn_{0.97}Li_{0.03}O_3$ and $Ba_{0.97}K_{0.03}MnO_3$. The central findings of this work are: **(1)** these materials possess a usually large, high-temperature magnetoelectric effect that amplifies the dielectric constant by more than an order of magnitude near their respective Néel temperature; **(2)** Li and K doping can readily vary the ratio of cubic to hexagonal layers and cause drastic changes in dielectric and magnetic properties. These findings provide a new paradigm for developing *novel, high-temperature magnetoelectric materials* that may eventually contribute to technology.

[1]This work was supported by NSF through grants DMR-0552267, DMR-0856234 (GC) and EPS-0814194 (GC, LED), and by DoE through grants DE-FG02-97ER45653 (LED) and DE-FG02-98ER45707 (PS).

11:39AM J33.00003 Electric-field control of magnetic orderings in the tetragonal $BiFeO_3$[1] , CHUN-GANG DUAN, East China Normal University — We present a systematic first-principles study on the magnetic properties of the tetragonal $BiFeO_3$ (P4mm) with various in-plane lattice constants. The Heisenberg model is applied to study the behaviors of exchange constants (J_{1a}, J_{1c}, J_{2a}, J_{2c}) under the influence of the in-plane strain. We find that in certain region of the in-plane lattice constant, switching the direction of polarization from out of plane to in-plane by electric field could result in transition of magnetic orderings, e.g., from G-type to C-type antiferromagnetic states in tetragonal $BiFeO_3$. This may open a new avenue to controlling magnetoresistance using electric field.

[1]Supported by the NSF of China (Grant No. 50771072 and 50832003).

11:51AM J33.00004 Ferroelectric polarization in the magnetic world , JUN HEE LEE, Department of Physics and Astronomy, Rutgers University — Switchable spontaneous polarization in ferroelectrics is produced by a structural distortion of a high-symmetry reference phase which lowers the symmetry to a polar space group. Under certain conditions, this structural distortion and symmetry breaking can also induce ferromagnetism and other changes, such as a metal-insulator transition, allowing the possibility of electric and magnetic field control. In this talk, I will present first-principles illustrations of specific materials realizations of the rich variety of this behavior in magnetic perovskite oxides, identified using a database of first-principles calculations of the full phonon dispersions of a range of magnetic perovskites, including the d3 compounds SrMnO3and SrCaO3, the d5 compounds BiFeO3, and the series SrMO3 (M= V, Cr, Mn, Fe, Co). First, I will discuss an epitaxial-strain-induced multiferroic phase produced by large spin-phonon coupling in SrMnO3 [1]. Then, I will turn to colossal magnetoresistance based on a ferromagnetic- metal/antiferromagnetic-ferroelectric phase boundary with epitaxial strain in SrCoO3, which exhibits typical ferromagnetic metallic character in room-temperature but with a large spin-phonon coupling by which antiferromagnetic ordering favors a polar distortion. Lastly, I will discuss the identification of perovskite superlattice systems in which the symmetry lowering produced layer-by-layer ordering produces a phase with ferroelectrically-induced weak ferromagnetism. I will present first-principles calculations demonstrating these behaviors in BaMnO3/SrMnO3 superlattices and other systems which could provide robust experimental realizations.

[1] J. H. Lee and K. M. Rabe, "Epitaxial-strain-induced multiferroicity in SrMnO3 from first principles," Phys. Rev. Lett. 104, 207204 (2010)

12:27PM J33.00005 Magnetic and multiferroic phases of single-crystalline $Mn_{1-x}Co_xWO_4$, K.-C. LIANG, R.P. CHAUDHURY, Y.-Q. WANG, Y.Y. SUN, B. LORENZ, TCSUH and Department of Physics, University of Houston, Houston, Texas 77024-5002, USA, F. YE, J.A. FERNANDEZ-BACA, H.A. MOOK, Neutron Scattering Science Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6393, USA, C.W. CHU, TCSUH and Department of Physics, University of Houston, Houston, Texas 77024-5002, USA — The recent interest of $MnWO_4$ system is due to the strong correlation between the long-wavelength magnetic structure and the ferroelectric polarization. To understand the effects of Co substitutions on magnetic and multiferroic phases of $MnWO_4$, we studied the magnetic and dielectric properties of the single-crystalline $Mn_{1-x}Co_xWO_4$ compounds. At lower Co substitution, the commensurate (CM) AF1 phase was found suppressed but could be restored in external magnetic fields along b axis. We also observed the ferroelectric polarization along b axis suppressed by a b-axis magnetic field. On the other hand, the higher Co substitution such as 15% showed more complex magnetic phases, which warrants future investigation. With Neutron scattering data, more detailed magnetic orders of the various phases would be revealed, and the relationship between magnetic phases and ferroelectric polarization will be discussed.

12:39PM J33.00006 Magnetoelectricity in $BiFeO_3$ films - first-principles-based computations and phenomenology[1] , SERGEY PROSANDEEV, University of Arkansas, IGOR KORNEV, Ecole Centrale Paris, LAURENT BELLAICHE, University of Arkansas, UNIVERSITY OF ARKANSAS TEAM, ECOLE CENTRALE PARIS TEAM — A first-principles-based effective Hamiltonian is used to compute linear and quadratic magnetoelectric (ME) coefficients in epitaxial (001) $BiFeO_3$ thin films. Its predictions are analyzed within a phenomenological model that provides analytical expressions of the ME coefficients in terms of polarization, as well as, dielectric and magnetic susceptibilities. Main discoveries are: (i) the quadratic ME coefficient is dramatically enhanced by increasing the magnitude of the compressive strain within the Cc phase, as similar to the previously reported enhancement of the linear ME coefficient in these films; (ii) the enhancements of the linear and quadratic ME coefficients have the same macroscopic origin, namely an increase in the dielectric permittivity; and (iii) the relative contribution of two different free-energy terms on the total linear ME coefficient is extracted from the simulations. The analytical expressions also help in understanding other ME effects.

[1]ONR N00014-08-1-0915 and N00014-07-1-0825, DOE DE-SC0002220, NSF DMR-0701558 and DMR-0080054. Thanks to MRI NSF 0722625 providing computer facilities.

12:51PM J33.00007 First Principles Study on Magnetoelectric Effects in $Ba_2CoGe_2O_7$, KUNIHIKO YAMAUCHI, ISIR-SANKEN, Osaka University, Japan, SILVIA PICOZZI, CNR-SPIN, L'Aquila, Italy — Magnetoelectric (ME) effects, or magnetically-induced ferroelectricity, are attracting large interests due to promising applications for novel type of devices. While the microscopic origin of ME effects is mostly classified as relate to spin current and/or exchange striction, a novel mechanism originating in spin- dependent p-d hybridization has been proposed and well explained ME effects observed in antiferromagnetic $Ba_2CoGe_2O_7$. In this study, we theoretically confirmed the magnetically induced electric polarization, whose size is dependent on the direction of Co spins. By means of both Landau theory and density functional calculations, the behavior of the experimentally observed polarization was well reproduced. Microscopically, we suggest single-site spin orbit coupling to slightly change the Co-d orbital shape upon changing the direction of Co spins, resulting in "asymmetric" p-d hybridization and consequent change in the electric polarization.

1:03PM J33.00008 Magnetoelectric resonance in S=3/2 two-dimensional antiferromagnet $Ba_2CoGe_2O_7$, SHIN MIYAHARA, Multiferroics Project (MF), ERATO, Japan Science and Technology Agency (JST), NOBUO FURUKAWA, Aoyama Gakuin University — We have investigated dynamical magnetoelectric effects in S = 3/2 two-dimensional antiferromagnet $Ba_2CoGe_2O_7$. It is a quasi two-dimensional antiferromagnet. Below T_N = 6.7 K, the Co magnetic moments show an antiferromagnetic ordering [1]. Recently, the material is paid attention to due to the magnetic field induced ferroelectric polarization [2,3]. Such multiferroics behaviors can be explained well by considering a spin-dependent metal-ligand hybridization mechanism on a Heisenberg model with strong uniaxial anisotropy term [3,4]. Through the spin dependent polarization, electric component of light can modulate the spin structures. As a result, electric component of light can excite magnetic excitations. We can clarify selection rules and resonance peak positions in absorption. When both magnetic and electric components induce the same magnetic excitation, cross correlated term, where electric component induced excitation is deduced to the ground state by magnetic component and vice versa, is realized. The effects of such cross correlation can be observed directly as linear directional dichroism in absorption process.[1] A. Zheludev *et al.*, Phys. Rev. B **68** 024428 (2003). [2] H.T. Yi *et al.*, Appl. Phys. Lett. **92** 212904 (2008). [3] H. Murakawa et al., Phys. Rev. Lett. **105** 137202 (2010). [4] T. Arima, J. Phys. Soc. Jpn. **76** 073702 (2007).

1:15PM J33.00009 Investigation of Multiferroic properties of the Co doping $SrBi_2Nb_2O_9$, WILLIAM PEREZ, NORA ORTEGA, ASHOK KUMAR, RAM KATIYAR, University of Puerto Rico — Multiferroics (MF) are novel class of next generation multifunctional materials, however there are very few single-phase MF materials existing in nature. Thin films (TF) of $(Sr_xCo_{1-x})Bi_2Nb_2O_9$ (SCBN) with x = 0, 0.05, 0.1, 0.15, 0.2, 0.25, 0.3 with thickness ∼400 nm were fabricated from individual SCBN targets on $Pt/Ti/SiO_2/Si$ substrate by pulsed laser deposition technique. The x-ray diffraction studies revealed orthorhombic structure of SCBN for up to 20% Co doped TF without any phase segregation, the splitting in (200) peak was observed above 25% of Co doping. The room temperature (RT) Raman spectra of SCBN TF showed $SrBi_2Nb_2O_9$ peaks in all compositions, however additional modes appeared in the 600-800 cm^{-1}frequency region. The dielectric constant of all SCBN films showed linear frequency dispersion above 1 kHz, and their values are in the range of 400 to 650 at 1 kHz. An increase in tangent loss from ∼ 0.040 to 0.135 at 1 kHz was observed with increase in Co concentration. All SCBN TF show well defined hysteresis loop with remanent polarization of about 16 $\mu C/cm^2$. However, less saturation in the ferroelectric loop was observed with increase of Co content. Both magnetic and magneto-electric behavior of TF along with the ferroelectric properties will be discussed.

1:27PM J33.00010 Large crystal-symmetry-induced magnetoelectric coupling in the quadruple perovskite $BiMn_3Mn_4O_{12}$, A. GAUZZI, G. ROUSSE, Univ. Pierre et Marie Curie, F. MEZZADRI, G. CALESTANI, Parma Univ., G. ANDRE, F. BOUREE, LLB CEA-CNRS, M. CALICCHIO, E. GILIOLI, R. CABASSI, F. BOLZONI, A. PRODI, IMEM-CNR, P. BORDET, Inst. Neel-CNRS, M. MAREZIO, CRETA-CNRS — The remarkable properties of manganese oxides AMnO$_3$ with perovskite structure, such as the colossal magnetoresistance and the multiferroicity, arise from peculiar charge, spin and orbital orderings of the Mn e_g electrons driven by cooperative Jahn-Teller distortions of the MnO$_6$ octahedra. Mastering these orderings remains a challenge owing to local structural distortions and electronic inhomogeneities enhanced by chemical substitutions and oxygen defects. We show that these difficulties are absent in *quadruple* perovskites AMn$_3$Mn$_4$O$_{12}$. These compounds share with *simple* perovskites AMnO$_3$ a similar pseudo-cubic network of corner-sharing MnO$_6$ octahedra and similar electronic properties associated with the Mn^{3+} and Mn^{4+} ions. However, they display smaller distortions thanks to the higher crystal symmetry an no defects. For A=Bi, by means of neutron powder diffraction we give direct crystallographic evidence of a large coupling between the electric dipole of the 6s lone pair of Bi^{3+} and the magnetic structure of the Mn^{3+} ions, which provides a hint for enhancing the magnetoelectric coupling in proper ferroelectrics in view of multiferroic applications.

1:39PM J33.00011 Micorscopic theory of temperature-dependent magnetoelectric effect in Cr_2O_3 , ANDREA SCARAMUCCI, MAXIM MOSTOVOY, Zernike Institute for Advanced Materials, University of Groningen, NICOLA A. SPALDIN, Materials Department, University of California Santa Barbara / Department of Materials, ETH Zurich, KRIS T. DELANEY, Materials Research Laboratory, University of California Santa Barbara — We study the temperature dependence of the magnetoelectric effect in Cr_2O_3 by considering the coupling between electric polarization and spins induced by Heisenberg exchange interactions. The form of the coupling is obtained by symmetry analysis and its strength is calculated by *ab initio* methods. Using Monte Carlo simulations, we evaluate the temperature dependence of the largest component of the magnetoelectric susceptibility. The quantitative agreement of our results with experimental measurements shows that the dominant contribution to the linear magnetoelectric effect originates from nonrelativistic exchange interactions and spin fluctuations. The approach used can be applied to study other magnetoelectrics with collinear spin ordering and opens a new route for the design of materials with large magnetoelectric effect at high temperatures.

1:51PM J33.00012 Pressure- and field-dependent Raman studies of magnetodielectric behavior in Mn_3O_4[1] , M. KIM, S. YUAN, S.L. COOPER, Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois, Urbana, Illinois, 61801 — We present simultaneous pressure- and field-dependent Raman scattering studies of the magnetodielectric spinel, Mn_3O_4, which allow us to investigate both the microscopic origins and pressure dependence of magnetodielectric phenomena in this material. We identify the specific phonon modes responsible for the dramatic magnetodielectric behavior observed in this material, and show that these modes provide quantitative information regarding magnetodielectric behavior in Mn_3O_4 via the Lyddane-Sachs-Teller (LST) relationship. We also show that pressure can induce monoclinic distortions accompanied with magnetic ordering in Mn_3O_4. Finally, by exploring the field-dependent phonon spectrum at different pressures, we are able to map out the pressure-field structural phase diagram of Mn_3O_4 and explore the pressure-dependence of magnetodielectric behavior in this material.

[1]Work supported by the National Science Foundation under Grant NSF DMR 08-56321 and by the U.S. Department of Energy under Award No. DE-FG02-07ER46453.

2:03PM J33.00013 Infrared optical properties of multiferroic $FeTe_2O_5Br$ single crystal[1] , KEVIN H. MILLER, C. MARTIN, X. XI, University of Florida, H. BERGER, Ecole Polytechnique Federal de Lausanne, G.L. CARR, Brookhaven National Laboratory, D.B. TANNER, University of Florida — Reflection as a function of temperature has been measured on a single crystal of the anisotropic multiferroic $FeTe_2O_5Br$ utilizing light spanning the far infrared to the visible portions of the electromagnetic spectrum. The complex dielectric function and optical properties along all three principal dielectric axes were obtained via Kramers-Kronig analysis and by fits to a Drude-Lorentz model. Transmission in the terahertz region as a function of temperature and magnetic field is also described, with particular focus on temperatures around the $\sim$10 K transition to the multiferroic state.

[1]Supported by the US DOE through contract DE-FG02-02ER45984 at UF and DE-AC02-98CH10886 at the NSLS.

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J34 DMP: Focus Session: Interfaces in Complex Oxides - Microscopy and Local Structure C141

11:15AM J34.00001 Unexpected ordering at the atomic scale interface of $SrRuO_3$ and $BaTiO_3$[1] , ARTHUR P. BADDORF, Oak Ridge National Laboratory — Atomically engineered oxide multilayers and superlattices display unique properties responsive to the electronic and atomic structures of the interfaces. Interfaces can exhibit not only two-dimensional functionality, but have the power to dictate the properties of thin films. A clear example is found in ferroelectric thin films, where the domain size, orientation, and transport properties are controlled by top and buried interfaces. We have explored a prototypical ferroelectric - bottom electrode interface by characterizing $BaTiO_3$ grown on $SrRuO_3$. Films were grown on $SrTiO_3$ substrates by pulsed laser deposition, monitored by high-pressure reflection high-energy diffraction, exhibited high crystalline quality in electron diffraction and cross-sectional transmission electron microscopy (STEM), and were flat according to atomic force microscopy. Despite multiple indicators commonly accepted to confirm a sharp interface, atomically the structure is more complex. When grown in a typical oxygen pressure, at or below 10 mTorr, in situ scanning tunneling microscopy (STM) revealed the $SrRuO_3$ surface is littered with oxygen vacancies. For growth or post-annealing above $\sim$100 mtorr, vacancies were removed, but STM and low energy electron diffraction (LEED) disclosed a surface reconstruction consisting of parallel rows with periodicity doubled in one direction. Density function theory (DFT) suggests these rows are chains of Sr and O raised by excess oxygen. Both LEED and cross-sectional STEM revealed that this reconstruction persists at the buried interface and modifies the structure of subsequent $BaTiO_3$ layers. By four layers, the $BaTiO_3$ surface returns to a bulk-like structure with upward polar distortion. This study emphasizes the importance of atomic scale structural studies of what may otherwise appear as sharp interfaces.

[1]Research at ORNL's CNMS was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. DOE.

11:51AM J34.00002 Highly confined 2D electron gas in $SrTiO_3/SrRuO_3$ superlattices[1] , MARCOS VERÍSSIMO-ALVES, CITIMAC, Universidad de Cantabria, Spain, DANIEL BILC, Universite de Liège, Belgium, PABLO GARCÍA-FERNÁNDEZ, CITIMAC, Universidad de Cantabria, Spain, PHILIPPE GHOSEZ, Universite de Liège, Belgium, JAVIER JUNQUERA, CITIMAC, Universidad de Cantabria, Spain — In recent years, experimental advances in the creation of atomically smooth interfaces between complex oxides have made possible the observation of unusual electronic phenomena such as the formation of 2D electron gases confined to the interface between insulating compounds. In this work, we explore an alternative for creating a 2D electron gas in oxide interfaces by means of a $(SrTiO_3)_5/(SrRuO_3)_1$ superlattice. LSDA+U and hybrid functional B1-WC DFT calculations with full relaxation of atomic geometry show the presence of a 2D electron gas, and the system can be described with $U = 4$ eV. Electronic correlations thus become important with quantum confinement: the system is a minority spin half metal with a magnetic moment of $\mu = 4\mu_B$. Degenerate Ru $4d_{(xz,yz)}$ states are the main responsible for the DOS at the Fermi level, whose shape strongly resembles that of 1D free-electron gases. Our results suggest that the material could find uses in spintronic devices.

[1]We thank financial support from FIS2009-12721-C04-02 and CP-FP 228989-2 Projects.

12:03PM J34.00003 Ferroelectric thickness effects on LaSrMnO3/PbZrTiO3 Heterostructures , JINLING ZHOU, West Virginia University, EVAN WOLF, CHARLES FRYE, DISHENG CHEN, SRINIVAS POLISETTY, MIKEL HOLCOMB, DAVID LEDERMAN COLLABORATION, YING-HAO CHU COLLABORATION — Magnetoelectric (ME) coupling is the coupling of magnetic and electric properties within a material. It allows the possibility of dual control of the material through the manipulation of either electric or magnetic fields and therefore could potentially revolutionize the current technology. However, little is known about the factors that influence the strength of this magnetoelectric coupling. In the presented research, ferromagnetic LSMO and ferroelectric PZT are constructed as wedged adjacent layers for the purpose of studying the coupling effects and physical properties in each layer and the resulting interface. X-ray absorption spectroscopy (XAS) and photoemission electron microscopy (PEEM) are used as the major techniques to map out magnetism, ferroelectricity, and the interfacial coupling. The XAS spectra illustrate a strong effect on the magnetic properties depending on ferroelectric thickness. PEEM images display the magnetic and ferroelectric domains in each material layer, allowing further insight into why the coupling depends on layer thickness. This research will aid the understanding of coupling in not only magnetoelectric heterostructures, but also in other similar complex oxide systems.

12:15PM J34.00004 $SrTiO_3$ on silicon: interface chemistry, polarization pinning, and electronic states , SOHRAB ISMAIL-BEIGI, Yale University, ALEXIE KOLPAK, Massachusetts Institute of Technology, FRED WALKER, JIM REINER, CHARLES AHN, Yale University — We use $SrTiO_3$/Si as a model system to examine the effects of interface atomic structure and composition on the functional properties of epitaxial oxide films on silicon. Using first-principles computations, we show that intrinsic chemo-mechanical boundary conditions at the interface fix a single polarization direction in the SrTiO3 thin film independent of the interface composition, inhibiting ferroelectric functionality. In contrast, the transport properties of the interface are quite sensitive to the interface composition, which can be used to tune the interface from an insulator to an interfacial 2D electron gas. We describe the origins of both functionalities and discuss their applicability to the general class of epitaxial oxides on semiconductors.

12:27PM J34.00005 First Principles Study of Resonant Phonon Coupling across the LSMO / STO Interface , KEVIN F. GARRITY, YARON SEGAL, CARLOS A.F. VAZ, JASON D. HOFFMAN, FRED J. WALKER, CHARLES A. AHN, SOHRAB ISMAIL-BEIGI, Yale University — Epitaxial interfaces permit dynamical modification of the properties of a thin film via coupling to the substrate. In particular, the coupling of phonons between two materials allows one to manipulate the atomic structure and vibrational modes near an interface. We use first principles density functional theory (DFT) to study the octahedral oxygen rotations at and across an interface between $La_xSr_{(1-x)}MnO_3$ (LSMO) and $SrTiO_3$. By performing finite temperature Monte Carlo sampling on a classical potential built to reproduce our DFT energetics, we demonstrate that as the $SrTiO_3$ is driven through the phase transition where its octahedral rotations become frozen in place, phonons from the $SrTiO_3$ couple into the interfacial LSMO. These couplings can then modify the LSMO transport properties, as observed in our experiments. The decay length of the phonon coupling into the LSMO agrees with our experimental determinations on this system. We demonstrate that the observed changes in resistance are not due to static changes in the LSMO structure, confirming the phonon coupling.

12:39PM J34.00006 Coupling of strain and magnetism in LPCMO films[1] , SURENDRA SINGH, M. FITZSIMMONS, Los Alamos National Laboratory, HYOUNGJEEN JEEN, AMLAN BISWAS, University of Florida — Complex oxides show extraordinary structural, magnetic and magneto-transport properties and these properties are closely coupled with atomic structure and strain. The temperature- magnetic field phase diagram and transport studies of $La_{0.27}Pr_{0.40}Ca_{0.33}MnO_3$ (LPCMO) films suggest the existence of two phases at low temperatures, i.e. ferromagnetic metallic (FMM) phase and charge order insulating (COI) phase. We report the magneto transport properties of LPCMO films on application of external strain using mechanical jig. The study shows the shift in metal to insulator transition (MIT) temperature on application of external strain. To understand the effect of strain as well as kinematics of formation of FMM phase from COI phase of LPCMO films and vice versa, we have performed detailed in situ transport and specular polarized neutron reflectivity measurements across the MIT as functions of temperature, magnetic field and applied strain. The study reveals a variation of magnetic scattering length density along the depth of the film, which may be attributed to chemical inhomogeneity of the film as a function of depth.

[1]This work is supported by Department of Energy and National Science Foundation.

12:51PM J34.00007 Coupling between oxygen octahedron rotations, Jahn-Teller distortion, magnetic ordering and epitaxial strain in LaMnO3 from first principles , JUN HEE LEE, KARIN M. RABE, Rutgers University, KRIS DELANEY, ERIC BOUSQUET, NICOLA SPALDIN, University of California Santa Barbara — LaMnO3 is known to have rich physics due to coupling among orbital ordering, Jahn-Teller distortions and magnetism. However, less attention has been paid to the role of oxygen octahedron rotations and epitaxial strain. In this talk, we show from first principles calculations that oxygen octahedron rotations induce weak ferromagnetism in *Pbnm* LaMnO3 and that octahedral rotations are cooperatively coupled to the Jahn-Teller distortion.. Furthermore, we predict that compressive epitaxial strain drives bulk A-type antiferromagnetic Pbnm insulating phase to a ferromagnetic metallic phase. At the phase boundary between the ferromagnetic-metallic and antiferromagnetic-insulating phases, colossal magneto-resistance is expected.

1:03PM J34.00008 Local Octahedral Distortions and Magnetic Properties Controlled by Substrate Symmetry at Perovskite Oxide Interfaces[1] , JUN HE, Vanderbilt University, ALBINA BORISEVICH, SERGEI KALININ, STEPHEN PENNYCOOK, Oak Ridge National Laboratory, SOKRATES PANTELIDES, Vanderbilt University — We have investigated the oxygen octahedral distortions and local magnetism at the interfaces of magnetic perovskite oxide heterostructures using first principles calculations. The studied prototype oxide heterostructures include $La_{0.7}Sr_{0.3}MnO_3$, $SrRuO_3$, and $BiFeO_3$. The results show that the symmetry mismatch at interfaces between two perovskite oxides imposes an interfacial layer with distortion modes that do not exist in either bulk material, creating new interface properties by symmetry alone. The thickness of such interface layer depends on the resistance of the octahedra to deformation.

[1]Work supported by the Division of Materials Sciences and Engineering, BES, U.S. DoE., Computations were performed at NERSC.

1:15PM J34.00009 Atomic Resolution and First Principles Study of the Structure and Bonding at $SrTiO_3$/GaAs Hetero-interfaces[1] , QIAO QIAO, ROBERT KLIE, SERDAR OGUT, University of Illinois at Chicago — Ultrathin metal-oxide films on polar semiconductor surfaces have received much attention in recent years due to occurrence of novel functional properties, including ferroelectricity, superconductivity and the presence of an interfacial 2-dimensional electron gas. In this study, we examine the atomic and electronic structures of epitaxial ultrathin $SrTiO_3$ (100) films on GaAs (001) using aberration corrected atomic-resolution Z-contrast imaging and electron energy loss spectroscopy (EELS) in combination with first principles calculations to develop a fundamental understanding of the interfacial structure-property relationships. Using atomic-column resolved EELS, we show that Ti diffuses into the first few monolayers of GaAs depending on the thin film growth condition. The effects of Ti diffusion into subsurface GaAs (001) with (4x2)-β2 surface reconstructions will be investigated via first principles calculations. We will also discuss the results for the formation energies of Ti-related impurity defects in the bulk and surface regions of GaAs to help in the interpretation of electron microscopy experiments.

[1]Supported by NSF Grant No. DMR-0846748

1:27PM J34.00010 Accessing hidden isosymmetric phase transitions in perovskite thin films , JAMES RONDINELLI, Argonne National Laboratory, SINISA COH, Rutgers University — Isosymmetric phase transitions (IPT), which show no change in occupied Wyckoff positions or crystallographic space group, are exceedingly rare in crystalline matter because most condensed systems respond to external stimuli by undergoing "conventional" symmetry-lowering displacive, martensitic or reconstructive transitions. In this work, we use first-principles density functional calculations to identify an elusive IPT in orthorhombic ABO_3 perovskite oxides with tendency towards rhombohedral symmetry. Using perovskite $LaGaO_3$ as our prototypical system, we show that the latent isosymmetric phase transition, which manifests as an abrupt change in the octahedral rotation axis, is accessible only with an external elastic constraint—bi-axial strain. We show the transition originates from a soft phonon that describes the geometric connectivity and relative phase of the GaO_6 polyhedra. By connecting the origin of IPT to a chemical and structural incompatibility between the lattice and the elastic constraints, we describe how subtle changes in bulk orthorhombic and monoclinic symmetries are critical to the complete engineering of structure-correlated electronic properties in thin films. Because bi-axial strain is the critical parameter controlling the IPT, we suggest heteroepitaxial synthesis of IPT materials is a plausible route to realize high-κ dielectric actuators with variable band gaps and dielectric anisotropies.

1:39PM J34.00011 Electronic properties of ultrathin GdTiO3 thin films and GdTiO3/SrTiO3 interfaces , POUYA MOETAKEF, BHARAT JALAN, JACK ZHANG, University of California, Santa Barbara, S. JAMES ALLEN, SUSANNE STEMMER, University of California, Santa Barbara — Interfaces between Mott insulators, such as the rare earth titanates, and band insulators, such as SrTiO3, have recently attracted much attention. We report on the transport properties of epitaxial rare earth titanate thin films, GdTiO3, grown by molecular beam epitaxy (MBE) and those of heterostructures with SrTiO3 and GdTiO3. Growth of GdTiO3 was performed by shuttered growth of alternating titanium tetra isopropoxide (TTIP) and Gd fluxes, in the absence of any additional oxygen. We show that to stabilize the GdTiO3 perovskite phase, SrTiO3 buffer layers are needed for growth on perovskite substrates, such as LSAT ((LaAlO3)0.3(Sr2AlTaO6)0.7). The contribution of n-type SrTiO3 buffer layers and that of the SrTiO3/GdTiO3 interfaces to the transport properties are determined by measurements of the electrical resistance and Hall coefficient as a function of temperature and magnetic field.

1:51PM J34.00012 Atomically-resolved mapping of polarization and electric fields across ferroelectric-oxide interfaces by Z-contrast imaging[1] , ALBINA BORISEVICH, HYE JUNG CHANG, SERGEI KALININ, Oak Ridge National Laboratory, ANNA MOROZOVSKA, NAS Ukraine, YING-HAO CHU, PU YU, RAMAMOORTHY RAMESH, University of California Berkeley, STEPHEN PENNYCOOK, Oak Ridge National Laboratory — Polarization, electric field, charge and potential across ferroelectric-oxide interfaces are obtained from direct atomic position mapping by aberration corrected scanning transmission electron microscopy combined with Ginsburg-Landau-Devonshire theory. We compare two antiparallel polarization orientations, which allows separation of the polarization and intrinsic interface charge contributions. Using the Born effective charges, the complete interface electrostatics is obtained in real space, providing an alternative method to holography. The results provide new microscopic insight into the thermodynamics of polarization distribution at the atomic level.

[1]Research is sponsored by the of Materials Sciences and Engineering Division, U.S. DOE.

2:03PM J34.00013 Inherited (In)stabilities in Transition Metal Superlattices , SVEN RUDIN, Los Alamos National Lab — Many transition metals exhibit a solid phase with a body-centered cubic (bcc) crystal structure. For some elements, e.g., tungsten (W), bcc is the only solid phase; for others, e.g., titanium (Ti), the bcc phase only appears at high temperatures. Titanium's high-temperature bcc phase exhibits soft phonon modes. These reflect the atomic movements upon transformation into the low-temperature phases. One such mode shows atomic displacements that also appear in the top few layers of tungsten's surface reconstruction. Superlattices constructed from alternating nanometer-thick layers of W and Ti would allow the two displacement patterns to interact. The work presented here uses density functional theory calculations to predict how the structure and mechanical response of such superlattices depends on the choice of transition metal elements and the layer thicknesses.

Tuesday, March 22, 2011 11:15AM - 2:15PM –
Session J35 DCMP: Topological Insulators: Optics C140

11:15AM J35.00001 Far-infrared magneto-spectroscopy study of ultrathin Bi^2Se^3 layers in high magnetic field , WENLONG YU, GA Inst Tech, LI-CHUN TUNG, NHMFL, XUNCHI CHEN, DMITRY SMIRNOV, IRENEUSZ MIOTKOWSKI, HELIN CAO, YONG P. CHEN, ZHIGANG JIANG — We present a far-infrared (FIR) magneto-spectroscopy study of thin Bi2Se3 layers. Transmittance and reflectance measurements are performed in the Faraday geometry at 4.2 K and in a magnetic field up to 17.5 T. The thin samples (much less than 1 micron) are stabilized on the Scotch tape, which enable us to obtain reliable FIR transmission signals. A pronounced electron-phonon coupling, i.e., the coupling of a FIR phonon of Bi2Se3 with the continuum free-carrier spectrum, is observed and strongly enhanced by the applied magnetic field. The phonon lineshape is asymmetric and can be fit by a Fano formula. After examining the fitting parameters, we find no systematic broadening of the lineshape in our measurements.

11:27AM J35.00002 Terahertz and magneto-optical studies of HgTe films , JASON HANCOCK, University of Geneva, GEORGY ASTAKHOV, CHRISTOPHE BRUENE, Wuerzburg, DIRK VAN DER MAREL, University of Geneva, LAURENS MOLENKAMP, Wuerzburg — We present a frequency-domain infrared, time-domain terahertz, and magneto- optical study of thin films of high-mobility HgTe. The conductivity at low frequency and a wide range of temperature is described, and clear cyclotron effects are observed at low temperature and frequency. The context of these findings to the possible 3D topological phase will be discussed.

11:39AM J35.00003 Magneto-Optics in the search for the topological insulating state , ALEXANDER SCHAFGANS, Department of Physics, University of California, San Diego, ANDREW LAFORGE, Department of Physics, University of California, Santa Cruz, A. TASKIN, YOICHI ANDO, Institute of Scientific and Industrial Research, Osaka University, Ibaraki, Osaka 567-0047, Japan, DIMITRI BASOV, Department of Physics, University of California, San Diego — We present infrared spectroscopic data for the thermoelectric material Bi-Sb at the insulating composition, taken in magnetic field applied both in the Voight and Faraday geometries, in order to gain insight into the recently discovered topological insulating state. We observe a metallic plasma edge that displays significant blue shift at high temperatures. The form of the plasma edge shows broadening suggestive of sample inhomogeneities. The plasma edge is remarkably sensitive to the applied magnetic field, resulting in a complicated spectral lineshape. We compare these results with magneto-optics of the topological insulator Bi_2Se_3.[1]

[1]A. D. LaForge, *et. al.*, Phys. Rev. B 81, 125120 (2010).

11:51AM J35.00004 Magneto-optical spectra of topological insulators Bi_2Te_3, Sb_2Te_3 and Bi_2Se_3 in magnetic fields up to 18 Tesla , M.S. WOLF, S.V. DORDEVIC, The University of Akron, N. STOJILOVIC, University of Wisconsin Oshkosh, HECHANG LEI, C. PETROVIC, Brookhaven National Lab, L.C. TUNG, National High Magnetic Field Lab — Topological insulators are a novel class of materials that behave as insulators in the bulk, but have conducting states on the surface. Studies of their behavior in magnetic field is an important avenue towards understanding their complex properties. We will report the results of our magneto-optical measurements of topological insulators Bi_2Te_3, Sb_2Te_3 and Bi_2Se_3 in magnetic fields up to 18 Tesla. In all three compounds we detect magnetic-field induced changes in optical properties, which are most pronounced around the plasma edge. The induced changes are much bigger in Bi_2Se_3 than in Bi_2Te_3 and Sb_2Te_3.

12:03PM J35.00005 Optical properties of novel topological insulators[1] , ANDREI SUSHKOV, G.S. JENKINS, H.D. DREW, N.P. BUTCH, J. PAGLIONE, University of Maryland at College Park, K.R. CHOI, S.-W. CHEONG, Rutgers University — The recent discovery of topological insulators (TI) with the spin-polarized Dirac-like electrons on their surfaces have attracted a lot of attention and theoretical and experimental research efforts. One of the fascinating properties of TIs is the presence of the linear magneto-electric coupling which is responsible for coupled charge-spin modes in dynamical response. We will report our results on the search for such modes together with the conventional optical properties of materials predicted to be TI such as 5d oxide Na_2IrO_3, SmB_6, and Bi_2Se_3 and other materials. Measurement results include optical reflectance and/or transmission in the frequency range 5 - 50,000 cm^{-1} and Faraday or Kerr rotation and circular dichroism at selected THz frequencies.

[1]This work was supported in part by the NSF MRSEC under Grant No. DMR-0520471.

12:15PM J35.00006 Terahertz Kerr and Reflectivity Measurements on the Topological Insulator Bi_2Se_3[1] , GREGORY S. JENKINS, A.B. SUSHKOV, D.C. SCHMADEL, N.P. BUTCH, P. SYERS, J. PAGLIONE, M.-H. KIM, H.D. DREW, Center for Nanophysics and Advanced Materials, University of Maryland, College Park, J.G. ANALYTIS, I.R. FISHER, Geballe Laboratory for Advanced Materials, Departments of Physics and Applied Physics, Stanford University, Stanford — We report the first terahertz Kerr measurements on bulk crystals of the topological insulator Bi_2Se_3 with and without Fe doping at 4 K and magnetic fields up to 8 T. Transport evidence and characterization of the surface states will be presented. By employing a gate that creates a small depletion layer, the optical signals from the surface state carriers are modulated with no contribution arising from the bulk carriers. The real and imaginary parts of the Kerr angle yeild the transport scattering rate, spectral weight, and mass of the surface state carriers. FTIR and magneto-optical measurements characterize the bulk carriers. Comparisons with ARPES and other transport measurements will be discussed.

[1]Work supported in part by DOE grant #DESC0005436.

12:27PM J35.00007 Magneto-optical and Magneto-electric Effects of Topological Insulators in Quantizing Magnetic Fields[1] , WANG-KONG TSE, A.H. MACDONALD, University of Texas, Austin — Topological insulators show novel magneto-electric effect when the surface Dirac cone dispersion is gapped by a weak Zeeman field. In this talk, we present our study of the magneto-optical and magneto-electric effects of a thin-film topological insulator in the presence of a strong quantizing magnetic field. We find that low-frequency magneto-optical properties depend only on the sum of top and bottom surface Dirac-cone filling factors, whereas the magneto-electric response depends only on the difference. The Faraday rotation is quantized in integer multiples of the fine structure constant α and the Kerr effect exhibits a full-quarter rotation. Strongly enhanced cyclotron-resonance features appear at higher frequencies that are sensitive to the filling factors of both surfaces. When the product of the bulk conductivity and the film thickness in e^2/h units is small compared to α, magneto-optical properties are only weakly dependent on accidental doping in the interior of the film.

[1]This work was supported by the Welch grant F1473 and by DOE grant DE-FG03-02ER45985.

12:39PM J35.00008 Photo-Induced Kerr Rotation in the Bulk and Surface of a Topological Insulator , FAHAD MAHMOOD, DAVID HSIEH, JAMES MCIVER, DILLON GARDNER, YOUNG LEE, NUH GEDIK, Department of Physics, Massachusetts Institute of Technology, Cambridge MA 02139 — We report ultrafast bulk- and surface-sensitive optical pump-probe spectroscopy from Bi_2Se_3 (111). Using second harmonic generation, we demonstrate that the bulk and surface electronic contributions can be separated and exhibit qualitatively different relaxation dynamics. Ultrafast surface-sensitive optical measurements reveal a large photo-induced Kerr rotation from the surface that is dependent on the helicity of the circularly polarized excitation pulse. We will discuss the microscopic origin of this observation and how it relates to the strong spin-charge coupling on the surface of a topological insulator.

12:51PM J35.00009 Infrared studies of topological insulators Bi_2Te_3, Sb_2Te_3 and Bi_2Se_3 , S.V. DORDEVIC, M.S. WOLF, The University of Akron, N. STOJILOVIC, University of Wisconsin Oshkosh, HECHANG LEI, C. PETROVIC, Brookhaven National Lab — In this study we have used infrared spectroscopy to probe the electrodynamic response of topological insulators Bi_2Te_3, Sb_2Te_3 and Bi_2Se_3. Infrared spectra are collected over a broad frequency and temperature range. The results reveal similar spectra in all three compounds, with well defined plasma edge located in the far-infrared part of the spectrum. However there are some important differences in the temperature evolution of the spectra. Namely, as temperature decreases the plasma edge shifts to lower frequencies in Bi_2Se_3, whereas in Bi_2Te_3 and Sb_2Te_3 it shifts to higher frequencies.

1:03PM J35.00010 Surface optical study of topological insulator Bi2Se3 , DAVID HSIEH, JAMES MCIVER, DARIUS TORCHINSKY, DILLON GARDNER, YOUNG LEE, NUH GEDIK, Department of Physics, Massachusetts Institute of Technology, Cambridge MA 02139 — We report the observation of optical surface second harmonic generation from the (111) surface of Bi2Se3 using ultrafast laser pulses. We demonstrate that second harmonic generation is sensitive to both the surface crystal structure as well as the surface carrier density, which we tune through surface molecular doping. Protected nodes in the second harmonic circular dichroism spectroscopy provide a method to study time-reversal symmetry breaking effects from a single surface in a contact free manner.

1:15PM J35.00011 Ultrafast carrier and phonon dynamics in Bi_2Se_3 crystals , XUNCHI CHEN, GA Inst of Tech, JINGBO QI, GA Inst of Tech, NHMFL, WENLONG YU, GA Inst of Tech, PAUL CADDEN-ZIMANSKY, DMITRY SMIRNOV, NHMFL, NORMAN TOLK, Vanderbilt University, IRENEUSZ MIOTKOWSKI, HELIN CAO, YONG P. CHEN, Purdue University, YIZHENG WU, SHAN QIAO, Fudan University, ZHIGANG JIANG, GA Inst of Tech — Ultrafast time-resolved differential reflectivity of Bi_2Se_3 crystals is studied using optical pump-probe spectroscopy. Three distinct relaxation processes are found to contribute to the initial transient reflectivity changes: a sub-ps and a few-ps electron-phonon relaxation process due to different phonon modes and a defect-induced charge trapping process. After the crystal is exposed to air, the relative strength of these processes is altered and becomes strongly dependent on the excitation photon energy. We argue that the observed behavior is likely due to the presence of Se vacancies. Further, weaker charge trapping process and vanishing air doping effect are observed in magnetically doped samples, supportive of our argument. Part of this work is published on Appl. Phys. Lett. 97, 182102(2010).

1:27PM J35.00012 Photo-induced currents in the topological insulator Bi2Se3 , JAMES MCIVER, DAVID HSIEH, HADAR STEINBERG, PABLO JARILLO-HERRERO, NUH GEDIK, Department of Physics, MIT, Cambridge, MA 02139 — We report the observation of photo-induced currents in micro-devices built from exfoliated single crystals of Bi2Se3. Our experiments are performed using ultrashort laser pulses at 800 nm and in the absence of an applied bias. We find that the induced currents scale quadratically with laser field strength, confirming their second order nature. We will present the temperature dependence of these second order currents and discuss their microscopic origin.

1:39PM J35.00013 Circular photogalvanic effect on topological insulator surfaces: Berry curvature-dependent response[1] , PAVAN HOSUR, University of California at Berkeley — Strong spin-orbit coupling is commonly exploited for generating electric currents using circularly-polarized light. We study, theoretically, the direct current generated by circularly-polarized light on the surface of a topological insulator, focusing on the part that reverses on switching the light-helicity. Interestingly, the dominant current, due to an interband transition, is controlled by the Berry curvature of the surface bands. This extends the connection between photocurrents and Berry curvature beyond the quasiclassical approximation where it has been shown to hold. Explicit expressions are derived for the (111) surface of the topological insulator Bi_2Se_3 where we find significant helicity-dependent photocurrents when the rotational symmetry of the surface is broken by an in-plane magnetic field or a strain. Moreover, the dominant current grows linearly with time until a scattering occurs, which provides a means for determining the scattering time. DC spin density is generated on the surface as well, and is also dominated by a linear-in-time, Berry curvature-dependent contribution.

[1]This work was supported by LBNL DOE-504108

1:51PM J35.00014 Raman studies of irradiation-induced defects in thin flakes of Bi2Se3 and related materials , ISAAC CHILDRES, JIFA TIAN, IRENEUSZ MIOTKOWSKI, YONG P. CHEN, Purdue University — We report a Raman spectroscopy study of exfoliated Bi2Se3 flakes of various thicknesses after exposure to irradiation by lasers, electron-beam and oxygen plasma. We observe little effect of irradiations on Raman spectra of thicker (>50 nm) Bi2Se3 flakes, which exhibit characteristic Raman peaks at ∼130 cm-1 and ∼170 cm-1 similar to bulk Bi2Se3. However, spectra from irradiated thinner (<20 nm) flakes show the appearance of an extra Raman peak (∼250 cm-1) and attenuation and broadening of the peaks at ∼130 cm-1 and ∼170 cm-1. This additional peak is not seen in flakes exposed to electron-beam irradiation and lower-power lasers. We interpret the new peak in the Raman spectra as due to irradiation-induced disorder. We also performed similar Raman studies on Bi2Te3, Sb2Se3 and Sb2Te3.

2:03PM J35.00015 Tuning optical and electrical transport properties of Bi2Se3 with Ca[1] , ZHIYONG WANG, TAO LIN, PENG WEI, XINFEI LIU, Department of Physics and Astronomy, UC Riverside, RANDY DUMAS, KAI LIU, Department of Physics, UC Davis, JING SHI, Department of Physics and Astronomy, UC Riverside — We have systematically tuned the carrier type and density in Bi_2Se_3 single crystals by introducing a calcium dopant. By controlling Ca-concentration x in $Ca_xBi_{2-x}Se_3$, a minimum carrier density of $\sim 1 \times 10^{17}$ cm^{-3} is achieved in both n- and p-type materials. The Fourier transform infrared (FTIR) measurements were carried out in samples with different doping levels to obtain the inter-band transition energy, sample thickness, and the plasma frequency. The band gap and reduced effective mass of carriers were determined from the relation between the inter-band transition energy and carrier density. The undoped samples show a high electron density ($\sim 5 \times 10^{18}$ cm^{-3}) and the electrical resistivity shows a typical metallic behavior. At high magnetic fields (up to 14 T), the undoped samples show the Shubnikov-de Haas oscillations. Near the compensation point or x=1.2%, the electrical resistivity shows an insulating behavior with a low temperature saturation. This work was supported in part by DOE and NSF.

[1]This work was supported in part by DOE and NSF.

Tuesday, March 22, 2011 11:15AM - 2:03PM –

Session J36 DMP: Focus Session: Graphene Growth, Characterization and Devices: SiC and Metal Substrates C142

11:15AM J36.00001 SiC structuring and step bunching for C-face epitaxial graphene growth , JOHN HANKINSON, Georgia Tech, YIKE HU, MING RUAN, BAIQIAN ZHANG, CLAIRE BERGER, WALT DE HEER — Recent research at Georgia Tech has focused on understanding and improving the epitaxial graphene growth process. Electronic experiments have demonstrated the excellent properties that high quality epitaxial graphene can posses when grown by the confinement controlled sublimation (CCS) method in an induction furnace [1]. Here we focus on the mechanisms at work in the early stages of graphitization. Experimental observations of C-face epitaxial graphene growth have revealed that when step-pinning defects are present they seem to act as preferential graphene nucleation sites. In addition we have observed preferential graphene growth on silicon carbide sidewalls and mesas. Ongoing work seeks to take advantage of the correlation between silicon carbide structure and graphene growth by pre-patterning the SiC substrate in order to better control the graphene grown on it. With CCS growth we have created flat graphene regions extending over tens of microns with RMS roughness below 2.5 angstroms. Growth results and electronic measurements on graphene grown on structured SiC mesas will be presented.

[1] R. Ming et al. Materials Science and Engineering – Reports (submitted)

11:27AM J36.00002 Novel epitaxy of graphene using substrate microfabrication , HIROKAZU FUKIDOME, MASATO KOTSUGI, TAKUO OHKOUCHI, TOYOHIKO KINOSHITA, THOMAS SEYLLER, KARSTEN HORN, YUSUKE KAWAI, MAKI SUEMITSU, YOSHIO WATANABE — Epitaxy of graphene on SiC is promising for device applications owing to the capability to produce large-area film. For the further applications toward integrated devices, the microscopic thickness variation of graphene should be minimized because the thickness of graphene critically determines the electronic properties, such as carrier mobility and bandgap. One of the effective solutions is the epitaxy on microfabricated substrates to spatially control surface reactions involved in the epitaxy. The controllability of the epitaxy using substrate microfabrication has been already proven for the homoepitaxy on microfabricated Si substrates. We therefore study heteroepitaxy of graphene on microfabricated 6H-SiC(0001) substrates as a model system to produce epitaxial graphene without thickness variation. It has been in fact demonstrated by using photoemission and low energy electron microscopies that the epitaxial graphene exhibits no thickness variation when the size of microfabrication pattern is small (below 10 micrometer). Further the shape of the microfabrication pattern is also influential to the microscopic variation of the graphene. The controlled epitaxy of graphene by substrate microfabrication is thus demonstrated to be vital for future integrated graphene devices.

11:39AM J36.00003 Selective Epitaxial Graphene Growth on SiC via AlN Capping , FARHANA ZAMAN, MIGUEL RUBIO-ROY, MICHAEL MOSELEY, JONATHAN LOWDER, WILLIAM DOOLITTLE, CLAIRE BERGER, RUI DONG, JAMES MEINDL, WALT DE HEER, Georgia Institute of Technology, GEORGIA INSTITUTE OF TECHNOLOGY TEAM — Electronic-quality graphene is epitaxially grown by graphitization of carbon-face silicon carbide (SiC) by the sublimation of silicon atoms from selected regions uncapped by aluminum nitride (AlN). AlN (deposited by molecular beam epitaxy) withstands high graphitization temperatures of 1420^{o}C, hence acting as an effective capping layer preventing the growth of graphene under it. The AlN is patterned and etched to open up windows onto the SiC surface for subsequent graphitization. Such selective epitaxial growth leads to the formation of high-quality graphene in desired patterns without the need for etching and lithographic patterning of graphene itself. No detrimental contact of the graphene with external chemicals occurs throughout the fabrication-process. The impact of process-conditions on the mobility of graphene is investigated. Graphene hall-bars were fabricated and characterized by scanning Raman spectroscopy, ellipsometry, and transport measurements. This controlled growth of graphene in selected regions represents a viable approach to fabrication of high-mobility graphene as the channel material for fast-switching field-effect transistors.

11:51AM J36.00004 Multi-Layer Epitaxial Graphene Formed from Poly-Crystalline Silicon Carbide Grown on C-Plane Sapphire[1] , TIMOTHY MCARDLE, JACK CHU, YU ZHU, ZIHONG LIU, MAHADEVAIYER KRISHNAN, CHRIS BRESLIN, CHRISTOS DIMITRAKOPOULOS, ROBERT WISNIEFF, ALFRED GRILL, IBM T. J. Watson Research Center, Yorktown Heights, NY — Growth of epitaxial graphene on substrates as large as eight inches in diameter is of great interest for integration with current CMOS technology. We use ultra-high vacuum chemical vapor deposition to grow poly-crystalline silicon carbide (SiC) on c-plane sapphire wafers, which are then annealed at high temperature in vacuum to create multi-layer epitaxial graphene films. Despite the roughness and small domain size of the poly-crystalline SiC films, a thick, conformal layer of graphene is formed. Reducing the surface roughness by chemical-mechanical polishing the SiC surface prior to the anneal results in a dramatic reduction of the Raman defect band observed in the final graphene film. Additionally, the graphene formed on polished SiC demonstrates significantly more ordered layer-by-layer graphene growth and increased carrier mobility for the same carrier density as the unpolished samples.

[1]This work is supported by DARPA under Contract FA8650-08-C-7838 through the CERA program.

12:03PM J36.00005 Theory of the Growth of Epitaxial Graphene on Silicon Carbide , FAN MING, ANDREW ZANGWILL, School of Physics, Georgia Institute of Technology, Atlanta, GA 30332 — We present a one-dimensional kinetic Monte Carlo model for the growth of epitaxial graphene on 6H-SiC. The model parameters are effective energy barriers for the nucleation and subsequent propagation of graphene at step edges. For growth on vicinal substrates with half-unit-cell height steps, we predict first and second layer graphene coverages and the distribution of first-layer graphene strip widths as a function of total coverage, vicinal angle, and the model parameters. Comparing our results to experiment will provide the first quantitative insights into the kinetics of growth for this unusual epitaxial system.

12:15PM J36.00006 A density-functional theory study for the mobility of carbon atoms on 6H SiC(0001) , CHRISTIAN RATSCH, UCLA — Graphene is a very promising material for many microelectronic applications because of its unique electronic properties. Among the several proposed routes to fabricate (single) layers of graphene, the growth of epitaxial graphene on 4H and 6H SiC(0001) appears to be particularly promising. The 6H SiC(0001) surface has 3 different polytypes. In this talk, results from density-functional theory calculations will be presented for the potential energy surfaces and different diffusion rates of C atoms on these different polytype surfaces. Both, the Si or C terminated surfaces will be investigated. Results for the adsorption of single and multiple graphene layers will also be presented.

12:27PM J36.00007 Epitaxial graphene on SiC(0001) , THOMAS SEYLLER, University of Erlangen-Nuremberg — Epitaxial graphene on SiC is considered to open a route towards graphene based electronics such as, e.g., high frequency transistors. Recently considerable progress has been made in the growth of epitaxial graphene on SiC. On the Si-face of SiC, where the growth is slower as compared to the C-face, monolayers can be grown reliably. However, several open questions remain. Transport studies as well es photoelectron spectroscopy has shown that the pristine layers on SiC(0001) are heavily electron doped ($n = 1 \times 10^{13}$ cm^{-1}). This results in rather low electron mobilities of the order of 2000 cm^2/Vs at 25 K. In addition, the carrier mobility shows a strong temperature dependence so that it drops to around 1000 cm^2/Vs at 300 K. In my presentation I will first show how chemical gating of graphene by deposition of F4TCNQ affects the carrier mobility. Hall effect measurements on samples close to charge neutrality show a carrier mobility of 29,000 cm^2/Vs at 25 K. Then I will discuss measurements demonstrating inertial-ballistic transport in nanoscale cross junctions fabricated from epitaxial graphene on SiC(0001). Finally, I will review recent results obtained by hydrogenation of the interface between graphene and SiC(0001). The latter process leads to a decoupling of the bufferlayer which is converted into quasi-freestanding graphene (QFMLG). The electronic, structural, and transport properties of QFMLG will be discussed in detail.

1:03PM J36.00008 Structural and Electronic Properties of Graphene on Cu(111) and SiC(0001) , LI GAO, PAOLO SESSI, JONGWEON CHO, JEFFREY R. GUEST, NATHAN P. GUISINGER, Center for Nanoscale Materials, Argonne National Laboratory — Graphene has shown attractive physical properties and is a promising new material. The structural and electronic properties of graphene on Cu(111) and SiC(0001) have been investigated by scanning tunneling microscopy and spectroscopy and Raman spectroscopy. The growth of graphene on these two substrates was achieved by thermal decomposition of ethylene on Cu(111) and thermal decomposition of SiC(0001) surface, respectively, in an ultra high vacuum chamber. On Cu(111), the nucleation of monolayer islands and two predominant domain orientations have been observed, which leads to the formation of numerous domain boundaries with increasing coverage [1]. Raman spectroscopy verifies the single layer thickness and shows the defect-induced bands for graphene on Cu(111). On SiC(0001), the electronic structure of the first two carbon layers on top of the $6\sqrt{3}$ surface reconstruction has been studied by scanning tunneling spectroscopy.

[1] L. Gao, J. R. Guest, and N. P. Guisinger, Nano Lett. 10, 3512 (2010).

1:15PM J36.00009 Wafer scale synthesis of bilayer graphene film[1] , KYUNGHOON LEE, SEUNGHYUN LEE, ZHAOHUI ZHONG, Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, MI 48109, USA — The discovery of electric field induced bandgap opening in bilayer graphene paves the way for making semiconducting graphene without aggressive size scaling, or using expensive substrates. Despite intensive research, synthesizing homogeneous bilayer graphene in large size has proven extremely challenging, and the size of bilayer graphene was limited to micrometer scale by exfoliation Here we demonstrate homogeneous bilayer graphene films over at least square inch area, synthesized by chemical vapor deposition on copper foil and subsequently transferred to arbitrary substrates. Bilayer coverage of over 99% is confirmed by spatially resolved Raman spectroscopy. The result is further supported by electrical transport measurements on bilayer graphene transistors with dual-gate configuration, where field induced bandgap opening is observed in 98% of the devices. The size of our bilayer graphene film is only limited by the synthesis apparatus and can be readily scaled up, thus enabling wafer scale graphene electronics and photonics.

[1]Authors Kyung-Hoon Lee and Seunghyun Lee contributed equally to this work.

1:27PM J36.00010 Visualizing graphene grown by chemical vapor deposition on metal substrates at the atomic scale , LIUYAN ZHAO, KWANG RIM, CHRISTOPHER GUTIERREZ, RUI HE, KEUNSOO KIM, HUI ZHOU, TONY HEINZ, PHILIP KIM, ARON PINCZUK, GEORGE FLYNN, ABHAY PASUPATHY, Columbia University — We present an atomic-scale scanning tunneling microscopy (STM) study of large-area graphene films grown by chemical vapor deposition (CVD) on metal substrates. We will first describe experiments where pristine graphene is grown in UHV conditions on single crystal Cu(111) and Cu(100) surfaces. We will compare this with graphene grown on copper foils and thin films in a typical low-pressure tube furnace. We will describe the effect of substrate quality and orientation on the quality and electronic structure of the graphene film produced. Finally, we will describe experiments where the graphene film is doped by nitrogen during growth. We will describe the bonding environment and the local electronic structure caused by the incorporation of nitrogen atoms into the graphene lattice.

1:39PM J36.00011 Graphene Growth and Defects on Ni(111) , MATTHIAS BATZILL, University of South Florida, JAYEETA LAHIRI — Using scanning tunneling microscopy (STM) and Auger electron spectroscopy (AES) we have investigated the growth of graphene on Ni(111) surfaces by carbon segregation from the bulk. We reveal two distinct growth modes for graphene growth. Between 480 and 650 C graphene forms on clean Ni(111) and below 480 C graphene grows by an in-plane conversion of a surface carbide phase. This is the first time that graphene formation is observed by transformation of a surface carbide. STM indicates that a lattice-matched, one-dimensional in-plane domain boundary between graphene and the carbide forms and graphene grows by replacing Ni-atoms with carbon at this interface. In addition to the growth of graphene we will also briefly discuss atomic-scale defects that can be synthesized in Ni-supported graphene. In particular we emphasize the formation of an extended line-defect with metallic properties [1].

[1] J. Lahiri, Y. Lin, P. Bozkurt, I.I. Oleynik, M. Batzill Nature Nanotechnol. 5, 326 (2010).

1:51PM J36.00012 Atomic Structures and Electronic Scattering of Graphene Edges , JIFA TIAN, HELIN CAO, Department of Physics, Purdue University, JONGWEON CHO, LI GAO, JEFFREY R. GUEST, NATHAN P. GUISINGER, Center for Nanoscale Materials, Argonne National Laboratory, WEI WU, QINGKAI YU, Center for Advanced Materials, University of Houston, YONG P. CHEN, Department of Physics, Purdue University — The success of growing monolayer gaphene on Cu foils has stimulated intense interests to study its structural and electronic properties at the atomic scale. Here we present a scanning tunneling microscopy (STM) investigation on single crystalline graphene islands synthesized on polycrystalline Cu foils by chemical vapor deposition (CVD). Our studies reveal that most of the graphene edges are macroscopically parallel to the zigzag directions with microscopic roughness. The observed rough edges follow the zigzag directions at atomic scale and make many 120-degree turns. Strong electron scattering was observed from a rarely-occurring armchair-oriented edge, and there is little such scattering observed from zigzag-oriented edges. In addition, we also observed nearly periodic parallel lines attributed to the surface dislocations of the Cu underneath graphene.

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J37 DMP: Focus Session: Graphene Growth, Characterization, and Devices: Surface Studies C146

11:15AM J37.00001 Scanning Tunneling Microscopy of Graphene on a Boron Nitride Substrate , YANG WANG, Dept. of Physics at U.C. Berkeley, REGIS DECKER, VICTOR BRAR, Dept. of Physics at U.C. Berkeley / Lawrence Berkeley National Lab, WILLIAM REGAN, HSIN-ZON TSAI, QIONG WU, Dept. of Physics at U.C. Berkeley, ALEX ZETTL, MICHAEL CROMMIE, Dept. of Physics at U.C. Berkeley / Lawrence Berkeley National Lab — Graphene placed on a boron nitride (BN) substrate has been shown to result in increased mobility and improved Quantum Hall measurements.[1] It is therefore of great interest to understand how BN substrates differently influence graphene compared to more standard SiO_2 substrates. I will present new scanning tunneling microscopy measurements of graphene placed on a BN substrate. Differences in the local behavior of graphene on a BN substrate versus a SiO_2 substrate will be discussed.

[1]Dean, CR *et al.* Boron nitride substrates for high-quality graphene electronics. *Nature Nanotechnology* **5**, 722-726 (2010)

11:27AM J37.00002 STM study of graphene on boron nitride , JIAMIN XUE, Department of Physics, University of Arizona, Tucson, Arizona 85721, USA, DANNY BULMASH, JAVIER SANCHEZ-YAMAGISHI, Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA, K. WATANABE, T. TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan, PABLO JARILLO-HERRERO, Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA, B.J. LEROY, Department of Physics, University of Arizona, Tucson, Arizona 85721, USA — We have performed low-temperature STM topographic and spectroscopic measurements of graphene on h-BN. We found that the topographic variations are reduced as compared to graphene on SiO2. We also performed scanning tunneling spectroscopy measurements to study the spatial variation of the Dirac point. We will present our latest results on the topographic and spectroscopic features for graphene on h-BN and compare them with similar measurements for graphene on SiO2.

11:39AM J37.00003 Atomic-Scale Topographic and Electronic Structure of Graphene Films on Ultraflat Insulating Materials , CHRISTOPHER GUTIERREZ, LIUYAN ZHAO, FERESHTE GHAHARI, CORY DEAN, KWANG RIM, JAMES HONE, GEORGE FLYNN, PHILIP KIM, ABHAY PASUPATHY, Columbia University — Graphene, a unique two-dimensional material, has attracted much attention for its exotic electronic properties. But owing to its nature as a single monolayer, many of these interesting properties depend heavily on the substrate on which the graphene rests. Scanning tunneling microscope (STM) experiments offer the unique ability to investigate the effect of the substrate on the surface roughness (via topography maps) as well as the local electronic properties (via spectroscopy maps) of graphene. In this talk we will present such experimental results of graphene on atomically flat insulating substrates such as mica and boron nitride, as well as suspended graphene sheets. We will describe experiments performed both on exfoliated graphene flakes as well as large-area graphene films grown by chemical vapor deposition (CVD).

11:51AM J37.00004 Structural and electronic properties of epitaxial graphene on SiC(0001): Growth, transfer doping and atomic intercalation , ULRICH STARKE, Max-Planck-Institut fur Festkorperforschung, Stuttgart, Germany — Epitaxial graphene on SiC(0001) promises a scalable graphene technology. Growth methods and experimental techniques for layer counting will be reviewed. The graphene layers are n-doped due to the influence of a covalently bonded carbon interface layer. This doping level can be precisely tailored and completely neutralized by functionalizing the graphene surfaces with electronegative molecules. In particular the Fermi level can be shifted into the band gap of bilayer graphene. The influence of the interface can be completely eliminated by hydrogen intercalation. Hydrogen migrates under the interface layer, passivates the underlying SiC layer and decouples the graphene from the substrate. The interface layer alone transforms into a quasi-free standing monolayer and epitaxial monolayer graphene turns into a decoupled bilayer. By intercalation of Germanium the graphene layers can also be decoupled. In this process both p- and n-doping can be obtained, depending on the amount of Ge intercalated. Both phases can be prepared simultaneously on the surface, so that lateral p-n junctions can be envisioned.

12:27PM J37.00005 Scanning Tunneling Spectroscopy of Suspended Graphene in the Quantum Hall Regime , NIKOLAI N. KLIMOV, Maryland NanoCenter, UMD / CNST, PML, NIST, MD, SUYONG JUNG, Maryland NanoCenter, UMD / CNST, NIST, MD, GREGORY M. RUTTER, NIKOLAI B. ZHITENEV, CNST, NIST, Gaithersburg, MD, DAVID B. NEWELL, PML, NIST, Gaithersburg, MD, JOSEPH A. STROSCIO, CNST, NIST, Gaithersburg, MD — The discovery of graphene, a unique two-dimensional electron system with extraordinary physical properties, has ignited tremendous research activity in both science and technology. Graphene interactions with a substrate such as, for example, SiO_2/Si are known to strongly limit the electrical performance of graphene devices. Suspended graphene devices, where interaction with substrates can be strongly reduced, have been studied by macroscopic transport measurements and shown to have a 10-fold increase in mobility. However, a detailed investigation on a microscopic scale is still missing. In this talk we present a scanning probe microscopy (SPM) study of a free-standing graphene membrane. The device was fabricated from a graphene flake exfoliated over an array of 1μm holes etched in SiO_2/Si substrate. Electronic spectra of both suspended and supported regions of single-layer graphene can be probed using SPM in a perpendicular magnetic field and in varying back gate voltages applied to the Si substrate. The significant differences found in electronic spectra of suspended and non-suspended graphene will be discussed.

12:39PM J37.00006 Quantized Landau level spectrum and its density dependence in graphene supported by SiO_2[1] , ADINA LUICAN, GUOHONG LI, EVA ANDREI, Department of Physics and Astronomy, Rutgers University, DEPARTMENT OF PHYSICS AND ASTRONOMY, RUTGERS UNIVERSITY TEAM — Scanning tunneling microscopy and spectroscopy in magnetic field was used to study Landau quantization in graphene and its dependence on charge carrier density. Measurements were carried out on exfoliated graphene samples deposited on a chlorinated thermal SiO_2 which allowed observing the Landau level sequence characteristic of single layer graphene while tuning the carrier density through the Si back-gate. Upon changing the carrier density we find abrupt jumps in the Fermi level after each Landau level is filled. Moreover, at low doping levels a marked increase in the Fermi velocity is observed which is consistent with the logarithmic divergence expected due to the onset of many body effects close to the Dirac point.

[1]Work supported by DOE under DE-FG02-99ER45742, partial NSF under NSF-DMR-0906711 and Lucent

12:51PM J37.00007 The effect of the tip in scanning tunneling spectroscopy of graphene Landau levels[1] , KEVIN KUBISTA, DAVID MILLER, MING RUAN, WALT DE HEER, PHILLIP FIRST, Georgia Institute of Technology, GREGORY RUTTER, JOSEPH STROSCIO, NIST-Gaithersburg — Landau Level (LL) spectroscopy measurements were performed on multilayer epitaxial graphene using 4 K scanning tunneling spectroscopy in magnetic fields up to 8 T. Fits of the LL energies to the form expected for graphene show a slight difference in the Fermi velocity of hole and electron states. We show that this may be a consequence of the work function difference between graphene and the tip material (iridium). Data sets consisting of LL energies versus magnetic field are used to fit a model tip potential. The calculated spectrum of tip-perturbed LLs reveals the possible source of some "extra" peaks.

[1]Supported in part by NSF and NRI-INDEX

1:03PM J37.00008 Scanning tunneling spectroscopy of adsorbates and vacancies on graphene , JYOTI KATOCH, MASA ISHIGAMI, Department of Physics and Nanoscience Technology Center, University of Central Florida, Orlando, FL 32816 — Adsorbates and vacancies sensitively influence transport properties of graphene. We have investigated the impact of adsorbates, such as atomic hydrogen and potassium, and vacancy defects on electronic properties of graphene at atomic scale using scanning tunneling microscopy and spectroscopy Our results will be discussed in comparison with previous transport measurements to understand the effect of extrinsic disorder on transport properties of graphene.

1:15PM J37.00009 A Scanning Tunneling Microscopy and Spectroscopy Study of K-doped Graphene , JEONGHOON HA, HONGWOO BAEK, BEOMYONG HWANG, MINJUN LEE, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea, JUNGSEOK CHAE, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA, YOUNG KUK, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea — Understanding the role of impurity scattering is crucial in explaining the carrier transport phenomena in a graphene device. Although unique two-dimensional Dirac fermion behavior have been confirmed by many transport experiments, direct observation of the local electronic structure around impurities may provide detailed picture of carrier scattering. In this study the local electronic structure of potassium deposited graphene film were studied using scanning tunneling microscopy (STM) and spectroscopy (STS). Chemical vapor deposition (CVD) graphene were transferred on a SiO_2 substrate after confirming the thickness and flatness by Raman spectroscopy and atomic force microscopy. STM images show relatively long-range screening around K impurities and the spatially resolved STS revealed unique electronic structure within the screening range. It was found that the screen range varies with the applied back gate bias, suggesting carrier density dependence.

1:27PM J37.00010 Scanning Tunneling Microscopy Study of Fluorinated Graphene on Copper , SCOTT SCHMUCKER, JOSHUA WOOD, RICK HAASCH, JOSEPH LYDING, University of Illinois at Urbana-Champaign — We probe by ultrahigh vacuum scanning tunneling microscopy (UHV-STM) the structural and electronic properties of monolayer fluorinated graphene (C_xF, $x \approx 4$) synthesized by chemical vapor deposition on copper substrates and fluorinated by xenon difluoride gas [1]. The chemical composition and structure of the resulting film is probed by x-ray photoelectron spectroscopy (XPS), Raman spectroscopy, and scanning tunneling spectroscopy (STS). In contrast to metallic graphene, this material exhibits a large (>3 eV) band gap with a muted gap state corresponding to a copper surface state near -0.4 eV. We further investigate by STM alignment between the fluorographenic surface layer and copper substrate, uniformity of fluorination, and stability of fluorinated graphene under electron bombardment and thermal annealing.

[1] J.T. Robinson, et al., Nano Lett. 10, 3001-2005 (2010)

1:39PM J37.00011 Scanning tunneling spectroscopy of chemical vapor deposition grown graphene , DANIEL CORMODE, COLLIN REYNOLDS, BRIAN LEROY, University of Arizona — The electronic properties of CVD grown graphene were investigated by scanning tunneling microscopy. Mono and multi layered samples were prepared by growth on copper and transferred to 300 nm SiO_2 substrates. Raman spectroscopy mapping was used to determine the thickness of the samples as well as characterize regions of higher disorder as evidenced by an increased D peak. The samples were then measured in ultra high vacuum by scanning tunneling spectroscopy at 5 K. The type and density of defects measured with the STM were compared with measured D peak intensity. We have examined the correlation between changes in the local density of states and disorder in monolayer graphene.

1:51PM J37.00012 Directed Assembly of Iron Phthalocyanine and Pentacene Molecules on a Graphene Monolayer Grown on Ru(0001) , SHIXUAN DU, Institute of Physics, CAS, PR China, H.G. ZHANG, J.T. SUN, L.Z. ZHANG, Q. LIU, J.H. MAO, Y. PAN, M. GAO, H.T. ZOU, H.M. GUO, W.A. HOFER, H.-J. GAO, INSTITUTE OF PHYSICS, CHINESE ACADEMY OF SCIENCES, PR CHINA TEAM, SURFACE SCIENCE RESEARCH CENTRE, UNIVERSITY OF LIVERPOOL, UK COLLABORATION — Monolayer graphene was successfully fabricated on 4*d*transition metal surfaces. The resulting ordered Moiré pattern was found to be an ideal template for the formation of ordered nanoclusters and molecules. Using scanning tunneling microscopy we show the selective adsorption process and assembly of iron phthalocyanine and pentacene molecules with different structural symmetries on a graphene monolayer, epitaxially grown on Ru(0001). The combination of first principles calculations and experimental measurements suggests that the lateral dipole field is the main driving mechanism for assembling molecules into ordered arrays. These findings should be important for achieving a large scale well-defined molecule-graphene interface. And such a detailed understanding of the molecular assembly will be essential in the actual fabrication process.

2:03PM J37.00013 Ab initio scanning tunneling spectroscopy simulation of graphene with metal adatoms: weak and strong coupling regimes[1] , GUNN KIM, Department of Physics, Kyung Hee University, Korea, JAE-HYEON PARQ, JAEJUN YU, Department of Physics & Astronomy, Seoul National University, Korea, YOUNG-KYUN KWON, Department of Physics, Kyung Hee University, KYUNG HEE UNIVERSITY COLLABORATION, SEOUL NATIONAL UNIVERSITY COLLABORATION — Metal atoms on graphene, when ionized, can act as a point-charge impurity to probe a charge response of graphene with the Dirac cone band structure. To understand charge and spin polarization in graphene, we present scanning tunneling spectroscopy STS simulations based on density-functional theory calculations. We find that a Cs atom on graphene is fully ionized with a significant band-bending feature in the STS whereas the charge and magnetic states of Ba and La atoms on graphene appear to be complicated due to orbital hybridization and Coulomb interaction. By applying external electric field, we observe changes in charge donations and spin magnetic moments of the metal adsorbates on graphene.

[1]This work was supported by the National Research Foundation of Korea through the ARP (Grant No. R17-2008-033- 01000-0) (J.Y.) and the Basic Science Research Program through the NRF of Korea (Grant No. 2010-0007805) (G.K.).

Tuesday, March 22, 2011 11:15AM - 1:39PM –

Session J38 DCP: Focus Session: Ultrafast Dynamics and Imaging II A130/131

11:15AM J38.00001 Probing Ultrafast Solution-Phase Chemistry in the X-ray Water Window and beyond via Soft X-ray Spectroscopy[1] , NILS HUSE[2], Chemical Sciences Division, Lawrence Berkeley National Laboratory — A prerequisite for a microscopic understanding of chemical reactions is knowledge of the ultrafast interplay of valence charge distributions, spin states, and nuclear degrees of freedom. These degrees of freedom are often intricately coupled, leading to very complex dynamics. Femtosecond core-level spectroscopy is very well suited to study such dynamics via x-ray absorption near-edge structure (for information on changes in valence charge distribution / spin-state) and via the extended x-ray absorption fine structure (for information in nuclear arrangements) due to the very localized nature of the initial states of well-defined symmetry and the high chemical specificity of core-level excitations. We have employed femtosecond core-level spectroscopy to study metal-ligand interactions in solvated transition metal complexes as an important class of model systems to demonstrate the feasibility and merit of ultrafast solution-phase soft X-ray spectroscopy.[3,4] Laser-induced charge transfer reactions on sub-100 fs time scales trigger structural dynamics in first-row transition-metal complexes that display multiple spin-state changes within 300 fs upon photo-excitation. The combined analysis of vibrational, optical, and core-level spectroscopy reveals a complex interplay of nuclear, electronic, and spin degrees of freedom in these systems that leads to detailed insights into the underlying reaction mechanisms. These are prototypical in nature for a variety of organometallic systems. The chemical specificity of core-level spectroscopy is exploited by probing metal-centered transitions to elucidate the "metallic view." We have very recently succeeded in also following the "ligand view" via soft X-ray spectroscopy in the X-ray water window. The later experiment has far-reaching consequences as it demonstrates the feasibility of studying ultrafast processes and short-lived species of solvated organic compounds via Nitrogen K-edge spectroscopy to deliver a detailed picture of the evolving valence charge density in chemical reactions.

[1]This work was supported by the Department of Energy under Contract No. DE-AC02-05CH11231.

[2]Co-authors: H. Cho, K. Hong, L. Jamula, F. M. F. de Groot, T. K. Kim, J. K. McCusker, and R. W. Schoenlein

[3]N. Huse, T. K. Kim, L. Jamula, J. K. McCusker, F. M. F. de Groot, R. W. Schoenlein, *J. Am. Chem. Soc.*, **132**, 6809.

[4]H. Wen, N. Huse, R. W. Schoenlein, A. M. Lindenberg, *J. Chem. Phys.*, **131**, 234505.

11:51AM J38.00002 Ultrafast Dynamics in Helium Nanodroplets Probed by Femtosecond Time-Resolved EUV Photoelectron and Ion Imaging , OLEG KORNILOV, Max-Born-Institut, OLIVER BÜNERMANN, Georg-August-University, ALI EFTEKHARI-BAFROOEI, Lawrence Berkeley National Laboratory, STEPHEN R. LEONE, DANIEL M. NEUMARK, University of California-Berkeley, OLIVER GESSNER, Lawrence Berkeley National Laboratory — Femtosecond time-resolved EUV photoelectron and ion imaging are employed to study the relaxation dynamics of electronically excited helium nanodroplets. Excitation into a broad droplet absorption band ($\sim$23.8 eV) is followed by ionization with a delayed IR pulse. The transient photoelectron spectra and angular distributions indicate that electronically excited helium atoms are predominantly emitted in either an aligned 1s4p Rydberg state within less than $\sim$100 fs or in a non-aligned 1s3d state within $\sim$200 fs. The transient ion imaging results suggest that different Rydberg atoms are emitted with significantly different kinetic energy distributions that closely resemble Maxwell-Boltzmann distributions with temperatures of 2700 K (1s3d) and 490 K (1s4p). The results are interpreted in terms of a dynamic model that is based on the local density dependent blue shift of atomic Rydberg states in the droplet environment.

12:03PM J38.00003 "Molecular spectrometers" in the condensed phase: local THz-FIR response from femtosecond fluorescence , NIKOLAUS ERNSTING, Humboldt University Berlin — We examine dye molecules whose color depends on the polarity of the environment. Following fast optical excitation, their fluorescence band typically red-shifts by 0.5 eV on femtosecond to nanosecond time scales. This "dynamic Stokes shift" reflects the joint molecular and environmental reorganisation of the system. Solvation dynamics has been studied for decades in the hope that the dynamics of the environment itself can be extracted. We contribute with two research lines: (1) development of rigid polar solvation probes whose vibrational response is removed from that of water, for example, and (2) fluorescence techniques which measure the dynamic Stokes shifts more precisely. Two results will be shown. The frequency-dependent permittivity $\varepsilon(\omega)$ of water surrounding N-Methyl-6-Quinolone is extracted up to about 100 cm^{-1} from the time-resolved fluorescence shift R(t). The key consists in an analytical connection $\varepsilon(\omega) \quad \rightarrow$ R(t) which is needed for data fitting. Measurements with the cryoprotectant disaccharide trehalose in water serve to establish the method. Its unique feature is locality, *i.e.* the possibility to measure $\varepsilon(\omega)$ around a supramolecular structure with a covalently connected or embedded probe. THz vibrational activity of a biopolymer is thus measured locally, on the effective length scale for polar solvation, with an embedded molecular probe. For this purpose 2-hydroxy-7-nitro-fluorene was linked into a 13mer duplex opposite an abasic site. The NMR solution structure shows that the fluorene moiety occupies a well-defined position in place of a base-pair. The dynamic Stokes shifts for solution in H_2O and D_2O are quantified. Their difference is much larger than expected for free water, suggesting that only bound water is observed. A weak 26 cm^{-1} spectral oscillation of the emission band is observed which is not present when the probe is free in solution, and is therefore caused by the supramolecular structure (DNA and hydration water).

12:39PM J38.00004 Tunable acoustic terahertz generation in InGaN quantum wells effected by metal nanocrystals , MEG MAHAT, ANTONIO LIOPIS, Department of Physics, University of North Texas, Denton, TX, 76201,USA, SERGIO PERIERA, CICECO, University of Aveiro, 3810-193 Aveiro, Portugal, IAN WATSON, Institutes of Photonics, SUPA, University of Strathclyde, Glasgow, G4NW, UK, TAE CHOI, Departments of Mechanical Engineering, University of North Texas, Denton, TX, 76203, USA, ARKADII KROKHIN, ARUP NEOGI, Department of Physics, University of North Texas, Denton, TX, 76201,USA — The strained semiconductor multiple quantum wells have the capability to generate acoustic terahertz emission via coherent acoustic phonon oscillations. The frequency of the THz emission is usually limited by the periodicity of the quantum wells or superlattice structures. We propose a novel technique to modify the frequency and amplitude of THz oscillations by the inclusion of the metal nanocrystals (NCs) within InGaN/GaN multiple quantum wells via the self-assembled inverted hexagonal pits. Time resolved differential transmission measurements demonstrate a four-five folds decrease in the THz frequency under band edge excitation conditions. A theoretical model predicts a strong dependence of the amplitude and period of the oscillations on the radius of the metal NCs.

12:51PM J38.00005 "Making the Molecular Movie": First Frames , R.J. DWAYNE MILLER, Max Planck Research Group for Atomically Resolved Dynamics, University of Hamburg, CFEL/DESY and University of Toronto — Femtosecond Electron Diffraction has enabled atomic resolution to structural changes as they occur, essentially watching atoms move in real time–directly observe transition states. This experiment has been referred to as "making the molecular movie" and has been previously discussed in the context of a gedanken experiment. With the recent development of femtosecond electron pulses with sufficient number density to execute single shot structure determinations, this experiment has been finally realized. A new concept in electron pulse generation was developed based on a solution to the N-body electron propagation problem involving up to 10,000 interacting electrons that has led to a new generation of extremely bright electron pulsed sources that minimizes space charge broadening effects. Previously thought intractable problems of determining t=0 and fully characterizing electron pulses on the femtosecond time scale have now been solved through the use of the laser pondermotive potential to provide a time dependent scattering source. Synchronization of electron probe and laser excitation pulses is now possible with an accuracy of 10 femtoseconds to follow even the fastest nuclear motions. The camera for the "molecular movie" is well in hand based on high bunch charge electron sources. Several movies depicting atomic motions during passage through structural transitions will be shown. Atomic level views of the simplest possible structural transition, melting, will be presented for a number of systems in which both thermal and purely electronically driven atomic displacements can be correlated to the degree of directional bonding. Optical manipulation of charge distributions and effects on interatomic forces/bonding can be directly observed through the ensuing atomic motions. New phenomena involving strongly correlated electron systems will be presented in which an exceptionally cooperative phase transitions has been observed. The primitive origin of molecular cooperativity has also been discovered in recent studies of molecular crystals. These new developments will be discussed in the context of developing the necessary technology to directly observe the structure-function correlation in biomolecules–the fundamental molecular basis of biological systems.

1:27PM J38.00006 Two-dimensional dynamical reconstruction of the valence exciton in LiF[1] , XIAOQIAN M. CHEN, YU GAN, PETER ABBAMONTE, University of Illinois at Urbana-Champaign, CHEN-LIN YEH, Tamkang University, Taiwan, DIEGO M. CASA, Argonne National Laboratory, WEI KU, Brookhaven National Laboratory — The structure and dynamics of excitons are interesting because excitons are model many-body excitations with technological relevance, e.g. to the behavior of photocells. In a previous study, we used inelastic X-ray scattering, together with inversion techniques, to reconstruct one-dimensional projection images of exciton propagation in LiF in real space and time, and showed that the exciton in LiF is of the Frenkel type. Here we generalize our previous work to a two dimensional plane in LiF. Our new images of exciton propagation show intricate shape changes arising from scattering off of the crystal lattice. Our results are compared to model Wannier function calculations for a more detailed test of the Frenkel model.

[1]This work was supported by the U.S. Department of Energy under grants DE-FG02-07ER46459 and DE-FG02-07ER46453.

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J39 DBP: Physics of Proteins III: Folding, Structure and Stability A124/127

11:15AM J39.00001 The Speed Limit of Protein Folding: Alpha-Helix Initiation Modeled and Observed[1] , MILO LIN, OMAR MOHAMMED, AHMED ZEWAIL[2], Physical Biology Center for Ultrafast Science and Technology, California Institute of Technology — As a primary event of protein folding, alpha-helix initiation is the starting point of macromolecular complexity. In this work, an analytic coarse-grained model which predicts the initiation rate as a function of temperature, is presented. Helix initiation was measured via ultrafast temperature-jump fluorescence refolding experiments on two penta-peptides, and the measured rates agreed well with those of the model. In addition, the temporal separation of rate-limiting diffusion from fast annealing stipulated by the model was confirmed via ensemble-converging all-atom molecular dynamics simulations, which reproduced both the diffusion and the picosecond annealing processes and rates observed experimentally. Some of these results were published in: Mohammed OF, Jas GS, Lin MM, Ma H, Zewail AH (2009) Primary peptide folding dynamics observed with ultrafast temperature jump. Angew Chem 48: 5628-5632.

[1]We are grateful to the National Science Foundation and the National Institutes of Health for funding of this research at Caltech. M.M.L. acknowledges financial support from the Krell Institute and the US Department of Energy for a graduate fellowship.
[2]principal investigator

11:27AM J39.00002 Protein folding microenvironments within the cytoplasm of living cells , MINGHAO GUO, APRATIM DHAR, MARTIN GRUEBELE, University of Illinois at Urbana-Champaign — The protein folding kinetics in a living cell strongly depends on the local environment. Viscosity of cytoplasm and crowding by macromolecules modulate stability, folding rates and folding mechanism in the folding progresses. We use Fast Relaxation Imaging (FRel) to map out the stability and folding kinetics of a FRET-labeled phosphoglycerate kinase (PGK) in the cytoplasm of individual eukaryotic cells with 500 nm spatial resolution. It shows that this modulation results in large variation of folding mechanism compared to in vitro experiment. We have developed the folding-diffusion model of protein folding in cell with hetergenous microenvironment, which includes spatial hetergenous of folding rates of the multiple-state folding of PGK and diffusion between pixels. It is shown that diffusion contributes little to the large variation of folding kinetics, which can only result from the change of folding mechanism due to microenvironment.

11:39AM J39.00003 First step in folding of nonconstitutive membrane proteins: spontaneous insertion of a polypeptide into a lipid bilayer and formation of helical structure[1] , YANA RESHETNYAK, ALEXANDER KARABADZHAK, DHAMMIKA WEERAKKODY, Physics, URI, DONALD ENGELMAN, Yale Univ., VLADISLAV MARKIN, Univ of Texas Southwestern Med School, OLEG ANDREEV, Physics, URI — There are two questions we would like to address: 1) what is the molecular mechanism of a polypeptide insertion into a lipid bilayer and formation of transmembrane helix? 2) Are there any transient changes of a lipid bilayer in process of a polypeptide insertion and folding? As a convenient system we are studying pHLIP (pH (Low) Insertion Peptide) insertion into a membrane and folding, which is modulated by pH. The insertion of pHLIP occurs with rapid (0.1 sec) interfacial helix formation followed by a much slower (100 sec) insertion pathway to form a transmembrane helix. The reverse process of unfolding and peptide exit from the bilayer core proceeds much faster than folding/insertion and through different intermediate states. Our kinetic studies with pHLIP variants indicate that insertion can occur 100 times faster and with less number of intermediate states. To study changes, which might occur with a lipid bilayer in a process of peptide insertion and folding, we employed stopped-flow SAXS.

[1]Supported by grant from the NIH RO1133890 to OAA, DME, YRK

11:51AM J39.00004 Protein barrel fluctuations and the barrel permeability: A comparison between Green and Red Fluorescent proteins , CHOLA REGMI, PREM CHAPAGAIN, BERNARD GERSTMAN, Department of Physics, Florida International University, THEORETICAL BIOPHYSICS TEAM — As compared to the Green Fluorescent Proteins (GFP), the monomeric variants of the Red Fluorescent Proteins (RFP), also known as mFruits, are substantially less photostable, possibly due to the barrel permeability for molecular oxygen into the protein barrel. We performed molecular dynamics simulations to compare the protein barrel fluctuations of the GFP as well as a monomeric variant of the RFP. We also performed implicit ligand sampling for uncovering the pathways for molecular oxygen entry into the barrels. We found that, as compared to the GFP barrel, the RFP barrel has significantly larger structural fluctuations and these large barrel fluctuations lead to clear pathways through which molecular oxygen or other ions can enter the barrel more easily.

12:03PM J39.00005 Heterogeneous helical propensity and its effects on dimerization and the stability of a model protein dimer , YUBA BHANDARI, PREM CHAPAGAIN, BERNARD GERSTMAN, Department of Physics, Florida International University, THEORETICAL BIOPHYSICS TEAM — We will present the results of Monte Carlo simulations of the dimerization and unfolding of a helical protein dimer. Using a three dimensional lattice model, we investigate the role of including sections of amino acids with strong alpha-helix propensity at different locations along the helices on the dimerization kinetics and the dimer stability. Specifically, we focus on the rate limiting steps in both folding and unfolding processes. We find that these processes can be optimized by tuning the ease of access through diffusion to the metastable intermediate state and its stability. The kinetics and thermodynamical stability is tuned by a combination of the locations of the amino acids with the high helical propensity and the salt bridges.

12:15PM J39.00006 Protein-like folding and free energy landscape of a homopolymer chain[1] , MARK TAYLOR, Dept. of Physics, Hiram College, Hiram, OH, WOLFGANG PAUL, Martin-Luther-Universitat, Halle, Germany, KURT BINDER, Johannes-Gutenberg-Universitat, Mainz, Germany — Many small proteins fold via a first-order "all-or-none" transition directly from an expanded coil to a compact native state. We have recently reported an analogous direct coil-to-crystallite transition for a flexible homopolymer [1]. Wang-Landau sampling was used to construct the 1D density of states for square-well chains up to length 256 and a microcanonical analysis shows that for short-range interactions the usual polymer collapse transition is preempted by a direct freezing transition. A 2D configurational probability landscape, built via multi-canonical sampling, reveals a dominant folding pathway and an inherent configurational barrier to folding. Despite the non-unique homopolymer ground state, the thermodynamics of this direct freezing transition are identical to those of two-state protein folding. Homopolymer folding proceeds over a free energy barrier via a transition state folding nucleus, displays a protein-like Chevron plot, and satisfies the van't Hoff two-state criterion.

[1] Phys. Rev. E 79, 050801(R) (2009); J. Chem. Phys. 131, 114907 (2009).

[1]Funding: NSF DMR-0804370, DFG SFB-625/A3

12:27PM J39.00007 Unfolding Kinetics of Egg Protein , DIPTI SHARMA, UML — This study explores denaturing kinetics of egg white using high resolution calorimetric technique. Fresh egg was scanned fro heating and cooling to see the thermodynamics 10° C to 100° C at different heating ramp rates varying from 1 to 20° C/min. An endothermic peak was found on heating scan showing denaturing of protein which was found absent at the cooling indicating the absence of any residue after heating. The denature peak shifted towards higher temperature as ramp rate increases following Arrhenius behavior and shows an activated denaturing kinetics of the egg protein. This peak was also compared with the water to avoid water effects. Behavior of denaturing peak can be explained in terms of Arrhenius theory.

12:39PM J39.00008 Probing the dynamics of biomolecules in liquid water by terahertz spectroscopy[1] , NGUYEN VINH, JIM ALLEN, Physics Department, UCSB, KEVIN PLAXCO, Department of Chemistry and Biochemistry, UCSB — Decades of molecular dynamics and normal mode calculations suggest that proteins are rife with collective vibrational modes with ps to ns time constants. Given that proteins are "decorated" with charged groups, these motions should lead to oscillating dipoles that, in turn, will lead to strong gigahertz to terahertz absorption. Investigation of these harmonic motions by absorption spectroscopy, however, is extremely challenging due to the strong absorption of water. In response, we have developed a sensitive Vector Network Analyzer based spectrometer that operates from 65 to 700 GHz and can measure both the absorbance and refractive index of protein solutions. In order to extract the complex dielectric response of the protein in solution we employ an effective medium approximation for the mixture of the protein and aqueous buffer. The extracted dielectric response suggests that each protein molecule is surrounded by a tightly held layer of 164 +/- 5 water molecules that behave as if they are an integral part of the protein. The size of this hydration shell and the dielectric response of the solvated protein are all independent of protein concentration. Our measured dielectric response, however, does not agree with published computation models of the protein: the measurements indicate a low frequency cutoff in the density of modes of $\sim$250 GHz.

[1]Supported by W.M. Keck Foundation.

12:51PM J39.00009 MD-simulations of Beta-Amyloid Protein Insertion Efficiency and Kinetics into Neuronal Membrane Mimics , LIMING QIU, CREIGHTON BUIE, MARK VAUGHN, KWAN CHENG, Texas Tech University — Early interaction events of beta-amyloid (Aβ) peptides with the neuronal membranes play a key role in the pathogenesis of Alzheimer's disease. We have used all-atom MD simulations to study the protein insertion efficiency and kinetics of monomeric Aβ_{40} and Aβ_{42} into phosphatidylcholine lipid bilayers (PC) with and without 40 mole% cholesterol (CHOL) that mimic the cholesterol-enriched and depleted lipid nanodomains of the neuronal plasma membranes. Independent replicates of 200-ns simulations of each protein pre-inserted in the upper lipid layer were generated. In PC bilayers, only 25% of Aβ_{40} and 50% of Aβ_{42} in the replicates showed complete insertion into the lower lipid layer, whereas the percentages increased to 50% and 100%, respectively, in PC/CHOL bilayers, providing evidence that cholesterol improves the protein insertion efficiency into the bilayers. The rate of protein insertion was proportional to the hydrophobic, transmembrane helix length of the inserted peptide and depended on the cholesterol content. We propose that the lysine snorkeling and C-terminus anchoring of Aβ to the PC headgroups at the upper and lower lipid/water interfaces represent the dual-transmembrane stabilization mechanisms of Aβ in the neuronal membrane domains.

1:03PM J39.00010 Characterization of Polyethylene Glycol Modified Hemoglobins , GIL SALAZAR, JAMES BARR, WAYNE MORGAN, LI MA, Physics Department Georgia Southern University — Polyethylene glycol modified hemoglobins (PEGHbs) was characterized by liquid chromatography and fluorescence methods. We prepared four samples of two different molecular weight PEG, 5KDa and 20KDa, modified bovine and human hemoglobin. We studied the oxygen affinities, stabilities, and peroxidase activities of PEGHbs. We have related oxygen affinities with different degrees of modifications. The data showed that the modification on the beta subunits was less stable than that of the alpha subunits on the human Hb based samples especially. We also compared peroxidase activities among different modified PEGHbs.

1:15PM J39.00011 Multi-scale structure of a protein (histone H3.1) via a knowledge-based potential[1] , RAS PANDEY, University of Southern Mississippi, BARRY FARMER, Air Force Research Laboratory — A coarse-grained computer simulation model is used to investigate the multi-scale structures of a histone H3.1, a protein with 136 residues in an effective solvent medium. The protein chain consisting of residues (nodes) tethered together by fluctuating bonds on a cubic lattice where empty lattice sites constitute the effective solvent matrix. Each residue interacts with surrounding solvent sites and other residues via Lennard-Jones (LJ) potential. A knowledge-based interaction matrix is used for the residue-residue interaction coefficient of the LJ potential. Interaction between the residue and solvent sites, a measure of the solvent quality, is varied. Each residue executes its stochastic motion with the Metropolis algorithm. We examine a number of local and global physical quantities some of which include mobility and energy profiles of each residue and their local structural histogram, radius of gyration (R_g), radial distribution function, and structure factor of the protein for a range of the solvent interactions. Variation of R_g with the solvent quality of solvent exhibits a maximum.

[1]This work is supported by the Air Force Research Laboratory.

1:27PM J39.00012 Calculating the shift in pKa of the position 66 for an Staphylococcal nuclease mutant with the Replica Exchange Free Energy Perturbation method , DANIAL SABRI DASHTI, Physics Department and Quantum Theory Project at University of Florida, ADRIAN ROITBERG, Quantum Theory Project at University of Florida — The Experimental pKa value of Glutamate66 in a hyperstable mutant of Staph Nuclease, which has been measured by Moreno et al., shows a large shift of around 5 pKa units with respect to a glutamate in solution. In order to reproduce the large experimental shift by single structure continuum solvent computational methods, it is required that the dielectric constant of the interior of the protein be set to around ten in the simulations. The physical reason behind this is not understood as of yet and hypotheses have been produced by the Moreno group regarding solvent penetration, protein reorganization etc. We tried to resolve this inconsistency between experimental and continuum methods by introducing a four-state thermodynamic cycle that has couples conformational states with protonation state of the side chain of E66. We propose that what the experimental methods, (which are mostly sensitive to configurational changes) are measuring is actually the equilibrium constant between the two configurational states rather than between the two protonation states. In this regard we applied our recently developed Replica Exchange method Free Energy Perturbation (REFEP) in implicit solvent to calculate the pKa value of E66 for each of the configurational states as well as the mixed configuration, and our results are in almost perfect agreement with the experiments of Moreno.

1:39PM J39.00013 Brownian dynamics simulations of amelogenin microribbons formation[1] , WEI LI, ANTHONY PEREZ LOPEZ, YA LIU, Lehigh University, AMIT CHAKRABARTI, Kansas State University, JAMES GUNTON, Lehigh University — Recent advances in chemical particle synthesis have emphasized the fundamental role of surface colloidal heterogeneities and their detailed chemical composition, which is particularly significant for an important subclass of colloidal systems, namely, proteins. Recently, the process of self-assembly of amelogenin monomers with a hydrophobic/hydrophilic bipolar nature into ordered ribbon structures has been studied experimentally. In this work, we study this dynamical process by means of a Brownian dynamic simulation of a simple model which represents the bipolar character of the globular amelogenin molecule and the hydrophilic C-terminal tail. We monitor the kinetics of self-assembly through a study of the structure factor. We also calculate the phase diagram of the model using Gibbs ensemble Monte Carlo simulation and thermodynamic perturbation theory.

[1]This work is supported by grants from the NSF and Mathers Foundation.

1:51PM J39.00014 Stability of proteins inside a hydrophobic cavity , MITHUN RADHAKRISHNA, Columbia University, SUMIT SHARMA, Princeton University, SANAT K. KUMAR, Columbia University — Previous studies have shown that enclosing a protein in an athermal cavity stabilizes the protein against reversible unfolding by virtue of eliminating many open chain conformations. Examples of such confined spaces include pores in chromatographic columns, Anfinsen's cage in Chaperonins, interiors of Ribosomes or regions of steric occlusion inside cells. However, the situation is more complex inside a hydrophobic cavity. The protein has a tendency to adsorb on the surface of the hydrophobic cavity, but at the same time it loses conformational entropy because of confinement. We study this system using a simple Hydrophobic Polar (HP) lattice protein model. Canonical Monte Carlo (MC) simulations at different temperatures and surface hydrophobicity show that proteins are stabilized at low and moderate hydrophobicity upon adsorption. The range of surface hydrophobicity over which a protein is stable increases with a decrease in radius of the cavity.

2:03PM J39.00015 Wang-Landau sampling of protein adsorption using the HP model[1] , YING-WAI LI, D.P. LANDAU, Center for Simulational Physics, University of Georgia, T. WUEST, Swiss Federal Research Institute — We have applied Wang-Landau sampling[2] with appropriate trial moves[3] to investigate the thermodynamics and structural properties of lattice hydrophobic-polar heteropolymers (commonly known as the HP protein model) interacting with an attractive substrate. We estimate the density of states of the system, from which the partition function and all thermodynamic quantities, e.g. specific heat, radius of gyration, end-to-end distance and surface contacts, can be calculated. "Transitions" between "phases" are then identified based on a comprehensive analysis of these observables. Generally speaking, three transition processes are observed: adsorption-desorption, collapse (formation of hydrophobic core), and "flattening" of adsorbed structures. These have been confirmed by "snapshots" of typical states of the system. Depending on the surface attractive strength, these transitions take place in different order upon cooling, giving rise to different thermodynamic behaviors. Such dependence of folding hierarchy on the surface attraction is found to be universal for different HP sequences.

[1]Research supported by NSF.

[2]F. Wang and D. P. Landau, Phy. Rev. Lett. **86**, 2050 (2001).

[3]T. Wüst and D. P. Landau, Phy. Rev. Lett. **102**, 178101 (2009).

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J40 DCP: Theory of Clusters and Nanoscale Systems A122/123

11:15AM J40.00001 Nanomaterials synthesized by electrochemical discharges: qualitative and quantitative performance , ANIS ALLAGUI, ROLF WUTHRICH, Concordia University — During the electrochemical discharges in aqueous solutions, the electronic avalanches induce several reactions of dimerization and recombination of the hydrated electrons and H* and OH* radicals, generated by the radiation of water molecules. With the introduction of metallic ions M^{z+}, the successful manufacture of nanoparticles is controlled by the continuous competition of reduction of M^{z+}, by the powerful reducing agents e_H^- and H* to lower levels of valency, and the back reaction of oxidation by OH*. With the assumption that the concentration of metal ions is high enough when compared to those of species e_H^-, H* and OH*, the differential yield G between the formation and consumption of M^{z+} in a given finite volume around the electron-emitting electrode is modeled by homogeneous kinetics. It is found G to be proportional to the concentration of metal ions, the speed and penetration depth of the electrons, and the ratio of rate constants of reactions of nucleation and polymerization, which are supported by previous contributions on the dynamics and stability of the phenomenon.

11:27AM J40.00002 ABSTRACT WITHDRAWN —

11:39AM J40.00003 Structural Oscillation in Pd_{13} During Oxidation/Reduction[1] , D.R. ROY, J. ULISES REVELES, S. VINCENT ONG, S.N. KHANNA, Virginia Commonwealth University, A.M. KÖSTER, P. CALAMINICI, CINVESTAV, DEPARTMENT OF PHYSICS, VIRGINIA COMMONWEALTH UNIVERSITY COLLABORATION, DEPARTAMENTO DE QUíMICA, CINVESTAV COLLABORATION — First principles electronic structure calculations within a gradient corrected density functional formalism have been carried out to investigate the electronic structure and magnetic properties of bare and oxidized Pd_{13} clusters. It is shown that the ground state of neutral Pd_{13} is a bilayer structure that can be regarded as a fragment of the bulk, while a compact icosahedron is higher in energy. The addition of an electron, however, reverses the ordering of structures and Pd_{13}^- has an icosahedral ground state. Similar reordering of structure occurs as an O_2 molecule is added to the neutral cluster. The talk will focus on the oscillations between the two structures during catalysis process.

[1]We gratefully acknowledge support from the Air Force Office of Scientific Research through a grant FA9550-08-1-0400.

11:51AM J40.00004 Computational Studies on the Energy Landscape of Pt-Pd nanoparticles , ALVARO POSADA-AMARILLAS, Dept. de Inv. en Física, Unison, RAFAEL PACHECO-CONTRERAS, Dept. de Química, Cinvestav, DORA J. BORBÓN-GONZÁLEZ, LAURO OLIVER PAZ-BORBÓN, Fritz Haber Institut, ROY L. JOHNSTON, School of Chemistry, University of Birmingham, J. CHRISTIAN SCHÖN, Max Planck Institute for Solid State Research — Bimetallic nanoparticles such as Pt-Pd are currently the subject of intense research mainly due to their important catalytic properties. Clusters structure, composition and degree of mixing or segregation all play important roles in determining their chemical activity. It is presented here an exhaustive study of the structure of Pt-Pd nanoparticles, obtained by a Genetic Algorithm (GA) which incorporates the Gupta potential to mimic interaction for bimetallic atoms. This procedure provided an icosahedral structure as the lowest in energy. The threshold method (TM) is used to analyze the energy landscape of 13-atom $Pt@Pd_{12}$ nanoparticle, as well as the transition probabilities for those structures with pentagonal symmetry found by the TM. Disconnectivity graphs are obtained for both a vast exploration of the potential energy surface (PES) and the exploration around the lowest energy structure. We found low interconversion transition rates for the putative global minimum provided by the GA code, which was confirmed by the TM algorithm.

12:03PM J40.00005 Negative ions of transition metal-halogen clusters[1] , KALPATARU PRADHAN, Department of Physics, VCU, Richmond, VA, 23284, USA, GENNADY L. GUTSEV, Department of Physics, Florida A&M University, FL 32307, USA, PURUSOTTAM JENA, Department of Physics, VCU, Richmond, VA, 23284, USA — A systematic density functional theory based study of the structure and spectroscopic properties of neutral and negatively charged MX_n clusters formed by a transition metal atom M (M=Sc, Ti, V) and up to seven halogen atoms X (X=F, Cl, Br) has revealed a number of interesting features: (1) Halogen atoms are bound chemically to Sc, Ti, and V for $n < n_{max}$, where the maximal valence n_{max} equals to 3, 4, and 5 for Sc, Ti, and V, respectively. For $n > n_{max}$, two halogen atoms became dimerized in the neutral species, while dimerization begins at n = 5, 6, and 7 for negatively charged clusters containing Sc, Ti, and V. (2) Magnetic moments of the transition metal atoms depend strongly on the number of halogen atoms in a cluster and the cluster charge. (3) The number of halogen atoms that can be attached to a metal atom exceeds the maximal formal valence of the metal atom. (4) The electron affinities of the neutral clusters abruptly rise at $n=n_{max}$, reaching values as high as 7 eV. The corresponding anions could be used in the synthesis of new salts, once appropriate counterions are identified.

[1]We acknowledge the DTRA grant.

12:15PM J40.00006 Crystal Field Splitting and Stabilization of CuMgx- Clusters[1] , VICTOR M. MEDEL, J. ULISES REVELES, A.C. REBER, M.C. QIAN, S.N. KHANNA, Virginia Commonwealth University, DEPARTMENT OF PHYSICS, VIRGINIA COMMONWEALTH UNIVERSITY TEAM — The electronic states in clusters group into shells much in the same way as in atoms. Clusters with filled electronic shells exhibit enhanced stability as manifested through observed magic numbers in metal clusters. An important issue is if stable species can be attained at sub-shell fillings. In this work we have carried out first principles electronic structure calculations on $CuAl_x^-$ and $CuMg_x^-$ clusters to demonstrate this intriguing effect. It is shown that the ionic cores in the clusters can order to generate internal electric fields that lead to splitting of the supershells, much in the same way as the crystal field splitting of atomic states in crystals. The studies offer a new approach to forming magic species though control of the composition and the arrangement of atoms. The talk will highlight these effects and how they can be seen in experiments.

[1]We gratefully acknowledge support from the Air Force Office of Scientific Research through a grant FA9550-09-1-0371.

12:27PM J40.00007 *Ab initio* study of dimer and one-dimensional chain structures of $M@Au_{12}$ (M = W, Mo) clusters , SORA PARK, GUNN KIM, YOUNG-KYUN KWON, Kyung Hee University — Using density functional theory, we investigate the structural and electronic properties of the dimer and one-dimensional (1D) chain structures composed of metal-encapsulated Au_{12} nanoclusters ($M@Au_{12}$, M = W, Mo) with icosahedral (I_h) and cuboctahedral (O_h) symmetries. We consider various dimer configurations with different compounds and symmetries to find the most stable dimer structure in each case. We find that during dimerization (either homogeneous or heterogeneous dimer), Au atoms in the one cluster tend to form triangular bonds with counterpart Au atoms in the other. By maximizing the number of Au-Au bonds by dimerization, any cluster is stabilized by about 3 eV. We further find their stable 1D chain structures by considering various 1D chain configurations with different compounds and symmetries. Our results demonstrate that the spin-orbit coupling effects are significant on the electronic and magnetic properties as well as the structural stability due to 5*d* electrons in a transition metal atom M of the $M@Au_{12}$ nanocluster. We also present interesting differences in electronic and magnetic properties between I_h- and O_h-symmetric 1D polymerized $M@Au_{12}$ chain structures.

12:39PM J40.00008 Interpretation of Cp(*) - protected Aluminum Clusters as Superatom Complexes[1] , P. ANDRE CLAYBORNE, OLGA LOPEZ-ACEVEDO, Department of Chemistry, NSC, University of Jyväskylä, ROBERT WHETTEN, University of Jyväskylä and Georgia Insitute of Technology, HENRIK GRÖNBECK, Competence Centre for Catalysis and Department of Applied Physics, Chalmers University of Technology, HANNU HÄKKINEN, Department of Chemistry and Department of Physics, NSC, University of Jyväskylä — Metal clusters stabilized by a surface ligand shell represent an interesting intermediate state of matter between molecular metal-ligand complexes and bulk metal. Such "metalloid" particles are characterized by the balance between metal-metal bonds in the core and metal-ligand bonds at the exterior of the cluster. In previous studies, the electronic stability observed for selected ligand-protected aluminum clusters is not fully understood. By density functional theory calculations, we illustrate here that the electronic stability of various experimentally isolated Cp(*) – protected aluminum clusters can be explained using the electron shell model for the aluminum core, coupled with an ionic Al-Cp(*) interaction at the surface. Thus, one may classify ligand-protected aluminum clusters as "superatom complexes" similar to the ligand-protected gold clusters.

[1]Financial support by the Academy of Finland. The computational resources were provided by the CSC - the Finnish IT Center for Science in Espoo.

12:51PM J40.00009 Probing the existence of energetically degenerate cluster isomers by chemical tagging , QIAN WANG, Virginia Commonwealth University, QIANG SUN, PURU JENA — Current methods for identifying the ground state geometry of a cluster require synergy between theory and experiment. However, this becomes a difficult problem when the accuracy of the theoretical methods is not sufficient to distinguish between nearly degenerate isomers. Using density functional theory based calculations we show that the near degeneracy between the planar and cage structures can be lifted by tagging these with halogens and superhalogens moieties such as Cl and BO_2. The energy of the planar Au16- isomer is lowered from 0.15 eV before tagging to 0.51 $\sim$ 0.55 eV after tagging, thus providing a way to probe its coexistence.

1:03PM J40.00010 Gold clusters at finite temperature: influence of fluxionality on ligand adsorption , LUCA M. GHIRINGHELLI, ELIZABETH C. BERET, JÖRG MEYER, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, Germany — Metal clusters, in particular in relation with their catalytic properties, have been the object of intensive experimental and theoretical studies, in the recent years. A great deal of effort has been devoted by many theoretical groups to understanding the zero kelvin properties of such clusters. Here, by focusing on small gas phase An_N clusters $(3 \leq N \leq 20)$ and their interaction with CO and O_2 as a showcase, we illustrate a methodology for the study of small clusters and their interaction with atoms and molecules at finite temperature. We combine all-electron density functional theory, including scf-density dependent van-der-Waals tail corrections, with finite temperature sampling techniques, like Biased MD and Parallel Tempered MD. We find an unusual flexibility of the clusters, at room and lower temperature. At certain sizes, Au_N clusters at room temperature are liquid droplets. This has an important implication, when accounting for the dynamics of ligand adsorption. One has to consider that the energy released by an exothermic ligand adsorption heats up the newly formed complex, and the equilibration with the environment is much longer than the typical timescale for conformational rearrangement. In this respect, the very concept of a preferred adsorption site in the bare cluster might be meaningless.

1:15PM J40.00011 Pseudohalogens as Building Blocks of Hyperhalogens: A Case Study with $Au(CN)_x$ Complexes , DEVLEENA SAMANTA, Virginia Commonwealth University, MIAO MIAO WU, Peking University, China, PURUSOTTAM JENA, Virginia Commonwealth University, VIRGINIA COMMONWEALTH UNIVERSITY TEAM, PEKING UNIVERSITY, CHINA COLLABORATION — Electron affinity (EA) is one of the major factors that govern reactivity. Halogen atoms possess the highest electron affinities among the elements in the periodic table since it takes only one electron to close their shell. Pseudohalogens also require one electron to close their shell and thus mimic the properties of halogens. A typical example is the CN moiety whose electron affinity (3.8 eV) is slightly larger than that of Cl. Using calculations based on density functional theory we show that when a Au atom is surrounded by CN moieties, the electron affinity of $Au(CN)_x$ complexes rise above that of CN for $x \geq 2$ and reach a value as high as 8.4 eV, thus forming hyperhalogens. Electron affinities also show odd even alternation with the clusters with even x having higher EA values. Equilibrium geometries, electronic structure and spectroscopic properties of these complexes will be presented and results will be compared with available experimental data.

1:27PM J40.00012 Chirality in Metallic Clusters , IGNACIO L. GARZON, LUIS A. PEREZ, Universidad Nacional Autonoma de Mexico — In this work, we present a theoretical study on the structural, vibrational, electronic, and optical properties of chiral bare gold clusters. We consider the case of the Au_{34}^- cluster for which extensive experimental studies on its structural and electronic behavior had been published recently. Our results show that the lowest-energy isomers of the Au_{34}^- cluster correspond to two chiral structures with C_1 and C_3 point symmetry groups, being the C_1 isomer slightly more stable than the C_3 one. The calculated structure factors, which have been measured using trapped ion electron diffraction, indicate that these isomers are almost indistinguishable. On the other hand, their electronic DOS show different features around the HOMO-LUMO energy gap, which may be detected through optical spectroscopies. In fact, our calculated absorption and circular dichroism spectra show clear differences in the optical behavior of these chiral clusters. Another important property that distinguishes the C_1 and C_3 isomers is the different spatial distribution of the atomic coordination on the cluster surface, which would generate distinct enantiospecific adsorption patterns with chiral molecules. These results confirm the existence of intrinsically chiral bare gold clusters.

1:39PM J40.00013 Free gold clusters in CO and O_2 atmosphere: an ab initio study , ELIZABETH C. BERET, LUCA M. GHIRINGHELLI, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin — The marked catalytic activity of gold nanoparticles has inspired a large number of scientific contributions from different fields. However, many questions still lack a satisfying answer, for example what are the structures and stoichiometries of the gold particles in the presence of the reactive gases, and how do their catalytic properties depend on the particle size [1]. We answer these questions for neutral gold clusters modeled in a gas phase atmosphere containing CO and O_2 in variable compositions, and in a temperature range between 100 and 600 K. To this aim, DFT (PBE)–based *ab initio atomistic thermodynamics* technique [2] is applied, including full account of the vibrational contribution to the free energy. As a result, the preferred cluster+adsorbate structures for different environmental conditions are obtained and interpreted as candidate intermediates in the catalytic CO oxidation reaction.

[1] R. Meyer, C. Lemire, S. K. Shaikhutdinov and H. J. Freund, *Gold Bull.* **2004**, *37*, 72–124.
[2] K. Reuter and M. Scheffler, *Phys. Rev. B* **2001**, *65*, 035406; C. M. Weinert and M. Scheffler, *Mat. Sci. Forum* **1986**, **10–12**, 25–30; M. Scheffler and J. Dabrowski, *Phil. Mag. A* **1988**, *58*, 107–121.

1:51PM J40.00014 Structure-specific spectroscopy of plasmon-supporting nanoparticles , KENNETH KNAPPENBERGER, Florida State University — Recent advances in the development of sensitive ultrashort laser-based spectroscopic probes to investigate dynamics of high surface-to-volume metal and alloy nanostructures will be discussed. Electronic relaxation and interparticle electromagnetic coupling processes in hollow gold nanospheres (HGNs) and HGN aggregates were studied using femtosecond pump-surface plasmon probe and second harmonic generation spectroscopies, including single-particle measurements. In the case of HGNs, an unexpected, but systematic, blue shift of the spectral position of the surface plasmon resonance was observed upon nanoparticle aggregation. Femtosecond time-resolved measurements, high-resolution TEM, and Finite-Difference Time-Domain calculations demonstrate that this blue shift results from interparticle cavity coupling, an effect not possible for solid nanospheres. The efficiency of this coupling was tailored by controlling HGN aspect ratio over a vast range of sizes (20 nm to 80 nm outer diameters). This effect may be applied to developing more efficient optical and electronic devices, including photovoltaics.

2:03PM J40.00015 Rare Earth Doped Magnetic Clusters of Gold for Medical Application , BRAHM DEO YADAV, VIJAY KUMAR, Dr. Vijay Kumar Foundation — In recent years gold clusters have been studied extensively due to their unusual properties and applications in cancer treatment and catalysis. Small gold clusters having up to 15 atoms are planar as shown in figure 1. Thereafter a transition occurs to 3D structures but the atomic structures continue to have high dispersion. Doping of these clusters could transform them in to new structures and affect the properties. Gold clusters with cage structures such as W@Au12 can be prepared with large highest occupied-lowest unoccupied molecular orbital (HOMO-LUMO) gap by doping with a transition metal atom such as W. By changing the transition metal atom, cage structures of different sizes as well as different HOMO-LUMO gaps can be formed which could be useful in different optical applications. In these structures gold clusters are generally non-magnetic. However, it is also possible to form magnetic clusters of gold such as Gold clusters have been found to be good for cancer treatment. We have performed ab initio calculations on doping of rare earths in small gold clusters to obtain magnetic clusters using projector augmented wave pseudopotential method within generalized gradient approximation for the exchange-correlation energy. Elemental gold clusters having up to 15 atoms are planar and thereafter 3D structures become favorable. We have explored the changes in the growth behavior when a rare earth atom is doped and studied the variation in the magnetic behavior as a function of size. Our results suggest that gold clusters may have twin advantage of treating cancer as well as be helful in magnetic imaging such as by MRI.

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J41 DMP DPOLY GERA: Focus Session: Polymers for Energy Storage and Conversion – Structure in Organic Semiconductor Blends A115/117

11:15AM J41.00001 Organic devices. New perspectives provided from soft x-ray characterization , CHRIS MCNEILL, University of Cambridge — Organic semiconductors are continuing to receive significant interest for application in photovoltaic cells, field-effect transistors and light-emitting diodes. Conjugated polymers in particular offer the convenience of solution processibility with the flexibility of materials design afforded by synthetic chemistry. One of the disadvantages of conjugated polymers is the complexity of their film structure that, while key for understanding and optimizing device performance, is difficult to characterize. Here I will present new insights into the structure of films based on conjugated polymers using synchrotron-based soft x-ray techniques. By exploiting molecular resonances near the carbon K-edge, soft x-ray techniques such as x-ray spectromicroscopy and resonant soft x-ray scattering afford enhanced material contrast with high spatial resolution. This enhanced material specificity has been exploited to reveal the complex, hierarchical structure of conjugated polymer blends used in polymer solar cells. Furthermore, we have recently demonstrated a significant degree of miscibility of fullerene derivatives used in high-efficiency polymer/fullerene blends calling into question the assumed paradigm of phase-separated, pure phases. The polarized nature of synchrotron radiation can also be exploited to probe local molecular orientation and order using soft x-rays. This facilitates mapping of domain orientation and molecular order important for understanding charge transport in polycrystalline polymer films used in field-effect transistors.

11:51AM J41.00002 Systematic Multiscale Modeling of Polymers , ROLAND FALLER, UC Davis, DAVID HUANG, Univ of Adelaide, BESTE BAYRAMOGLU, ADAM MOULE, UC Davis — The systematic coarse-graining of heterogeneous soft matter systems is an area of current research. We show how the Iterative Boltzmann Inversion systematically develops models for polymers in different environments. We present the scheme and a few applications. We study polystyrene in various environments and compare the different models from the melt, the solution and polymer brushes to validate accuracy and efficiency. We then apply the technique to a complex system needed as active layer in polymer-based solar cells. Nano-scale morphological information is difficult to obtain experimentally. On the other hand, atomistic computer simulations are only feasible to studying systems not much larger than an exciton diffusion length. Thus, we develop a coarse-grained (CG) simulation model, in which collections of atoms from an atomistic model are mapped onto a smaller number of "superatoms." We study mixtures of poly(3-hexylthiophene) and C_{60}. By comparing the results of atomistic and CG simulations, we demonstrate that the model, parametrized at one temperature and two mixture compositions, accurately reproduces the system structure at other points of the phase diagram. We use the CG model to characterize the microstructure as a function of polymer:fullerene mole fraction and polymer chain length for systems approaching the scale of photovoltaic devices.

12:03PM J41.00003 Exploiting solvent additives to introduce processability to organic solar cells , JAMES ROGERS, KRISTIN SCHMIDT, University of California, Santa Barbara, MICHAEL TONEY, Stanford Synchrotron Radiation Lightsource, GUILLERMO BAZAN, EDWARD KRAMER, University of California, Santa Barbara — Solution processable, highly efficient, organic photovoltaics typically consist of a two component donor-acceptor type system composed of a low bandgap conjugated polymer donor blended with a fullerene acceptor. Efficient charge extraction from these blends demands that donor and acceptor components form nanoscale phase separated percolating pathways to their respective electrodes. Although post deposition thermal annealing has been shown to degrade device performance in low bandgap polymer systems, the incorporation of a small concentration of solvent additive (e.g. diiodooctane) into the solution from which a bulk heterojunction solar cell is cast has been shown to nearly double device efficiency without the need for subsequent thermal annealing. In situ grazing incidence wide angle x-ray scattering measurements as a function of time after spin coating suggest that the role of additives is to induce nucleation of crystals of the polymeric component and to facilitate changes in the correlation length (size and/or perfection) of these crystallites during the film drying process. The resulting structural order in additive processed films suggests novel processing routes for existing organic photovoltaics.

12:15PM J41.00004 Kinetics of Structure Formation in Polymer-Fullerene Solutions for Organic Photovoltaics , MARGARET SOBKOWICZ, RONALD JONES, R. JOSEPH KLINE, DEAN DELONGCHAMP, National Institute of Standards and Technology — Bulk heterojunctions (BHJs) composed of poly(hexylthiophene) (P3HT) and phenyl-C61-butyric acid methyl ester (PCBM) are promising active layers for organic photovoltaics. The nanoscale morphology of the BHJ is critical to the performance of solar devices because exciton diffusion, charge separation, and carrier transport require domains that have specific optimal sizes and connectivity. Processing parameters have been shown to influence the morphology and thus device performance. Because P3HT crystallization during film formation is the driving force for phase segregation, casting solution properties are vital to film electronic properties. Small angle neutron scattering (SANS) is an ideal measurement technique to study the blend morphology and phase formation in P3HT:PCBM solutions due to the large difference in neutron scattering length density between P3HT and PCBM, the length scale probed, and the excellent sensitivity of SANS to concentration fluctuations. In this work SANS and solution rheology are developed as characterization tools for organic photovoltaic materials. Scattering data from P3HT:PCBM solutions are correlated to gelation kinetics to develop a picture of the nanoscale organization and the influence of processing on morphology.

12:27PM J41.00005 Molecular-Scale and Nanoscale Morphology of P3HT:PCBM Bulk Heterojunctions: Energy-Filtered TEM and Low-Dose HREM , LAWRENCE DRUMMY, Air Force Research Laboratory, ROBERT DAVIS, DIANA MOORE, Sandia National Laboratory, MICHAEL DURSTOCK, RICHARD VAIA, Air Force Research Laboratory, JULIA HSU, Sandia National Laboratory — The performance of bulk heterojunction organic photovoltaic devices is critically dependent on the morphology of the active layer. Here we describe the combination of two electron microscopy techniques to quantitatively examine the molecular level structure and mesoscopic domain morphology of the active layer of P3HT:PCBM bulk heterojunction solar cells. Energy-filtered transmission electron microscopy (EFTEM) revealed the nanoscopic, interpenetrating fibrillar structure of the phase separated blend, providing unique assignments of the P3HT-rich and PCBM-rich regions. Low-dose high-resolution electron microscopy (LD-HREM) provided direct images of the P3HT crystals and their orientation within the P3HT-rich domains.

12:39PM J41.00006 Neutron Scattering Provides a New Model for Optimal Morphologies in Organic Photovoltaics: Rivers and Streams , MARK DADMUN, NATHAN HENRY, WEN YIN, University of Tennessee, KAI XIAO, JOHN ANKNER, Oak Ridge National Laboratory — The current model for the ideal morphology of a conjugated polymer bulk heterojunction organic photovoltaic (OPV) is a phase-separated structure that consists of two pure phases, one an electron donor, the other an acceptor, that form an interpenetrating, bicontinuous, network on the length scale of 10-20 nm. In this talk, neutron scattering experiments that demonstrate that this model is incorrect for the archetypal conjugated polymer bulk heterojunction, poly[3-hexylthiophene] (P3HT) and the fullerene 1-(3-methyloxycarbonyl)propy(1-phenyl [6,6]) C_{61} (PCBM) will be presented. These studies show that the miscibility of PCBM in P3HT approaches 20 wt%, a result that is counter to the standard model of efficient organic photovoltaics. The implications of this finding on the ideal morphology of conjugated polymer bulk heterojunctions will be discussed, where these results are interpreted to present a model that agrees with this data, and conforms to structural and functional information in the literature. Furthermore, the thermodynamics of conjugated polymer:fullerene mixtures dominate the formation of this hierarchical morphology and must be more thoroughly understood to rationally design and fabricate optimum morphologies for OPV activity.

12:51PM J41.00007 Organic Photovoltaic Interfaces: Back Contact Study , BRETT GURALNICK, MICHAEL MACKAY, RAUL LOBO, University of Delaware — Charge transfer between the polymer and contact greatly affects organic photovoltaics' (OPV) performance. The processing conditions are key since depositing the contact incorrectly reduces the polymer cell efficiency by up to fifty percent. The back contact, typically aluminum, is thermally evaporated onto the OPV active layer which has long been suspected to be affected by the process. To analyze this, the aluminum layer was dissolved after deposition and the resulting surface was imaged with an atomic force microscope. A fast aluminum deposition rate pitted the polymer surface creating regions of high resistivity thereby reducing cell efficiency. The addition of a LiF blocking layer between the active layer and aluminum was found to eliminate pitting allowing faster deposition. Interestingly, thermally annealing the active layer prior to aluminum deposition was also found to eliminate pitting. Neutron reflectivity experiments were used to determine that the fullerene derivative, used as the electron acceptor in the active layer, migrated to the surface during the annealing step and apparently act as a shielding layer preventing damage. With this knowledge the optimum deposition conditions were determined and has led to the highest efficiencies from OPVs.

1:03PM J41.00008 Long-range Order in Self-assembled Poly(3-alkylthiophene)-Diblock Copolymers , VICTOR HO, BRYAN BOUDOURIS, RACHEL SEGALMAN, University of California, Berkeley — Poly(3-alkylthiophenes) (P3ATs) are used commonly as active layer components in plastic electronic devices due to their relatively high hole mobilities, low optical band gaps, and their ability to be processed from solution. To date, however, block copolymers containing these molecules as a functional component predominantly have shown nanofibrillar morphologies identical to that of the P3AT homopolymers due to the large thermodynamic driving force for crystallization. We show that by decreasing rod-rod interactions through rational side chain substitution, well-ordered ($e.g.$, lamellar and hexagonally-packed) geometries can be obtained with P3AT-containing diblock copolymers as evidenced by x-ray scattering and electron microscopy. Additionally, we demonstrate that the structural and optoelectronic properties of the P3EHT domains remain in place. The ability to pattern these functional macromolecules on the nanoscale opens many doors for advanced design of organic electronic active layers.

1:15PM J41.00009 P3HT-based copolymers as interfacial compatibilizers in P3HT/PCBM system , S. MICHAEL KILBEY II, JIHUA CHEN, XIANG YU, KAI XIAO, MARK DADMUN, DEANNA PICKEL, BOBBY SUMPTER, CENTER FOR NANOPHASE MATERIALS SCIENCES, OAK RIDGE NATL LAB; DEPT. OF CHEMISTRY, UNIV. OF TENNESSEE COLLABORATION — To lower the interfacial tension and control the donor-acceptor phase separation in organic photovoltaic devices, a poly(3-hexylthiophene)-*block*-poly(ethylene oxide) (P3HT-*b*-PEO) diblock copolymer compatibilizer was added to a binary blend of regioregular P3HT and the fullerene derivative 6,6-phenyl C_{61} butyric acid methyl ester (PCBM). We systematically examined the ternary phase behavior of spin-coated films of P3HT/ P3HT-*b*-PEO/ PCBM before and after annealing with selected area electron diffraction, grazing-incidence X-ray diffraction, AFM, optical and transmission electron microscopy. Neutron reflectivity experiments were also carried out to study thermodynamic behaviors of P3HT/P3HT-*b*-PEO/PCBM trilayer films. The addition of 5% P3HT-*b*-PEO (block molecular weights of 10kDa and 3kDa, respectively) to a 1:1 P3HT/PCBM blend reduces the size of P3HT-rich domains in P3HT/PCBM films by up to 40% while the $\pi - \pi$ stacking of P3HT (i.e. (020) crystallinity) remains nearly unchanged. In addition we will discuss the effect of compatibilizer type, additive concentration, and thermal annealing conditions on power conversion efficiencies of compatibilized organic photovoltaic cells.

1:27PM J41.00010 Cooperative Assembly of Hydrogen-bonded Block Copolythiophenes/Fullerene Blends for Photovoltaic Devices[1] , JAMES J. WATKINS, YING LIN, JUNG AH LIM, QINGSHUO WEI, ALEJANDRO L. BRISENO, Polymer Science and Engineering Department, University of Massachusetts Amherst — The current work provides a general approach to obtain reliable donor acceptor morphologies by H-bonding cooperative assembly and to achieve efficient photovoltaic devices with enhanced device stability. Herein, we utilize P3HT-based block copolymer (BCP), in which one block is P3HT and the other block is a P3HT derivative containing a poly(ethylene oxide) (PEO) oligomer side chain. This design both enables self-assembly of the devices via microphase segregation into lamellar, cylindrical or spherical morphologies depending on the relative volume fractions of the blocks and provides a means for establishing strong preferential interaction between fullerene derivatives containing hydrogen bond donating groups (such as COOH groups) and the PEO side chain. One advantage of this approach is excellent device stability due to the suppression of macrophase separation resulting from fullerene crystallization under harsh annealing condition.

[1]Funding from the NSF Center for Hierarchical Manufacturing, The NSF Materials Research Center on Polymers and the DOE Energy Frontier Research Center is gratefully acknowledged.

1:39PM J41.00011 Enhanced Photovoltaic Performance of All-Conjugated Poly(3-alkylthiophene) Diblock Copolymers , MING HE, WEI HAN, JING GE, YULIANG YANG, FENG QIU, ZHIQUN LIN — Control of the ratio of blocks in the all-conjugated poly(3-butylthiophene)-b-poly(3-hexylthiophene) (P3BHT) diblock copolymer provides a simple route to precisely tune the molecular organization and nanoscale morphology in the resulting bulk heterojunction (BHJ) solar cells made of P3BHT/ $PC_{71}BM$. An attractive high PCE of 4.02 % was found in P3BHT21 (i.e., P3BT/P3HT block ratio of 2:1 mol/mol)/$PC_{71}BM$, compared to that of 1.08 % in P3BT and 3.54 % in P3HT homopolymer-based devices. The enhanced performance is attributed to improved phase separation, interpenetrating pathway and the formation of crystalline domain size of 10.4 nm in the active layer; the latter also elucidated the importance of alkyl side-chain lengths in the molecular organization and final film morphology. In the P3BHT21/$PC_{71}BM$ blend films, P3BT block facilitated the self-assembly of P3BHT chains into interpenetrating crystalline pathway for efficient charge transport, while P3HT block provided P3BHT chains with necessary flexibility to form improved phase separation at the nanoscale with maximum interfacial areas for charge generation.

1:51PM J41.00012 Morphological Characterization of Low-Bandgap Crystalline Polymer:PCBM Bulk Heterojunction Solar Cells[1] , HAIYUN LU, THOMAS RUSSELL, University of Massachusetts Amherst, UNIVERSITY OF MASSACHUSETTS AMHERST TEAM — Understanding the morphology of polymer-based bulk heterojunction (BHJ) solar cells is key to improving device efficiencies. Blends of a low-bandgap silole-containing conjugated polymer, poly[(4,4'-bis(2-ethylhexyl)dithieno[3,2-b;2',3'-d]silole)-2,6-diyl-alt-(4,7-bis(2-thienyl)-2,1,3-benzothiadiazole)-5,5'-diyl] (PSBTBT) with phenyl-C61-butyric acid methyl ester (PCBM) were investigated using different processing conditions. Scanning force microscopy, X-ray photoelectron spectroscopy, near-edge X-ray absorption fine structure spectroscopy, dynamic secondary ion mass spectrometry and neutron reflectivity studies showed that thermal annealing did not induce obvious changes in the structure of the active layer. Grazing-incidence X-ray diffraction and small-angle neutron scattering showed that the crystallization of PSBTBT and segregation of PCBM occurred during spin coating, and a brief thermal annealing increased the ordering of PSBTBT and enhanced the segregation of the PCBM, forming domains with 10-nm in size, leading to an improvement in photovoltaic performance.

[1]DOE and Konarka Inc. are acknowledged.

2:03PM J41.00013 Donor-acceptor conjugated polymers used as electron acceptors in bulk heterojunction photovoltaics , CHRISTOPHER BAILEY, BARNEY TAYLOR, JIANGUO MEI, JOHN REYNOLDS, JOHN HENDERSON, BENJAMIN LEEVER, MICHAEL DURSTOCK — Synthetic control over the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) has been of significant importance in organic photovoltaics due to the nature of charge separation in donor/acceptor blends. One technique for obtaining tunability of the HOMO and LUMO levels with polymer synthesis is to combine electron donating and electron accepting moieties separated by a conjugated linkage unit. This technique has been utilized to produce highly efficient devices reaching power conversion efficiencies above 8% in polymer/fullerene blends. In this work, we report the characterization of poly(2,7divinylene fluorenecobenzothiadiazole) (F10DVBT), and performs best as an electron acceptor when mixed with poly(3-hexylthiophene) (P3HT) with an open circuit voltage of 1.2V. A combination of morphological and photo-physical studies highlights interesting properties of this material and its interactions with P3HT. The donor-acceptor conjugated structure of F10DVBT appears to strongly affect the photocurrent of these devices, and may result from the interactions between intramolecular and intermolecular charge transfer processes.

Tuesday, March 22, 2011 11:15AM - 1:03PM –

Session J42 DPOLY: Padden Award Symposium A302/303

11:15AM J42.00001 Directing crystallization of organic semiconductors around corners in solution-processed thin films , STEPHANIE S. LEE, SAMUEL TANG, Department of Chemical and Biological Engineering, Princeton University, MARSHA LOTH, JOHN E. ANTHONY, Department of Chemistry, University of Kentucky, DETLEF-M. SMILGIES, ARTHUR WOLL, Cornell High Energy Synchrotron Source, YUEH-LIN LOO, Department of Chemical and Biological Engineering, Princeton University — We demonstrate the ability to pre-specify the crystallization direction of triethylsilylethynyl anthradithiophene (TES ADT), an organic semiconductor, in solution-processed thin films. Manipulating the substrate surface energy allows us to control the crystallization rate of TES ADT, which ranges from 9 to 25 μm/s, during solvent-vapor annealing. Grazing-incidence x-ray diffraction experiments on as-spun TES ADT films indicate that the initial in-plane orientation of TES ADT is influenced by the surface energy of the underlying substrate, likely due to the competition between strong molecule-molecule interactions and its wettability on the substrate. By imposing surface energy specific patterns on the substrate prior to the deposition of TES ADT, we can preferentially direct TES ADT crystallization around bends and sharp corners to form channels with high hole mobility for charge transport.

11:27AM J42.00002 Solid-State Structure and Crystallization in Double-Crystalline Diblock Copolymers , SHENG LI, SASHA MYERS, RICHARD REGISTER, Princeton University — Crystalline-crystalline block copolymers, containing two or more chemically distinct crystallizable blocks, can potentially exhibit a rich array of complex solid-state structures. Double-crystalline diblock copolymers of linear polyethylene (LPE) and hydrogenated polynorbornene (hPN) were synthesized, and their crystallization behavior and morphology were examined using two-dimensional simultaneous time-resolved synchrotron small-angle and wide-angle x-ray scattering. Previously, we showed that in symmetric diblock copolymers of hPN and LPE, with molecular weights above 50 kg/mol, the hPN block crystallizes first and sets the solid-state microstructure. In the present work, we extend these studies to lower molecular weights, and more importantly, we examine the structural relationship between the crystals formed by the two blocks under different conditions of confinement. When the diblock molecular weight is reduced to 20 kg/mol, the LPE block crystallizes first, even when LPE is the minority component, and restricts hPN to crystallize between the LPE lamellae. Furthermore, in both the high and low molecular weight diblock copolymers, the second-to-crystallize block always orients its crystals orthogonally to the first-to-crystallize block.

11:39AM J42.00003 Electric Field Induced Ordering of a Battery Electrolyte , SCOTT MULLIN, NITASH BALSARA, University of California, Berkeley — A disordered mixture of a symmetric poly(styrene-*block*-ethylene oxide) (SEO) copolymer and lithium bis(trifluoromethanesulfonimide) (a lithium salt) was placed between two lithium metal electrodes. Application of a 3V potential across the electrodes results in a current density of 15 mA/cm^2 and order formation as evidenced by the instantaneous development of a sharp small-angle X-ray scattering (SAXS) ring and Bragg spots due to the presence of a few large coherent grains. With time, radial streaks emanated from the ring, leading to a scattering pattern that resembles a sun dial. Our preliminary hypothesis is that these streaks are due to salt concentration gradients that occur when the current is passed. This gradient results in coherent grains within which the domain size changes continuously. To our knowledge, this kind of structure has not been observed previously in block copolymers. The disordered phase is recovered in the bulk when the applied potential is turned off, and the open circuit voltage of the cell and the SAXS invariant relax with similar time constants. This work represents the first step toward designing responsive battery electrolytes wherein structure and ion transport depends on the state-of-charge of the battery.

11:51AM J42.00004 Gradient Solvent Vapor Annealing of Thin Films , JULIE ALBERT, TIMOTHY BOGART, RONALD LEWIS, THOMAS EPPS, University of Delaware — The development of block copolymer materials for emerging nanotechnologies requires an understanding of how surface energy/chemistry and annealing conditions affect thin film self-assembly. Specifically, in solvent vapor annealing (SVA), the use of solvent mixtures and the manipulation of solvent vapor concentration are promising approaches for obtaining a desired morphology or nanostructure orientation. We designed and fabricated solvent-resistant devices to produce discrete SVA gradients in composition and/or concentration to efficiently explore SVA parameter space. We annealed copolymer films containing poly(styrene), poly(isoprene), and/or poly(methyl methacrylate) blocks, monitored film thicknesses during annealing, and characterized film morphologies with atomic force microscopy. Morphological changes across the gradients such as the transformation from parallel cylinders to spheres with increasing solvent selectivity provided insight into thin film self-assembly, and the gradient device has enabled us to determine transition compositions and/or concentrations.

12:03PM J42.00005 Injectable solid peptide hydrogel: shear-thinning and instant recovery , CONGQI YAN, Materials Science and Eng., U. of Delaware, JOEL SCHNEIDER, National Cancer Institute, NIH, DARRIN POCHAN, Materials Science and Eng., U. of Delaware — Peptides were designed to fold into β-hairpins once exposed to physiological conditions and consequently self-assemble into rigid hydrogel. The network consists of branched and entangled 3nm-wide fibrils. These physical gels shear thin and flow under a proper shear stress but immediately recover back into solids on removal of stress with further rigidity restoring over time. To elucidate mechanisms of these physical properties, gel behavior during and after flow was investigated. Gel stiffness recovered immediately after shear, as well as gel stiffening over time post-recovery, were found dependent on shear rate and shear duration. From scattering measurements during flow, the gel network structure was observed unchanged from the static state at all shear rates investigated. Thus, the peptide gel networks fracture into gel domains (>200nm as determined by scattering) during shear thinning/flow but can instantly percolate back into a solid hydrogel after cessation of shear, stiffening further as particle boundaries relax. As these gels are essentially the same solid material, before and after shear, they offer great potential as well-defined, injectable carriers of biomedical therapies where a desired encapsulated therapeutic payload is delivered to an *in vivo* site by simple syringe injection.

12:15PM J42.00006 Transport properties of mechanically deformed polymer networks[1] , HASSAN MASOUD, ALEXANDER ALEXEEV, Georgia Institute of Technology — We develop a hybrid computational method to probe how the permeation and hindered diffusion change when an isotropic polymer network is deformed by an externally applied force. We use a bond-bending lattice spring model to capture the micromechanics of random networks of interconnected elastic filaments coupled with the dissipative particle dynamics to explicitly model the viscous fluid and diffusive solutes. Our simulations reveal that the network transport properties are defined by the network porosity and by the degree of network anisotropy due to network mechanical deformations. We also show that the internal network structure does not affect the permeation and diffusion of stressed and unstressed networks. Furthermore, our results indicate that permeability of mechanically deformed networks can be predicted based on the alignment of network filaments that is characterized by a second order orientation tensor. Our findings have implications for designing drug delivery agents, tissue engineering, and understanding the function of certain biological systems.

[1]Financial support from the Donors of the PetroleumResearchFund, administered by theACS, is gratefully acknowledged.

12:27PM J42.00007 Numerical coarse-graining of polymer field theories , MICHAEL VILLET, GLENN FREDRICKSON, University of California, Santa Barbara — Field theoretic models of polymers are widely used to investigate polymer self-assembly, but numerical simulations of these models that include full fluctuation physics are computationally demanding and infrequently conducted. To enable efficient multi-scale simulations, we propose the use of systematically coarse-grained field theories that can be simulated on coarse computational lattices while accurately incorporating the effects of important sub-lattice-scale physics. We present a rigorous formalism for generating such coarse-grained theories from data obtained from small-scale fine-grained simulations, and demonstrate our methodology's effectiveness for a representative polymer solution model.

12:39PM J42.00008 Molecular mobility and cation conduction in sulfonated polyester copolymer ionomers , GREGORY TUDRYN, DANIEL KING, Penn State, MICHAEL O'REILLY, KAREN WINEY, UPenn, RALPH COLBY, Penn State — Poly(ethylene oxide) ionomers are candidate materials for electrolytes in energy storage devices due to the ability of ether oxygen to solvate cations. Copolyester ionomers are synthesized via condensation of sulfonated phthalates with mixtures of PEG and PTMG to make random copolymer ionomers with identical ion content. Variation of the PEG/PTMG composition changes Tg, dielectric constant and ionic aggregation; each with consequences for ion transport. Dielectric spectroscopy is used to determine number density of conducting ions, their mobility and extent of aggregation. Conductivity and mobility show Vogel temperature dependence and increase with PEG content; even though PTMG ionomers have lower Tg. Conducting ion densities show Arrhenius temperature dependence and are nearly identical for polymers containing PEG. SAXS confirms the extent of aggregation and temperature response from dielectric results, and exposes phase separation as PTMG content is increased. The tradeoff between ion-solvation and low Tg in this study provides fundamental understanding of ionic aggregation and ion transport in polymer electrolytes.

12:51PM J42.00009 Strain Localization and Sliding Friction in Physically Associating Networks , KENDRA A. ERK, KENNETH R. SHULL, Northwestern University — Experimental evidence, constitutive models, and scaling law arguments are presented for shear-induced strain localization in triblock copolymer gels deformed at reduced rates spanning almost four orders of magnitude. Strain-stiffening behavior proceeded by rapid softening is believed to result from the formation of highly localized regions of deformation in the macromolecular network. This behavior is described by a constitutive model that incorporates the strain energy and relaxation of individual strands in the network. Flow curves predicted from the model are non-monotonic, consistent with the onset of flow instabilities at high shear rates. Connections are established between the stress response of the gel at large strain and traditional sliding friction experiments of gelatin gels on glass. The gel's well-defined network structure and tunable range of relaxation times allow for these gels to be useful model systems for future studies of flow instabilities in physically associating solutions.

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J43 DPOLY: Physics of Copolymers II A306/307

11:15AM J43.00001 Coil-globule Transitions in Model Bioinspired Polymers , HANNAH MURNEN, ADRIANNE ROSALES, University of California Berkeley, RONALD ZUCKERMANN, The Molecular Foundry, Lawrence Berkeley National Laboratory, RACHEL SEGALMAN, University of California Berkeley — The monomer sequence of a polypeptide chain has a profound effect on the coil to globule transition of the protein. Both theoretical and experimental efforts to probe the effect of monomer sequence have included the use of chemical modifications post chain collapse in a homopolymer/solvent system followed by further analysis of the chain to understand the resulting sequence. Polypeptoids, or N-substituted glycines, are a far more precise sequence specific model system that can be used to test the effect of monomer sequence on the coil to globule transition. In this study, we synthesized 50mer sequences of a blocky protein-like copolymer using 40 monomers of N-(methyl)glycine and 10 of N-(carboxyethyl)glycine). As predicted in theoretical simulations, the protein like copolymer forms a smaller globule than the periodic control sequence. In addition, decreasing the relative hydrophobicity of the two comonomers results in a looser globule size at room temperature. Future work will focus on using polypeptoids to further probe this transition and to gain insight into the fundamental forces at play in polypeptide folding.

11:27AM J43.00002 Modeling the Heat Capacity of Spider Silk Inspired Di-block Copolymers[1] , W. HUANG, S. KRISHNAJI, D. KAPLAN, P. CEBE, Tufts University — We synthesized and characterized a new family of di-block copolymers based on the amino acid sequences of Nephila clavipes major ampulate dragline spider silk, having the form HABn and HBAn (n=1-6), comprising an alanine-rich hydrophobic block, A, a glycine-rich hydrophilic block, B, and a histidine tag, H. Using temperature modulated differential scanning calorimetry (TMDSC), we captured the effect of bound water acting as a plasticizer for copolymer films which had been cast from water solution and dried. We determined the water content by thermogravimetry and used the weight loss vs. temperature to correct the mass in TMDSC experiments. Our result shows that non-freezing bound water has a strong plasticization effect which lowers the onset of the glass transition by about 10°C. The reversing heat capacities, Cp(T), for temperatures below and above the glass transition were also characterized by TMDSC. We then calculated the solid state heat capacities of our novel block copolymers below the glass transition (Tg) based on the vibrational motions of the constituent poly(amino acid)s, whose heat capacities are known from the ATHAS Data Bank. Excellent agreement was found between the measured and calculated values of the heat capacity, showing that this model can serve as a standard method to predict the solid state Cp for other biologically inspired block copolymers.

[1]Support was provided from the NSF CBET-0828028 and the MRI Program under DMR-0520655 for thermal analysis instrumentation.

11:39AM J43.00003 Effect of chain shape and monomer sequence on self-assembly of polypeptoid-polystyrene block copolymers , ADRIANNE ROSALES, HANNAH MURNEN, University of California, Berkeley, RONALD ZUCKERMANN, Molecular Foundry, Lawrence Berkeley National Laboratory, RACHEL SEGALMAN, University of California, Berkeley — Polymer chain shape has profound effects on block copolymer self-assembly. In nature, chain shape is controlled by the monomer sequence of biological polymers, but such precise control is difficult with classical synthetic systems. Polypeptoids, a class of sequence-specific bioinspired polymer, are shown to have a chain shape which can be tuned by the introduction of monomers with bulky, chiral side chains. Here, it is shown that introducing chiral monomers into the peptoid chain increases chain stiffness, as reflected by a 20C increase in the glass transition temperature for a chiral polypeptoid compared to its achiral analog. Incorporation into block copolymers enables systematic study of the effect of chain shape while maintaining similar enthalpic interactions. For two otherwise analogous block copolymers, conformational asymmetry is shown to affect both the self-assembled morphology and its order-disorder transition temperature. The ability to tune polymer properties with this biomimetic system will lend insight to the relationship between monomer sequence and self-assembled nanostructures.

11:51AM J43.00004 Self-Assembly of Globular Protein-Polymer Diblock Copolymers , C.S. THOMAS, B.D. OLSEN, MIT — The self-assembly of globular protein-polymer diblock copolymers into nanostructured phases is demonstrated as an elegant and simple method for structural control in biocatalysis or bioelectronics. In order to fundamentally investigate self-assembly in these complex block copolymer systems, a red fluorescent protein was expressed in *E. coli* and site-specifically conjugated to a low polydispersity poly(N-isopropyl acrylamide) (PNIPAM) block using thiol-maleimide coupling to form a well-defined model globular protein-polymer diblock. Functional protein materials are obtained by solvent evaporation and solvent annealing above and below the lower critical solution temperature of PNIPAM in order to access different pathways toward self-assembly. Small angle x-ray scattering and microscopy are used to show that the diblock forms lamellar nanostructures and to explore dependence of nanostructure formation on processing conditions. Circular dichroism and UV-vis show that a large fraction of the protein remains in its folded state after conjugation, and wide angle x-ray scattering demonstrates that diblock copolymer self-assembly changes the protein packing symmetry.

12:03PM J43.00005 Phase Behavior and Significantly Enhanced Toughness in Polylactide Graft Copolymers , MEGAN ROBERTSON, University of Houston, GRAYCE THERYO, FENG JING, MARC HILLMYER, University of Minnesota — Polylactide (PLA), a biodegradable polyester derived from plant sugars, is commercially available and used in a variety of applications ranging from serviceware to resorbable sutures. One limitation to diversifying the applications of the material is its inherent brittleness. Graft copolymers containing PLA arms and a rubbery aliphatic polymer backbone were synthesized by a combination of ring-opening metathesis and ring-opening transesterification polymerizations. The high degree of incompatibility between the arms and backbone resulted in microphase separation of the graft copolymer at increasingly low fractions of the backbone polymer, as evidenced by small-angle x-ray scattering. In graft copolymers with a rubbery content of only 5 wt percent, the tensile strain at break was observed to be as high as twenty times that of neat PLA. Studies are underway to provide insight into the critical polymer molecular parameters for enhanced toughness and the deformation mechanisms.

12:15PM J43.00006 Thermoresponsive Polymers and Block Copolymers in Ionic Liquids , HAUNAN LEE, University of Minnesota, ZHIFENG BAI, NAKISHA NEWELL, TIMOTHY LODGE — We recently discovered that poly(ethylene oxide) (PEO) and poly(n-butyl methacrylate) (PnBMA) exhibit two completely different types of lower critical solution temperature (LCST) phase behavior in certain ionic liquids (ILs). While typical LCST type phase diagrams were shown in PnBMA/IL systems, we observed unusual temperature-composition phase diagrams in the PEO/IL systems, in which the cloud point curves are strongly asymmetric, with the critical composition located at 80 wt % of PEO. In addition, an important feature of these thermosensitive polymer/IL systems is that the LCST can be easily tuned over a wide range by blending different ILs, without changing the chemical structure of the polymers. On the basis of the LCST of PEO and the upper critical solution temperature (UCST) of poly(N-isopropylacrylamide) (PNIPAm) in ILs, we designed a PEO-PNIPAm block copolymer that exhibits interesting doubly thermosensitive self-assembly. The block copolymer forms PNIPAm-core micelles at low temperatures and transforms into PEO-core micelles at high temperatures. The critical micellization temperatures (CMT) of both blocks can be manipulated by adjusting the mixing ratio of ILs.

12:27PM J43.00007 Effect of homopolymer additives on texture evolution in block copolymer composites , HYUNG JU RYU, JANE SUN, MICHAEL BOCKSTALLER, Carnegie Mellon University — This contribution presents a systematic study of the effect of homopolymer (hP) addition on the texture evolution in block copolymer (BCP) blends. The microstructures of poly(styrene-b-isoprene) based symmetric di-BCP blended with homopolystyrene additives at various filling fraction were analyzed after different thermal annealing time. For the analysis we utilized serial electron imaging in conjunction with image reconstruction & stereological analysis. Particular emphasis was on the elucidation of the evolution of type and frequency of grain boundary (GB) formation as well as average grain size and orientation. Relative GB energies were determined from triple junction analysis. The results demonstrate that the presence of even small amount of hP impurities significantly reduce grain growth and annealing of high energy GB surfaces. This is interpreted as a consequence of selective segregation of the fillers within high energy GB regions and the associated stabilization of the GB surfaces. These results have important implication on the use of BCPs in areas ranging from plastic electronics to tunable photonic crystals.

12:39PM J43.00008 Influence of Chemical Heterogeneity on the Viscoelastic Properties of Polystyrene-b-Poly(alkyl methacrylate) Baroplastics[1] , ASEM ABDULAHAD, CHANG Y. RYU, Rensselaer Polytechnic Institute — The development of purification and fractionation techniques of block copolymers is important for overcoming the synthetic difficulty of preparing well-defined block copolymers using various living polymerization techniques. A large scale separation technique would lead us to obtaining sufficient amounts of homopolymer-free block copolymers for subsequent physical characterization. This can potentially aid in the elucidation of the role of chemical heterogeneity on the thermodynamic transitions and viscoelastic properties of block copolymer materials. Atom transfer radical polymerization by the activators regenerated by electron transfer method (ARGET-ATRP) was used to prepare a series of polystyrene-b-poly(alkyl methacrylate) copolymers that would inherently consist of homopolymers and a high polydispersity. Leveraging the understanding of polymer adsorption/desorption in solution onto silica and C18-modified silica surfaces during HPLC, we demonstrate how a large scale purification and fraction is achievable using flash chromatography. Finally, the viscoelastic properties of the purified, homopolymer-free block copolymers will be discussed.

[1]NSF PIRE Polymer Program

12:51PM J43.00009 Effects of B Segment Polydispersity on ABA Triblock Copolymer Phase Behavior , MAHESH MAHANTHAPPA, JOAN SCHROEDER, ANDREW SCHMITT, ADAM SCHMITT, KYUHYUN IM, University of Wisconsin-Madison — Advanced polymerization techniques enable the synthesis of a variety of polymeric materials with well-defined chain architectures, compositions, and tunable molecular weights and molecular weight distributions. The inherent chain length polydispersity of polymers derived from these syntheses affects their ultimate materials properties and applications. Relying on tandem ring-opening metathesis polymerization with chain transfer (ROMP-CT) and atom transfer radical polymerization (ATRP), we have synthesized a series of poly(styrene-b-1,4-butadiene-b-styrene) triblock copolymers in which the polybutadiene blocks are polydisperse (Mw/Mn = 1.7-2.0) and the polystyrene end blocks are monodisperse (Mw/Mn = 1.05-1.30). We systematically explore the role of block polydispersity, a molecular chain length heterogeneity, on the melt-phase self-assembly behavior of these block copolymers. Using a combination of temperature-dependent X-ray scattering and transmission electron microscopy, we demonstrate that monodispersity is not a necessary condition for molecular self-assembly into well-defined supramolecular morphologies. The origins of these effects are discussed and a preliminary experimental phase portrait for this system is presented.

1:03PM J43.00010 Elucidation of an Unusual Pull Out Mechanism for the Additive-Driven Assembly of Poly(ethylene oxide)-Poly(propylene oxide)-Poly(ethylene oxide)Tri-block Copolymers , VIKRAM DAGA, University of Massachusetts Amherst, HUA-GEN PENG, Polymers Division, NIST, YING LIN, University of Massachusetts Amherst, WEN-LI WU, CHRISTOPHER SOLES, Polymers Division, NIST, JAMES WATKINS, University of Massachusetts Amherst — The addition of poly(acrylic acid) (PAA) to disordered poly(ethylene oxide)-poly(propylene oxide)-poly(ethylene oxide) tri-block copolymers induces microphase segregation to yield well ordered blends with sub-10 nm domain sizes. Unexpectedly, even with large changes in the chain length (up to 10 times that of tri-block copolymer) and loading of PAA (>40%), the domain spacing of the ordered blend remains nearly invariant although order-to-order transitions are still observed. Here we use neutron scattering and selective deuteration of the tri-block copolymer to probe phase segregation and structure in these systems. One interesting observation is the emergence of a pullout mechanism during ordering in which PEO chain segments are drawn across the interface of a mixed PEO-PPO phase to stabilize the addition for PAA and to create a mixed PAA-PEO phase.

1:15PM J43.00011 Influence of thermal fluctuations on nucleation in a diblock copolymer melt , RUSSELL SPENCER, ROBERT WICKHAM, University of Guelph — We study the effect of thermal fluctuations on the kinetics of nucleation of lamellar droplets from a metastable cylinder phase in a diblock copolymer melt by simulating the time-dependent Landau-Brazovskii model in three dimensions. We investigate the shift in the location of phase coexistence, due to fluctuations, as well as changes in nucleus shape, critical size and interfacial velocity. We also examine the kinetics of the transition in the spinodal regime.

1:27PM J43.00012 Disorder-to-Order Transition Induced by Alkyne/Azide Click Chemistry in Diblock Copolymer Thin Films , XINYU WEI, Department of Polymer Science and Engineering, University of Massachusetts Amherst, WEI CHEN, Center for Nanoscale Materials, Argonne National Laboratory, JOSEPH STRZALKA, Advanced Photon Source, Argonne National Laboratory, THOMAS RUSSELL[1], Department of Polymer Science and Engineering, University of Massachusetts Amherst — The thin film morphology of binary blends of poly(ethylene oxide)-*block*-poly(n-butyl methacrylate-*random*-propargyl methacrylate) (PEO-*b*-P(nBMA-*r*-PgMA)) diblock copolymer and Rhodamine B azide was investigated. During thermal annealing, the click reaction between the alkyne-bearing diblock copolymer and the azide lead to a significant increase in non-favorable segmental interaction and thus microphase separation of the block copolymer. Different morphologies were realized by controlling block copolymer composition and the mole ratio between the alkyne and azide groups. The effects of film thickness and annealing temperature on microdomain orientation and lateral ordering were also revealed. Our studies suggest a promising approach to fabricate nanostructured materials with long-range lateral ordering.

[1]To whom correspondence should be addressed

1:39PM J43.00013 Correlation in SANS χ upon heating and pressurization for a diblock copolymer[1] , JUNHAN CHO, JUMI LEE, Dankook University, DU YEOL RYU, Yonsei University — The response of phase behavior to pressure for an A-*b*-B diblock copolymer in the disordered state has been studied by small-angle neutron scattering (SANS). Deuterated polystyrene-*b*-poly(n-propyl methacrylate) (dPS-*b*-PPrMA) copolymer, which possesses ordering transition upon heating and baroplasticity (suppressed demixing by pressurization), was taken as our model system. It was shown that effective Flory-Huggins parameter χ_F from scattering intensity profiles upon heating and pressurization forms a characteristic curve that is a function of pressure increment ΔP ($\equiv P - P_0$) divided by temperature dependent bulk modulus B_0 at a reference pressure P_0. Each isotherm of χ_F is superposed into the curve by a scale factor τ determined by B_0. The scattering intensity maxima I_{max}, which is governed by χ_F, were also shown to reveal a similar superposition.

[1]The authors acknowledge support from NRF of Korea through Regional Scientist program and Nuclear R&D program.

1:51PM J43.00014 Rouse and Entangled Dynamics in Coarse Grain Polymeric Systems[1] , ABELARDO RAMIREZ-HERNANDEZ, DARIN PIKE, Department of Chemical and Biological Engineering, University of Wisconsin-Madison, USA, FRANCOIS DETCHEVERRY, Universite Lyon 1 and CNRS, France, JUAN DE PABLO, Department of Chemical and Biological Engineering, University of Wisconsin-Madison, USA — The understanding of the kinetics of microphase ordering of block copolymers is important for controlling the morphology of these polymeric materials. Much of our current understanding of the equilibrium morphologies of block copolymers has emerged from studies using Self-Consistent Field Theory (SCFT), in which the effect of non-crossability of chains is not taken into account. In this work, we use a particle-based coarse grain model of block copolymers, and introduced elastic slip-links to model the effect of entanglements on the dynamics of the melts. These effects can be important when the self-assembly occurs in non-equilibrium conditions. We show that our model is able to reproduce both Rouse and Entangled dynamical behavior for a homopolymeric melt. We apply our computational approach to block copolymer systems under equilibrium and non equilibrium (shear flow) conditions.

[1]This work is supported by the National Science Foundation through the Nanoscale Science and Engineering Center at the University of Wisconsin

2:03PM J43.00015 Facile Synthesis and Characterization of Well-Defined Rod-Coil Block Copolymers Composed of Regioregular Poly(3-hexyl thiophene) , HONG CHUL MOON, JIN KON KIM, Pohang University of Science and Technology — We synthesized rod-coil block copolymers composed of regioregular poly(3-hexyl thiopene) (P3HT) block via anionic coupling reaction. Three different coil blocks (poly(2-vinyl pyridine) (P2VP) and polyisoprene (PI)) and poly(methyl methacrylate) (PMMA)) were selected. For the synthesis of P2VP-*b*-P3HT-*b*-P2VP and P2VP-*b*-P3HT-*b*-P2VP, the chain ends of the P3HT were capped by the aldehyde group. On the other hand, phenyl acrylate (PA)-capped P3HT was prepared for coupling reaction with living PMMA anions. When the excess amount of the used living anions was removed by column chromatography, all of the neat block copolymers showed lower PDI without leaving any homopolymers. We also investigated the optical property and thin film morphology of synthesized various block copolymers.

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J44 DPOLY DFD: Focus Session: Kinetic Control of Solution Assemblies A309

11:15AM J44.00001 Helical Assembly of Janus Particles , JONATHAN WHITMER, Department of Physics, University of Illinois at Urbana-Champaign, QIAN CHEN, SHAN JIANG, SUNG CHUL BAE, STEVE GRANICK, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, ERIK LUIJTEN, Department of Materials Science and Engineering and Department of Engineering Sciences and Applied Mathematics, Northwestern University — Amphiphilic Janus particles, which have hydrophobic and hydrophilic hemispheres, assemble into a variety of clusters depending on salt concentration and particle volume fraction. At low salt concentration, repulsion due to surface charges keeps cluster sizes small, whereas at higher salt concentrations beautiful elongated helices of tetrahedra emerge. We demonstrate that the emergence of these helical structures is a nonequilibrium effect, and that kinetic selection drives formation of polytetrahedral shapes relative to polyhedral shapes which are entropically more favorable.

11:27AM J44.00002 Nucleation of Nanoparticle Superclusters from Solution[1] , SIDDIQUE J. KHAN, C.M. SORENSEN, A. CHAKRABARTI, Dept. of Physics, Kansas State University — Colloids of surface ligated nanoparticles (NP) often act as solutions with the NP displaying reversible temperature and solvent dependent solubility. In many cases when the nanoparticles are highly uniform, the precipitating solid is a two- or three-dimensional superlattice of the nanoparticles. Thus there is strong analogy to the phase behavior of molecular solutions, and it is reasonable to ask what controls the phase behavior of nanoparticle solutions and what is the nature of nucleation and growth of the insoluble phase? We have recently developed [1] a phenomenological model for the effective interaction potential between two ligated gold nanoparticles. In the current work, we carry out Brownian Dynamics simulations using this NP-NP interaction potential. We will report results from our simulations for both dynamics and shape of pre- nucleating and post-nucleating superclusters.

[1] S.J. Khan, F. Pierce, C.M. Sorensen and A. Chakrabarti, Langmuir, 25, 13861 (2009).

[1]Supported by NSF NIRT grant CTS0609318.

11:39AM J44.00003 Directing the self-assembly of polyhedral silver nanocrystals , MICHAEL GRUENWALD, University of California at Berkeley, JOEL HENZIE, ASAPH WIDMER-COOPER, PHILLIP GEISSLER, PEIDONG YANG — Self-assembly of nanocrystals with complex shapes requires precise control of nanoscale interactions and driving forces. Here we show with experiment and simulation that large 3D supercrystals with exceptional order can be assembled by tuning the shape and attraction between polyhedral building blocks. When passivated with adsorbing polymer, Ag nano-polyhedra can behave as quasi-hard particles, and assemble into their densest known packings under a simple gravitational driving force. Excess polymer in solution induces depletion attractions that can stabilize less dense, ordered packings. In the case of octahedra, controlling polymer concentration allows us to tune between the well-known Minkowski lattice, and a novel packing with complex helical motifs. Such large-scale ordered arrangements of Ag nanocrystals provide many possibilities for designing scalable 3D plasmonic metamaterials with applications including chemical and biological sensing, nanophotonics and photocatalysis.

11:51AM J44.00004 Nanoscale systems assembled with DNA: from principles to rational design , OLEG GANG, Brookhaven National Laboratory-Center for Functional Nanomaterials — This abstract not available.

12:27PM J44.00005 A direct comparison of crystallization transitions and glassy dynamics in polymers and colloids[1] , ROBERT S. HOY, COREY S. O'HERN, Yale University — Using computer simulations, we compare the freezing transitions in systems composed of N spherical particles with and without covalent-bonding constraints. Linear polymer chains with $N-1$ permanent covalent bonds are compared to "colloidal" systems with the same nonbonded interactions but no covalent bonds. In the "sticky hard sphere" limit, where covalent bonds act as holonomic constraints, the melting temperatures $T_{\rm melt}$ for both polymers and colloids (with the same N) are inversely proportional to the number of unconstrained degrees of freedom. We also examine the effect of the thermal quench rate $|\dot{T}|$ on collapse. At $|\dot{T}|$ below a lower "critical" value, which decreases rapidly with increasing N, polymers and colloids form similar ground states. This critical value is lower for polymers than colloids and has different N-dependence. In both cases, the dynamics of the systems slow down near $T_{\rm melt}$ as the system approaches isostaticity. For high $|\dot{T}|$, glassy dynamics produces disordered final states. At intermediate $|\dot{T}|$, we find complex nonmonotonic behavior in T, which we relate to the very different rearrangement kinetics of polymeric and colloidal clusters.

[1]Support from NSF grant no. CMMT-1006527 is gratefully acknowledged.

12:39PM J44.00006 Dynamics of Fatty Acid Single Molecule Islands on Metal-exchanged Mica , MOURAD CHENNAOUI, ALEKS PONJAVIC, JANET WONG, Imperial College London, London, UK — Under certain conditions, surface-active molecules are known to self-organise into SAMs according to two main driving forces: molecular surface adsorption via diffusive/convective transport, and surface reorganisation and growth. For the latter in-situ methods are required to deconvolute the complex underlying kinetics and dynamics. To this end, a single molecule fluorescence imaging technique is used to observe the dynamics of fatty acid molecules on different metal-exchanged Mica substrates (K, Li, H). It is shown that the molecular surface re-organisation proceeds via an initial islandisation step. These islands spread and grow until forming a stable and organised SAM. Islands formation kinetics/dynamics according to different surface metal types is investigated. Diffusive mechanisms within and between the islands are also explored.

12:51PM J44.00007 Multicompartment and multigeometry nanostructures with block copolymers and kinetic control , DARRIN POCHAN, University of Delaware — The combination of charged block copolymer architecture with the kinetic control of solvent processing offers great flexibility for the creation of new assembled morphologies in solution and outstanding ability to control and manipulate those morphologies. When charged, acidic blocks are present, assembled structures are tunable in a well-defined way via co-assembly of organic bases with adjustable chain structure and control of the solution assembly pathway. A rich variety of polymeric micelles have been made such as toroids, disks, and helical cylinders from poly(acrylic acid)-*block*-poly(methyl acrylate)-*block*-polystyrene (PAA-*b*-PMA-*b*-PS) triblock copolymers in THF/water mixtures with multiamines to complex with the PAA. Both the type and amount of multiamine were found to be critical for formation of specific micelles. Kinetic pathways and temporal stabilities of different micelles and nanoscale aggregates have also been studied. Due to low chain exchange dynamics between block copolymeric micelles in solution, global thermodynamic equilibrium is extremely difficult, if not impossible, to achieve. In our block copolymer/THF/water/multiamine quaternary systems, thermodynamics and kinetics of morphological evolution are governed by three important factors, including chain length of hydrophobic blocks, ratio of THF to water, and the interaction of multiamine with hydrophilic PAA block in the corona. Slow kinetics associated with these factors in solution greatly hinders the system from reaching a global equilibrium. However, by taking advantage of slow kinetics behavior of polymeric micelles in solution, one can purposely produce multicompartment micelles and mulitgeometry micelles by now mixing different PAA-containing block copolymers together but forcing them to ultimately reside in the same nanoscale structure through kinetic processing. While kinetically trapped in common nanostructures, local phase separation can occur producing compartments. This compartmentalization can be used within common micelle geometries to make complex spheres and cylinders or can be used to make new nanostructures such as multigeometry aggregates (e.g. hybrid cylinder-sphere aggregates). All is possible through the kinetic control of the assembly process.

1:27PM J44.00008 Determination of critical micelle concentrations in ionic liquid/block copolymer systems , MICHELLE MOK, TIMOTHY LODGE, University of Minnesota — The micellization of block copolymers in ionic liquids is of great interest, due to their potential as cargo carriers for separations, transfer and extraction applications. In this study, we investigate the critical micelle concentration (cmc) of block copolymers in ionic liquids using fluorescence-based techniques. Specifically, the cmcs of poly(styrene-b-ethylene oxide) and poly(styrene-b-methylmethacrylate) copolymers were determined from the polarity-sensitive emission spectra of pyrene probes. At the onset of micellization, the probes preferentially partition to the non-polar styrene cores, analogous to pyrene-based cmc studies of aqueous micelle systems. The cmcs are explored as a function of copolymer block molecular weight and composition, as well as ionic liquid composition.

1:39PM J44.00009 Hierarchical Helical-Assembly of Conjugated Poly(3-hexylthiophene)-*b*-poly(3-triethylene glycol-thiophene) Diblock Copolymers , EUNJI LEE, BRENTON HAMMER, TODD EMRICK, RYAN C. HAYWARD, Department of Polymer Science and Engineering, University of Massachusetts, Amherst — One-dimensional crystalline fibrillar assemblies of poly(3-hexylthiophene) (P3HT)-based materials hold significant potential for fabrication of low-cost optoelectronic devices. We have studied the crystallization-driven assembly of a series of poly(3-hexylthiophene)-*block*-poly(3-triethylene glycol-thiophene) (P3HT-*b*-P3TEGT) diblock copolymers, which provide a large contrast in solubility due to the presence of non-polar (hexyl) and polar (TEG) side-chains. P3HT-*b*-P3TEGT diblock copolymers were found to form well-defined fibrillar structures in mixed solvents of chloroform and methanol, with lengths could be tuned easily by changing the solvent composition or relative block lengths. For polymers containing relatively short P3TEGT blocks, the resulting fibers show twisted ribbon-like structures. For appropriate block ratios, complexation of the TEG side chains to alkali metal cations drives formation of clearly defined single helical ribbons and superhelical structures.

1:51PM J44.00010 Molecular simulation study of random block copolymer films prepared through solvent evaporation , DMITRY BEDROV, KEITH HAMBRECHT, GRANT SMITH, University of Utah — Molecular simulations have been used to study equilibrium and non-equilibrium morphologies of random block copolymer films prepared through solvent evaporation. The polymer chains are comprised of "A" and "B" beads connected by FENE springs. Chains comprised of six blocks (ten beads each) and representing all possible combinations of A and B blocks were used to form films with 50/50 A/B fraction. Bead-bead interactions were chosen such that one of the blocks had higher glass transition temperature than the other and that the A and B blocks were incompatible in absence of the solvent. Initially the polymer chains were dissolved in a monomeric solvent at 75/25 solvent/polymer ratio. Then, polymer films were formed through solvent evaporation at various processing parameters. The nanoscale structure and viscoelastic properties of the polymer were investigated as a function of solvent quality, segment incompatibility and rate of evaporation. It was found that when the temperature is below the glass transition temperature of one of homopolymers, the morphology and properties of the film are strongly dependent on evaporation rate.

2:03PM J44.00011 Blood Clotting-Inspired Control of Single-Chain Molecules in Flows , CHARLES SING, ALFREDO ALEXANDER-KATZ, MIT — Recent experimental evidence has demonstrated a clear link between mechanical stimuli and the activation of von Willebrand Factor (vWF), a protein that plays a critical role in the blood clotting cascade. This protein exhibits counter-intuitive conformational and adsorption responses that suggest novel ways of controlling the single-chain dynamics of polymer chains. Specifically, we are using simulation and theoretical approaches to elucidate the fundamental physics that govern globule-stretch transitions in collapsed polymers due to the effect of fluid flows. We begin to extend this general approach to the case of globule adsorption-desorption transitions in the presence of fluid flows, and demonstrate how kinetic considerations must be taken into account to describe the basic features of these transitions. We expect that these results will both allow the development of novel techniques for single-chain targeting and assembly and offer insight into the physiological behavior of vWF.

Tuesday, March 22, 2011 11:15AM - 2:15PM –

Session J45 DAMOP: Focus Session: Non-equilbrium Physics with Cold Quantum Gases A310

11:15AM J45.00001 Universal Dynamics Near Quantum Critical Points , ANATOLI POLKOVNIKOV, Boston University — asp@physics.bu.edu

11:51AM J45.00002 Dynamics of a finite-rate quantum quench in an ultra-cold atomic BCS superfluid[1] , CHIH-CHUN CHIEN, BOGDAN DAMSKI, Los Alamos National Laboratory — We study dynamics of an ultra-cold atomic BCS superfluid driven towards the BCS superfluid-Fermi liquid quantum critical point by a gradual decrease of the pairing interaction. We analyze how the BCS superfluid falls out of equilibrium and show that the non-equilibrium gap and Cooper pair size reflect critical properties of the transition. We observe three stages of evolution: adiabatic where the Cooper pair size is inversely proportional to the equilibrium gap, weakly non-equilibrium where it is inversely proportional to the non-equilibrium gap, and strongly non-equilibrium where it decouples from both equilibrium and non-equilibrium gap. These phenomena should stimulate future experimental characterization of non-equilibrium ultra-cold atomic BCS superfluids.

[1]This work is supported by U.S. Department of Energy through the LANL/LDRD Program.

12:03PM J45.00003 Slow quench dynamics of a trapped one-dimensional Bose gas confined to an optical lattice , JEAN-SEBASTIEN BERNIER, Centre de physique theorique, Ecole Polytechnique, GUILLAUME ROUX, LPTMS, Universite Paris-Sud, CORINNA KOLLATH, Centre de physique theorique, Ecole Polytechnique — We analyze the effect of a linear time-variation of the interaction strength on a trapped one-dimensional Bose gas confined to an optical lattice. The evolution of different observables such as the experimentally accessible onsite particle distribution are studied as a function of the ramp time using time-dependent exact diagonalization and density-matrix renormalization group techniques. We find that the dynamics of a trapped system typically display two regimes: for long ramp times, the dynamics are governed by density redistribution, while at short ramp times, local dynamics dominate as the evolution is identical to that of an homogeneous system. In the homogeneous limit, we show that the energy absorbed scales non-trivially with the ramp time.

12:15PM J45.00004 Quench dynamics of paired states of fermions in two dimensions with breaking of parity and time-reversal symmetries[1] , NOAH BRAY-ALI, Joint Quantum Institute, National Institute of Standards and Technology-Gaithersburg and University of Maryland, College Park — Resonantly paired fermions in two spatial dimensions with breaking of parity and time-reversal symmetry are believed to exhibit two topologically distinct phases at low temperature: the weak-pairing (Bardeen-Cooper-Schrieffer or BCS) phase and the strong-pairing (Bose-Einstein condensate or BEC) phase. We examine the dynamic response of each phase to a rapid quench towards and away from the quantum critical regime. The weak-pairing (BCS) phase has a higher residual defect concentration after the quench than the strong-pairing (BEC) phase. We relate this to the presence of a topologically protected, Majorana fermion edge excitation in the weak-pairing phase, and propose quench dynamics as a practical, experimental probe of this excitation in these systems.

[1]Funded by National Research Council Postdoctoral Research Associateship.

12:27PM J45.00005 Title: Time-Dependent Mean Field Theory for Quench Dynamics in correlated electron systems , MARCO SCHIRO', Princeton Center for Theoretical Science, Princeton University, MICHELE FABRIZIO, SISSA, International School for Advanced Studies — A simple and very flexible variational approach to the out-of-equilibrium quantum dynamics in strongly correlated electron systems is introduced through a time-dependent Gutzwiller wavefunction. As an application, we study the simple case of a sudden change of the interaction in the fermionic Hubbard model and find at the mean field level an extremely rich behaviour. In particular, a dynamical transition between small and large quantum quench regimes is found to occur at half-filling, in accordance with the analysis of Eckstein *et al.*, Phys. Rev. Lett. **103**, 056403 (2009), obtained by dynamical mean field theory, that turns into a crossover at any finite doping.

12:39PM J45.00006 Non-equilibrium dynamics and heating of cold atoms in optical lattices , ANDREW DALEY, University of Pittsburgh, HANNES PICHLER, PETER ZOLLER, University of Innsbruck — We study the dissipative many-body dynamics of cold atoms in optical lattices that is induced by incoherent scattering of light from the lattice lasers. The resulting heating process is intrinsically non-equilibrium, and involves an important interplay between the atomic physics of the spontaneous emission process and the many-body physics of the state present in the system. In particular, we observe important differences for strongly and weakly interacting regimes, as well as a strong dependence on the sign of the laser detuning from the excited atomic state. We compute heating rates and changes to characteristic correlation functions based on a microscopic master equation. In 1D this equation can be propagated exactly by combining time-dependent density matrix renormalization group (t-DMRG) methods with quantum trajectory techniques.

12:51PM J45.00007 Quantum effects on Fermi-Pasta-Ulam recurrence in ultracold lattice bosons[1] , IPPEI DANSHITA, RIKEN, RAFAEL HIPOLITO, Boston University, VADIM OGANESYAN, City University of New York, ANATOLI POLKOVNIKOV, Boston University — We propose an experimental scheme for studying the Fermi-Pasta-Ulam (FPU) problem in a quantum mechanical regime with use of ultracold one-dimensional Bose gases in an optical lattice. In the classical limit, we identify parameter regions in which FPU recurrence can occur in this system. The strength of quantum fluctuations can be widely controlled by tuning the number of atoms per lattice sites (filling factor). To investigate the effects of quantum fluctuations on the FPU recurrence, we simulate the real time dynamics of the Bose-Hubbard model by means of the exact numerical method of time-evolving block decimation. We show that strong quantum fluctuations cause significant damping of the FPU oscillation.

[1]I. D. is supported by KAKENHI (22840051) from JSPS.

1:03PM J45.00008 Dynamic Stimulation of Phase Coherence in Lattice Bosons[1] , ANDREW ROBERTSON, VICTOR GALITSKI, University of Maryland, GIL REFAEL, California Institute of Technology — The existence of superfluidity depends on the energy distribution of excitations in a system. However, the distribution at thermal equilibrium is rarely optimal for the manifestation of long-range phase coherence. We show that by pushing a system of lattice bosons out of equilibrium with periodic driving, it is possible to increase or decrease the phase coherent region in the phase diagram of the Bose-Hubbard model. We demonstrate this by calculating the non-equilibrium spatial correlation function using a synthesis of Keldysh and Floquet theories. This work is supported by DARPA-MTO.

[1]Supported by DARPA-MTO

1:15PM J45.00009 Phase Kink Dynamics in fluctuating Bose condensates , AMY CASSIDY, LUDWIG MATHEY, CHARLES CLARK, Joint Quantum Institute, NIST and University of Maryland — We study the dynamics of Bose gases following a phase imprint. Numerical results within truncated Wigner approximation, which includes both quantum and thermal fluctuations, are compared with analytical predictions. In order to emphasize the effects of fluctuations in these approximations, we also compare our results with dynamics governed by the Gross Pitaevskii equation. We study the dynamics of several observables, including the density and single-particle and density-density correlation functions, with particular focus on experimentally relevant quantities.

1:27PM J45.00010 Exploring topological phases with quantum walks[1] , TAKUYA KITAGAWA, MARK RUDNER, EREZ BERG, EUGENE DEMLER, Harvard University — The quantum walk was originally proposed as a quantum mechanical analogue of the classical random walk, and has since become a powerful tool in quantum information science. In this talk, we show that the dynamical protocols called discrete time quantum walks provide a versatile platform for studying topological phases, which are currently the subject of intense theoretical and experimental investigation. In particular, we demonstrate that recent experimental realizations of quantum walks simulate a non-trivial one dimensional topological phase. With simple modifications, the quantum walk can be engineered to realize all of the topological phases which have been classified in one and two dimensions. We further discuss the existence of robust edge modes at phase boundaries, which provide experimental signatures for the non-trivial topological character of the system. Reference: T.Kitagawa, M.Ruder, E.Berg, and E. Demler, Phys. Rev. A 82, 033429 (2010)

[1]NSF grant DMR 0705472, CUA, DARPA OLE, AFOSR MURI, NSF grants DMR-0757145(E.B), NSF Grants DMR 090647 and PHY 0646094(MSR).

1:39PM J45.00011 Universal energy distribution in thermally isolated driven systems , LUCA D'ALESSIO, Boston University, GUY BUNIN, Technion, Haifa, ANATOLI POLKOVNIKOV, Boston University, YARIV KAFRI, Technion, Haifa — The evolution of the energy distribution of a thermally isolated and repeatedly driven system is studied. A general formalism to calculate the width of the energy distribution is derived and the result is compared with the thermal width. This comparison allow us to identify two regimes: quasi-thermal and run-away. In the quasi-thermal regime the width on the energy distribution of the driven system is proportional to the thermal width with a protocol-dependent universal coefficient. In the run-away regime the width of the energy distribution is an universal function of the energy with an exponent different from the thermal case. A simple formulation in terms of entropy production allow us to distinguish these two regimes. Examples and application to both classical and quantum system (mainly cold atoms) are presented.

1:51PM J45.00012 Ramping through Superfluid-to-Mott transition in the Bose-Hubbard Model , BERNHARD WUNSCH, DAVID PEKKER, TAKUYA KITAGAWA, Harvard University, EFSTRATIOS MANOUSAKIS, Florida State University, EUGENE DEMLER, Harvard University — We discuss equilibrium and dynamic properties of cold bosonic atoms in optical lattices which can be described by the Bose-Hubbard Model. Motivated by recent experiments we study local density fluctuations and their correlations both in equilibrium and for a ramp from the superfluid to the Mott regime. We compare mean-field Gutzwiller approach with exact diagonalization studies and analyze the effect of a trapping potential. In order to describe fluctuations and finite temperature we include quadratic fluctuations on top of the mean field.

2:03PM J45.00013 Dynamics of thermalisation: a Gaussian regime[1] , SAM GENWAY, Imperial College London, ANDREW HO, Royal Holloway, University of London, DEREK LEE, Imperial College London — We study numerically the thermalisation and temporal evolution of subsystems in a fermionic Hubbard model prepared far from equilibrium at a definite energy. Taking motivation from cold atoms in optical lattices with single-site addressability, we consider measurements on a two-site subsystem. We ask the question: how do observables on the subsystem thermalise when the total system is in a pure state? Even for very small systems near quantum degeneracy, the subsystem can reach a steady state resembling thermal equilibrium. This occurs for a non-perturbative coupling between the subsystem and the rest of the lattice where relaxation to equilibrium sharply contrasts perturbative results. To examine the extent to which this behaviour is generic for small quantum systems, we also investigate small Bose-Hubbard model systems and fermionic systems with random couplings between the subsystem and the rest of the lattice.

[1]Work supported by EPSRC.

2:00PM - 2:00PM –
Session K1 APS: Poster Session II (2:00pm - 5:00pm) Hall D

K1.00001 QUANTUM FLUIDS AND SOLIDS –

K1.00002 Riemann-Hypothesis Millennium-Problem(MP) Physics Proof via CATEGORY-SEMANTICS(C-S)/F=C Aristotle SQUARE-of-OPPOSITION(SoO) DEduction-LOGIC DichotomY , J. BAEZ, M. LAPIDARYUS, EDWARD CARL-LUDWIG SIEGEL, FUZZYICS=CATEGORYICS(SON OF TRIZ)/CATEGORY-SEMANTICS — Riemann-hypothesis physics-proof combines: Siegel-Antonoff-Smith[AMS Joint Mtg.(2002)-Abs.973-03-126] digits on-average statistics HIII[Am. J. Math 123, 3, 887(1996)] logarithm-function's (1,0)-fixed-point base=units=scale-invariance proven Newcomb[Am. J. Math. 4, 39(1881)]-Weyl[Goett. Nachr.(1914); Math. Ann. 7, 313(1916)]-Benford[Proc. Am. Phil. Soc. 78, 4, 51(1938)]-law [Kac, Math. of Stat.-Reasoning(1955); Raimi, Sci. Am. 221, 109(1969)] algebraic-inversion to ONLY Bose-Einstein quantum-statistics(BEQS) with digit d = 0 gapFUL Bose-Einstein Condensation(BEC) insight that digits are quanta are bosons were always digits, via Siegel-Baez category-semantics tabular list-format matrix truth-table analytics in Plato-Aristotle classic "square-of-opposition" : FUZZYICS=CATEGORYICS/Category-Semantics, with Goodkind Bose-Einstein condensation(BEC) ABOVE ground-state with/and Rayleigh(cut-limit of "short-cut method";1870)-Polya(1922)-"Anderson"(1958) localization [Doyle and Snell, Random-Walks and Electrical-Networks, MAA(1981)-p.99-100!!!].

K1.00003 Drag effects in a system of electrons and microcavity polaritons , OLEG BERMAN, ROMAN KEZRASHVILI, New York City College of Technology of the City University of New York, YURII LOZOVIK, Institute of Spectroscopy — The theory of the drag effects in the system of spatially separated electrons and excitons in coupled quantum wells (QWs) embedded in an optical microcavity is developed. It is shown that for systems of spatially separated interacting quasiparticles is the possibility of controlling the motion of the quasiparticles of one subsystem by altering the parameters of state of the quasiparticles in the other subsystem, for example, controlling the flow of polaritons or exciton using a current of electrons. At low temperatures, the electron current dragged by the polariton flow is strongly suppressed and hence, the absence of the electron current indicates the superfluidity of polaritons. However, the polariton flow can be dragged by the electrons, and, therefore, there is a transport of photons along the microcavity, which decreases with rise of the superfluid component and can be observed through the change in angular distribution of photons discussed above. At high temperatures, from one hand, the existence of the electric current in the electron QW indicates the exciton flow in the other QW, and from the other hand, the electron current in one QW induces the exciton flow in the other QW via the drag of excitons by the electrons. The drag coefficients for the polariton-electron systems are calculated and analyzed.

K1.00004 UNDERGRADUATE RESEARCH / SOCIETY OF PHYSICS STUDENTS –

K1.00005 Celebrating Five Years of SPS: A lesson in building physics outreach from scratch , JEROME T. MLACK, ROBERTO RAMOS, Drexel University — It has been almost five years since SPS was revived at Drexel University. Until 2006 Drexel SPS had been inactive for two decades. In this poster we report the challenges of building a chapter from scratch and turning it into an active and award-winning group. The students are constantly involved in mentorship programs in the underserved Philadelphia school district, while regularly seeking opportunities to perform and present research. We report the various activities we have initiated, and the lessons we have learned from them.

K1.00006 Exploring the Depletion Layer: An Investigation into How Water Reacts when Confined to a Hydrophobic Surface , ISAAC MARX, ADELE POYNOR, Allegheny College Physics Department — We observe water interacting with surfaces everyday. It forms spherical drops on hydrophobic surfaces, such as a freshly waxed car, and it spreads out on hydrophilic surfaces. However, water acts much differently when it is confined to a hydrophobic area. In our experiment, Surface Plasmon Resonance (SPR) is utilized to find differences in surface conditions. Tests are done for the interface of a hydrophobic surface surrounded by water and also for a hydrophobic surface surrounded by methanol, which we know will not form a depletion layer. With this data we are able to analyze the optical properties of the depletion layer in much greater detail.

K1.00007 Exploring Isothermal Layers in the Stable Atmospheric Boundary Layer[1] , JOSEPH WILKINS, University of Louisville — Simulating the stable atmospheric boundary-layer presents a significant challenge to numerical models due to the interactions of several processes with widely varying scales. The goal of this project is to more clearly define the cause of isothermal layers observed during the Meteorological Experiment in Arizona's Meteor Crater and to test the National Taiwan University/Purdue University (NTU/P) model in stable environments with complex terrain. The NTU/P model is able to utilize the actual terrain data with minimal smoothing for stability. We have found that isothermal profiles can be generated by the standing wave that develops due to weak wind flowing over the crater. However, the horizontal heterogeneity is greater than observed. Continued effort will explore enhancing horizontal mixing due to turbulence and radiative transfer.

[1]Louis Stokes Alliances for Minority Participation Program, Summer Research Opportunities Program.

K1.00008 Drug Loading of Mesoporous Silicon[1] , ANNE MOFFITT, JEFF COFFER, MENGJIA WANG, Texas Christian University — The nanostructuring of crystalline solids with low aqueous solubilities by their incorporation into mesoporous host materials is one route to improve the bioavailability of such solids. Earlier studies suggest that mesoporous Si (PSi), with pore widths in the range of 5-50 nm, is a candidate for such an approach. In this presentation, we describe efforts to load curcumin into free-standing microparticles of PSi. Curcumin is a compound extracted from turmeric root, which is an ingredient of curry. Curucmin has shown activity against selected cancer cell lines, bacteria, and other medical conditions. However, curcumin has a very low bioavailability due to its extremely low water solubility (0.6μg/mL). Incorporation of curcumin was achieved by straightforward loading of the molten solid at 185°C. Loading experiments were performed using PSi particles of two different size ranges, 45-75 μm and 150-250 μm. Longer loading times and ratio of curcumin to PSi leads to a higher percentage of loaded curcumin in both PSi particle sizes (as determined by weight difference). The extent of curcumin crystallinity was assessed by x-ray diffraction (XRD). The solubility and release kinetics of loaded curcumin from the PSi was determined by extraction into water at 37°C, with analysis using UV-VIS spectrometry.

[1]NSF-REU and TCU

K1.00009 Identification of gram-negative and gram-positive bacteria by fluorescence studies , JONATHAN DEMCHAK, JOSEPH CALABRESE, MARIAN TZOLOV, Lock Haven University of PA — Several type strains of bacteria including Vibrio fischeri, Azotobacter vinelandii, Enterobacter cloacae, and Corynebacterium xerosis, were cultured in the laboratory following standard diagnostic protocol based on their individual metabolic strategies. The bacterial cultures were not further treated and they were studied in their pristine state (pure culture - axenic). The fluorescent studies were applied using a continuous wave and a pulsed excitation light sources. Emission and excitation spectra were recorded for the continuous wave excitation and they all show similar spectral features with the exception of the gram positive bacteria showing vibronic structures. The vibrational modes involved in these vibronic bands have energy typical for carbon-carbon vibrations. The fluorescence is quenched in addition of water, even a very thin layer, which confirms that the observed spectral features originate from the outer parts of the bacteria. These results allow to conclude that the fluorescence spectroscopy can be used as a method for studying the membranes of the bacteria and eventually to discriminate between gram positive and gram negative bacteria. The pulsed experiments show that the fluorescence lifetime is in the sub-microsecond range. The results indicate that the observed spectra are superposition of the emission with different lifetimes.

K1.00010 Electrocardiogram analysis through time discrete Fourier transform[1] , CAMERON LANCASTER, GUOPING ZHANG, Department of Physics, Indiana State University — The motivation for this research is to find an alternative method to diagnose heart conditions. This can be accomplished by analyzing wave patterns in EKG data, and using the Fourier Transform to compare steady wave patterns against fibrillating wave patterns. The two main contributors are the following: heart electricity and Fourier Transform. Also, it is recognized that ion movement has potential to change the frequency in any heart beat signal. This effect is caused due to a strong electrostatic attraction that causes the membrane capacitance to build charge. For a single ion focus, the Nernst Potential influences the equilibrium potential for the membrane of an ion. If two or more ions are contributing to an electric field charge, the Goldman-Hodgkin-Katz will find the membrane equilibrium potential. If a membrane has an efflux, or influx, of ions, then it is possible to get the passive flow of the electric current to zero. In continued research, we will gain knowledge of solving equations; such as ionic flux, quantitative diffusion, electric current density, and more. The finishing portion of this research will be to compare the Fourier Transformed wave graphs to determine heart conditions.

[1]Supported by U.S. Department of Energy under Contract No. DE-FG02-06ER46304 and Indiana State University.

K1.00011 In-Vivo Proton Therapy Dosimetry Using Scintillating Fiber Technology , ASHLEY CETNAR, Grove City College, PAUL GUEYE, Hampton University — Proton therapy is a cancer treatment modality that uses high-energy proton beams to irradiate cancerous cells while minimizing the radiation to healthy tissue. Because of its Bragg peak distribution, a proton is more efficient in localizing doses than conventional x-ray therapy. When the protons interact within the body, there are many reactions that induce secondary radiation. To date, there is still no accurate device available that is capable of measuring the beam profile and effective dose delivery during the treatment. This research focused on the use scintillating fibers technology to measure the secondary emitted radiation exiting a water phantom tank and the delivery system bombarded by proton beams. A realistic Geant4 Monte Carlo simulation was also developed to provide additional information to further optimize our prototype. This poster presents the results obtained from preliminary experimental and simulated studies for a possible real time radiation detection system using scintillating fibers.

K1.00012 Approximating the Production Rate for Neutrino-Induced Pair-Production in Intense Magnetic Fields[1] , JORDAN RUSSELL, Hendrix College — We consider the production of electron-positron pairs by neutrinos in an intense magnetic field. Calculating the total production rate of these pairs requires summing over all of the allowed Landau levels of the electron and positron for a range of incoming neutrino energies. Because of the computationally challenging nature of this summation, the focus of my research has been to institute a set of estimations and calculate the total rate over the dominant region of Landau-level space. I will present an approximate relationship for field strengths in excess of the critical field.

[1]Supported by Hendrix College and Arkansas Space Grant Consortium Grant No. HC20066

K1.00013 The Optimization and Implementation of the Qweak Database , UDAI GARIMELLA, DAMON SPAYDE, Hendrix College, QWEAK COLLABORATION — The Qweak experiment at Thomas Jefferson National Accelerator Facility (J-Lab) is an attempt to precisely measure the parity violation observed in low energy electron-proton scattering events. Specifically, the weak charge of the proton will be measured to 4% error, which will, in turn, be used to calculate the "running" Weinberg mixing angle $(\sin^2(\theta_w))$. Since the Standard Model makes a firm prediction for $(\sin^2(\theta_w))$ at low energies, the experiment presents an opportunity to test the limits of this model. Any significant variation in$(\sin^2(\theta_w))$ from the expected value would be indicative of new physics, while an agreement would place strict constraints upon the existing model. In order to make an exact measurement of the weak charge, large amounts of data (almost 2200 hours worth) will be gathered. A large, robust database is needed to store and organize this data, so it can be analyzed in an easy and effective manner. The optimization and implementation of this database will be discussed.

K1.00014 Optimizing the Josephson Parametric Amplifier - A numerical study , ZLATKO MINEV, RAJAMANI VIJAYARAGHAVAN, IRFAN SIDDIQI, QNL, UC Berkeley — Recent progress in quantum information processing using superconducting circuits has stimulated interest in low noise amplifiers which operate at the quantum limit. Josephson parametric amplifiers (paramp) based on low quality factor (Q) non-linear resonators are a promising candidate for quantum state readout. We present a numerical study to optimize the paramp for dynamic range and bandwidth by investigating the lowest resonator Q compatible with high gain and low noise performance in the 4– 8 GHz range. We also investigate designs involving multiple junctions and weak-link junctions to further optimize the dynamic range. Such an amplifier can be used for single shot readout of superconducting qubits and real time detection of the quantum state—crucial developments for implementing quantum feedback and error correction.

K1.00015 Image processing of transmission ion microscopy webcam video with Iris software , NICOLE NEWTON[1], ARTHUR PALLONE[2], Murray State University — Scientists and engineers build simple, low-cost, webcam-based instruments for use in many disciplines. Analysis of the optical signal received through the three broadband color filters – red, green and blue – form the basis of many of those instruments. The CMOS sensors in webcam pixels also produce signals in response to ionizing radiations – such as alpha particles from a radioactive source. Simple alpha radiography has been demonstrated with a commercially available antistatic Po-210 source and a webcam modified to expose the pixel sensors. Analysis of webcam video with the Iris software is presented as a way to demonstrate other transmission ion microscopy imaging modes.

[1]undergraduate student
[2]faculty sponsor

K1.00016 Cathodes with modified morphology for polymer light emitting devices[1] , JACOB COX, MARIAN TZOLOV, Lock Haven University of PA — This work is the result of a junior year research project on fabrication and characterization of Polymer Light Emitting Devices (PLEDs). The PLEDs were created on top of indium tin oxide coated glass substrates, starting with a 60 nm thick hole injection layer, followed by an 80 nm layer of PPV-MEH polymer. The structures were finalized by a thermally evaporated aluminum film acting as the cathode for the device. We have concentrated on modifying the structure and morphology of the aluminum cathode in conjunction with the variation of the polymer film thickness. The devices were tested using current- voltage and light-voltage characteristics, light emission spectroscopy, device lifetime testing, profilometry, and optical microscopy of device degradation. The structure of the aluminum films was evaluated by SEM imaging. The results from this complex study showed a correlation between the morphology of the metal electrodes with the performance of the PLEDs.

[1]This work was partly supported by the NSF grant # 0923047.

K1.00017 Spatio-temporal beam profiling of pulsed infrared laser sources , IAN REEVES, JEFFREY OLAFSEN, LINDA OLAFSEN, Baylor University — Development of viable infrared lasers relies not only on the power and wavelength generated by the source, but also on the spatial and temporal profile of the output beam. Thermal imaging is of particular interest to researchers working in the field of optically pumped semiconductor analysis as the output from many of these devices falls in the mid-infrared range. While knife edge and other beam profile analysis techniques typically are unable to capture the temporal evolution of beam profiles, real time imaging is employed in this work, using a thermal camera synchronized with a Nd:YAG pump laser via LabVIEW-controlled triggering. Coupling the synchronization with detailed image analysis using IDL, this new methodology is applied to the near-infrared output of an optical parametric oscillator and ultimately will be extended to mid-infrared semiconductor lasers.

K1.00018 Development of a Portable Automated Gas Environment System (PAGES2) , NATHAN CAMPBELL, JACOB BAXLEY, EDWARD KINTZEL, Western Kentucky University, BRUCE HILL, LOUIS SANTODONATO, KENNETH HERWIG, Oak Ridge National Laboratory — For the user community at the Spallation Neutron Source (SNS), a portable automated gas environment system (PAGES2), capable of remote operation at pressures up to 100 bar has been built and programmed. The function of this system will be to characterize a variety of high surface area materials and allow studies of energy significant gases such as methane on these surfaces to be carried out. Understanding the fundamental physics of interaction at the gas-surface interface is key for the generation of application-minded products such as fuel cells. PAGES2 can generate adsorption isotherms to determine surface area of the material as well as the number of gas molecules required for a specific surface coverage. This system will not only produce new science, but also allow for better experimental design. PAGES2 system testing is currently underway, and initial results indicate the system is operating as designed. Future tests will be done prior to use at the SNS.

K1.00019 Realization of a closed-cycle dilution refrigerator for nanoscale magnetometry , RAVI NAIK, ANIRUDH NARLA, YU-DONG SUN, NATANIA ANTLER, IRFAN SIDDIQI, QNL, UC Berkeley — We present the implementation of a mechanical pump-free, dilution refrigerator with an automatic cool-down protocol. The cooling process utilizes a liquid nitrogen pre-cool circuit, a pulse tube cooler, and a custom internal dilution unit manufactured by Chase Cryogenics. The dilution unit employs charcoal sorption pumps and electronic heat switches to regulate the condensation and subsequent evaporative cooling of ^{3}He, ^{4}He, and a mash of both in three separate chambers. We achieve a base temperature of 85 mK with a 10-15 hour hold time. The unit presents a simple, compact, low vibration platform for conducting a wide spectrum of low temperature transport experiments. As an example, we present microwave frequency SQUID magnetometry data collected in this unit.

K1.00020 Phase cycling for optical two-dimensional Fourier-transform spectroscopy[1] , TRAVIS AUTRY, Department of Physics, University of Texas, Austin TX 78712, GALAN MOODY, HEBIN LI, MARK SIEMENS, STEVEN CUNDIFF, JILA, University of Colorado and National Institute of Standards and Technology, Boulder CO 80309 — Phase-cycling has been implemented in optical two-dimensional Fourier-transform spectroscopy to extract signals from quantum wells and quantum dots and to eliminate noise such as pump scatter co-propagating with the four-wave mixing signal. Experiments using actively phase-stabilized interferometers to cycle the excitation pulse optical phases suffer from partial noise cancellation because excitation and phase-control laser wavelengths are incommensurate. To obtain full noise elimination, we have incorporated liquid crystal variable retarders capable of imposing a π phase shift for wavelengths 650-950 nm. We present non-rephasing spectra of potassium vapor contained in a $\sim$20 μm transmission cell and show that this phase cycling method removes all noise from pump scatter while drastically reducing the data acquisition time compared to mechanical phase-delay techniques.

[1]This work was supported by an NSF-REU grant at the University of Colorado- Boulder.

K1.00021 ABSTRACT WITHDRAWN –

K1.00022 Designing an Optical Dipole Trap for the Creation of Bose-Einstein Condensates[1]

, AMY VAN NEWKIRK, Grove City College, Department of Physics, L.S. LESLIE, University of Rochester, Institute of Optics, A. HANSEN, University of Rochester, Department of Physics and Astronomy, N.P. BIGELOW, University of Rochester, Department of Physics and Astronomy; University of Rochester, Institute of Optics — Bose-Einstein condensates have been produced with many different configurations of magnetic, optical, and hybrid traps. Pure optical dipole traps have the possibility of providing a spin state independent trapping potential, which is necessary in many BEC experiments. We are currently designing a red-detuned, single focused-beam dipole trap to be used in the production of BECs. The BEC is to be formed from rubidium-87 atoms. The lab currently has a magneto-optical trap and an Ioffe-Pritchard magnetic trap in place. The dipole trap will be the last step in the process to create a BEC. It will be formed with a single pass of a Yb fiber laser at 1064 nm. We developed a model for the dipole trap potential in mathematica. Using this model, we were able to see that our current lab configuration has the possibility of producing a dipole trap that will allow for Bose-Einstein condensation.

[1]This project was supported in part by NSF award PHY-0242483.

K1.00023 SEM and EDX Study of Al alloy Precipitant Surface Segregation due to Annealing[1]

, AUSTIN MOHNEY, INDRAJITH SENEVIRATHNE, Department of Geology and Physics, Lock Haven University of Pennsylvania — In Al alloys, precipitation hardening by impurity phase metallic microstructures in the main bulk metal is a norm. This results in resilience against dislocations, and improvement in other favorable attributes. We have studied Al 2024, Al 5052, Al 6061, and Al 7075 systems and their constituent precipitant migration due to thermal annealing. Scanning Electron Microscopy (SEM) was used to study the structure/morphology. Electron Dispersive X ray Spectroscopy (EDX) was used to study the near surface elemental variations. At annealing these alloys systems exhibit temperature activated relative segregation of the precipitants. Considering main constituents, it was observed Cu precipitant in 2024, and Mg precipitant in 6061 segregated to the surface. Further, increment in the ambient C absorption and O desorption on the surface layers were observed. Surface morphology variations were also studied at annealing using SEM. The data obtained will be discussed in terms of standard diffusion models for the alloys and corresponding diffusion coefficients.

[1]NSF Grant #: 0923047 and PASSHE FPDC (LOU # 2010-LHU-03)

K1.00024 AFM and EDX Study of Self Assembled Pt Nanostructures on PEDOT Thin Films under Ambient Conditions[1]

, INDRAJITH SENEVIRATHNE, AUSTIN MOHNEY, JOSHUA BUCHHEIT, ANURA GOONEWARDENE, Department of Geology and Physics, Lock Haven University of Pennsylvania — Noble metal nanostructure systems on conductive polymer thin films under ambient conditions are interesting due to their use in BioMEMS and hybrid systems further and considering the physics of the polymer - metal interactions The observed nanostructures have deformed spherical shape. The Pt was magnetron sputter deposited at RT (300K), PEDOT Baytron P 60nm thick, spin coated on glass slides cleaned with acetone and IPA. The system was studied using ambient IC mode Atomic Force Microscopy (AFM) for its structure. Elemental composition/distribution of the system was measured with Energy Dispersive X ray Spectroscopy (EDX). Pt nanostructures on the surface observed to be likely Volmer - Weber growth mode At Pt coverage of 120 ML, nanostructures had a mean diameter of 32 nm and mean height of 5 nm. When annealing at 15min at 473K systems changes to smaller nanostructures coexisting with bigger structures of mean diameter of 120 nm and mean height of 36 nm. Elemental/morphological variations when annealed at successively higher temperatures were also investigated.

[1]NSF Grant #: 0923047 and PASSHE FPDC (LOU # 2010-LHU-03).

K1.00025 AFM, and EDX Study of Self Assembled Au Nanostructures on P doped Si(100) Under Ambient Conditions[1]

, JOSHUA TATHAM, JOSHUA BUCHHEIT, INDRAJITH SENEVIRATHNE, Department of Geology and Physics, Lock Haven University of Pennsylvania — Noble metal nanostructures systems on semiconductor surface under ambient conditions are interesting but complex due to the presence of surface adsorbed species. Apart from various possible plasmonic and catalytic applications and these may give insights into thermodynamics and kinetics of such systems. The observed nanostructures have deformed spherical shape. The Au was magnetron sputter deposited at RT (300K), on Si(100) P doped cleaned with acetone and IPA. Ambient IC mode Atomic Force Microscopy (AFM) used to elucidate structure. Elemental composition and distribution on the deposited system was measured with Energy Dispersive X ray Spectroscopy (EDX). Self assembled Au nanostructures on the surface was observed with likely Stranski - Krastanov growth mode At 30 ML Au coverage of nucleated nanostructures observed to have a mean diameter of 2 nm and mean height of 2 nm. At Au coverage of 120 ML, nanostructures had a mean diameter of 25 nm and mean height of 4 nm. Observed variations when annealed at successively higher temperatures will also be discussed

[1]NSF Grant #: 0923047 and PASSHE FPDC (LOU # 2010-LHU-03).

K1.00026 Pt Nanostructures Self Assembled on P doped Si(100) Under Ambient Conditions: AFM, and EDX Study[1]

, ZACHARY BARCIKOWSKI, AUSTIN MOHNEY, INDRAJITH SENEVIRATHNE, Department of Geology and Physics, Lock Haven University of Pennsylvania — Noble metal nanostructures on surface support under ambient conditions are interesting but complex due to the presence of surface adsorbed species. System may have plasmonic and catalytic uses from the applications standpoint and may give insights into thermodynamics/kinetics of such systems. Observed Pt nanostructures have deformed spherical shape. The Pt was magnetron sputter deposited at RT (300K), on Si(100) P doped cleaned with acetone and IPA. The system was studied using ambient IC mode Atomic Force Microscopy (AFM) for its structure. Elemental composition / distribution were measured with Energy Dispersive X ray Spectroscopy (EDX). Self assembled Pt nanostructures on the surface was observed with a likely Stranski - Krastanov type growth mode At Pt 30 ML coverage nucleated nanostructures observed to have a mean diameter of 15 nm and mean height of 1.5 nm. At Pt coverage of 120 ML, structures exhibited mean diameter of 40 nm and mean height of 3 nm. System was also observed at incremental annealing as well

[1]NSF Grant #: 0923047 and PASSHE FPDC (LOU # 2010-LHU-03).

K1.00027 Thermal conductivity of a two-gap superconductor MgB_2in High Magnetic Field and Low Temperatures[1]

, MICHAEL GARMAN, SASHA DUKAN, Department of Physics and Astronomy, Goucher College — We calculate the thermal conductivity for a single MgB_2 crystal in a mixed state, placed in high magnetic field at zero temperature. We plot the thermal conductivity in the superconducting state κ(H) rescaled by the normal state value κ_N as a function of magnetic field for a realistic *i.e.* disordered MgB_2 superconductor. Our theoretical curve exhibits good qualitative agreement with the experimental data. We report on the self-consistent calculation of the influence disorder has on the thermal conductivity.

[1]This work was supported by the NSF grant No. DMR-0856415.

K1.00028 Low Temperature Study of the Electrical Properties of Sb-SnO_2 Nanofibers[1]

MARITZA REYNA, IDALIA RAMOS, NICHOLAS PINTO, University of Puerto Rico at Humacao — Antimony-doped tin oxide (ATO) can be used for many applications including the development of gas sensors, energy storage devices, and transparent electrodes. ATO nanofibers with sizes from 200 - 600 nm and a bandgap of 4.4 e.V were produced using the electrospinning method. The precursor was composed of tin chloride solution mixed with cellulose acetate solution and antimonium chloride. The XRD spectra of the nanofibers showed the characteristic peaks of Sb:SnO_2 with rutile structure. The electrical properties of single ATO nanofibers were studied following a cycle of cooling from 295 - 15 K and then heating from 15 - 295 K. These measurements were done in cold finger (close cycle helium refrigerator) in a vacuum. The conductivity measured at room temperature was 4.3 S/cm and decreases monotonically from 295 to 15K. As the temperature increases an anomalous peak is observed in the range of 250 to 300 K. This anomaly has been attributed to the chemi-absorbed molecules on the surface of the fiber and could be reduced by improving the vacuum conditions.

[1]PREM (NSF-DMR-0934195) and APS (Minority Scholarship for Undergraduates)

K1.00029 Modification of the growth mechanism of Zno nanowires by addition of oxidizing agents[1]

ERIC DRISCOLL, BRADLEY GOLDER, MARIAN TZOLOV, Lock Haven University of PA — Zinc oxide nanowires were grown catalytically on silicon (100) and (111) surfaces by means of chemical vapor deposition. A very thin layer of sputter deposited gold was used as the catalyst. Nanowires of different compositions were obtained by varying the ratio of carbon to zinc oxide in the source material and the flow rates of oxidizing gases. Results showed that the additional oxidizing gas changed the composition as well as the growth mode of the nanowires. The existence of several growth steps was observed. These steps were induced by the continuous presence of the source material during the system's heating and cooling processes. Remnants of gold found on the tips of the nanowires provided evidence for catalytic growth. The composition was analyzed by energy dispersive x-ray spectroscopy. Imaging by scanning electron microscopy showed random growth directions of nanowires, formation of sheets, and some instances of transitions from sheet to wire growth. The formation of defects was studied by photoluminescence spectroscopy.

[1]This work was partly supported by the NSF grant # 0923047.

K1.00030 Microstructure and Transport Studies of Functionalized Graphene[1]

RON GAMBLE, DARRYL LEWIS, NC A&T State University, DEREJE SEIFU, Morgan State University, JORGE CAMACHO, MYRON STRONGIN, Brookhaven National Laboratory, LIYUAN ZHANG, Brookkaven National Laboratory — The microstructure and transport studies of fuctionalized graphene are reported. These studies reveal that the minimum conductivity is sample dependent and within the range (2-12)e^2/h independent of gate voltage. The variation of the minimum conductivity is attributed to sample impurities, apparent in Atomic Force Microscopy and Raman Spectroscopy. The Raman peaks are in general consistent with graphene, but show shifts in the G and 2D peaks. These shifts are associated with strain and doping. The dependence of the current (I) on the bias voltage (V_{SD}) is linear for most samples. The current dependence on gate voltage (V_g)curves show asymmetric behavior, showing the imbalance between the hole and electron carriers. A 16 A deposition of Fe leads to a significant modification in the transport properties due mostly the formation of iron oxide. The AFM clearly shows the formation of Fe clusters.

[1]DOE/NSF Faculty-Student Teams Program

K1.00031 Thermal analysis study of polysterene-poly(methyl methacrylate) (PS-PMMA) diblock copolymer thin films morphologies when annealed and sheared under vacuum in inert atmosphere

LUIS POMALES, MELISSA DAVILA-SANTANA, MIRNA RIVERA-CLAUDIO, JOSEE VEDRINE-PAULEUS, University of Puerto Rico at Humacao — Diblock copolymers are made of two chemically bonded blocks, with incompatible monomers. This incompatibility gives the block the property to phase separate at temperatures above the glass transition (Tg). The ability to self-assemble into different mesophase structures is of great importance in nanolithography and nanofabrication. This research involves the morphological study of PS-PMMA thin films annealed under inert atmosphere. Our objective is to determine the microstructure properties of the PS-PMMA diblock copolymer as a function of film thickness, annealing temperature, and applied shear force. The PS-PMMA thin film is spin casted onto silicon substrates, and annealed under an inert atmosphere. Our initial results show that the samples have an incomplete formation of the microstructures. However, further film analysis is needed to study the morphological properties when annealed. Futures studies will focus on the effects of a shear force during annealing, to align the film microstructures.

K1.00032 Growth and characterization of $Ba_8Ga_{16}Ge_{30}$ Type I clathrate thin films grown by pulsed laser deposition[1]

JACOB DUSCHA, Macalester College/ University of South Florida, ROBERT HYDE, DEVAJYOTI MUKHERJEE, SARATH WITANACHCHI, University of South Florida — $Ba_8Ga_{16}Ge_{30}$thin films were successfully grown on Si (100) substrates using pulsed laser deposition process. Clathrates are studied for potential thermoelectric (TE) applications with few reports of thin film growth due to intrinsic difficulty in growing the caged structures in thin film form. Growth of stoichiometric $Ba_8Ga_{16}Ge_{30}$thin films is complicated by non-congruent evaporation during the ablation process resulting in Ga or Ge deficient films, degrading their properties. We report a systematic study of the growth parameters for stoichiometric $Ba_8Ga_{16}Ge_{30}$thin films. The laser ablated plasma plumes were analyzed using ICCD imaging and optical emission spectroscopy enabling optimization of growth parameters. Film thickness profiles of various target-substrate distances were plotted to estimate an optimum deposition rate. Surface morphologies and structure of the as-deposited films were examined using a scanning electron microscope and x-ray diffraction technique. This investigation provides a new direction towards the growth of high quality thin films for potential TE device applications.

[1]Supported by NSF REU,award No DMR-1004873.

K1.00033 Investigation of Silver Thin Film Reactivity via STM[1]

JEHOVANI LOPEZ, Department of Chemistry, California State University San Marcos, STEPHEN TSUI, Department of Physics, California State University San Marcos — The operation of a scanning tunneling microscope (STM) to some extent is nearly as much art as it is science. A recent attempt was made to examine the surface topography of glass by depositing a thin conducting silver film over the surface via plasma sputtering. Preliminary results show our instrument's inability to image this silver. Our hypothesis is that the silver nanoparticles may react in air, thereby creating a tunneling barrier that impedes the STM current. Silver nanoparticles deposited on highly orientated pyrolitic graphite at varying layers of thickness were imaged to analyze scatter patterns and deposition. Over time, STM images of the silver nanonclusters on HOPG showed some inconsistency in the diameters of the deposited clusters, possibly due to an artifact from the suggested reactivity of the silver. To confirm this, we also investigate depositions of gold, which is nonreactive.

[1]Support provided in part by the OBRT at CSUSM and the CTBP at UCSD.

K1.00034 Thin Film and Free Crystallite Formation of ZnO Nanorods from Solution Under Extreme Crystallization Conditions , ANAMIKA GOPAL, CHELSI KWITOSKI, MARIAN TZOLOV, Lock Haven University, Pennsylvania — ZnO nanorods, grown by the established Hexamethylenetetramine (HMTA) process, through the reaction of Zinc Nitrate with HMTA, are investigated. The nanorod morphology dependence on temperature, initial solution concentration and crystallization time is studied. Crystal growth on glass and ITO substrates and free crystallite precipitation in solution are characterized by SEM and EDX. Low concentrations and temperatures are investigated for production of rod-clusters with a high aspect ratio and low surface nucleation density. Such morphology is expected to enhance charge transport while preserving light transmissivity, for use in efficient ZnO photovoltaic devices. Free crystallite formation in solution with varied initial parameters is characterized by a time dependent light scattering study, supported by SEM and EDX data. A high aspect ratio of solitary, free crystallites is sought, which we believe would be most effective in solution processed, concentration gradient solar cells.

K1.00035 Time-resolved Four-terminal probe of ion transport in Schefflera leaves[1] , NICOLE PERIGO, GUOPING ZHANG, Department of Physics, Indiana State University — Plant growth relies on efficient ion transport. The rate of the ion transport depends on the concentration of each ion in the leaf. A common method is to use two-lead geometry. Here we employ a four-electrode set-up orienting the electrodes either parallel or perpendicular to each other. When the electrodes are parallel, two are at each end, with electric current running along the direction of the veins. When they are perpendicular, there are two along the direction of the veins (tip-tip) and two are perpendicular to the veins (side-side). The parallel set-up is similar to the Franck-Hertz experiment, but instead of using a vacuum tube we use a leaf. By using the parallel set-up, we find that two inner leads can directly control the movement of the ions in the time domain. By switching on/off the control current, a clear time-resolved current change is observed, where the signal decays less than one second. This time scale is similar to that of a typical ECG decay signal. Therefore, our method may be potentially a powerful tool to ion diffusion and transport in many biological and medical systems.

[1]Supported by U.S. Department of Energy under Contract No. DE-FG02-06ER46304 and Indiana State University .

K1.00036 PHYSICS EDUCATION —

K1.00037 Energy-Efficient Cooking of Spaghetti , AKASH LEVY, Allderdice High School — Spaghetti is a dual-career family dinner favorite. But how much energy is consumed in the process, and how can it be optimized? I performed an experiment to test two methods for preparing a spaghetti meal. In both cases, the water was rapidly heated to the boiling point. The flame was kept at maximum for the first experiment until the spaghetti was cooked. In the second experiment, the flame was reduced and the top covered, such that the water was kept at 100C. The two methods are compared in terms of the total time required to prepare the meal and amount of energy required. A discussion of potential savings for the latter method–and possible uses for that savings–is discussed.

K1.00038 Snail Mail: Kinematics Applied to an International Letter's Seventeen-Year Journey , ISHAN LEVY, Pittsburgh Obama 6-12 School — The average and instantaneous velocity of a letter sent in 1990 from India and arriving in 2007 in New York City is analyzed using the equations of kinematics. An important question to be addressed is: how does the average speed of "snail mail" compare with that of an actual snail? The distinction between instantaneous versus average kinematic quantities are highlighted in the process.

K1.00039 Heuristic Deduction of the Newton's Second Law , GREGORIO RUIZ-CHAVARRIA, JONAS TORRES-MONTEALBAN, Universidad Autonoma Chapingo — In this work we present a heuristic justification about the form of the second law of Newton. We start with a basic definition of force as the interaction between the body of study and everything that surrounds it. We define the mechanical state of a body through the momentum, because this gives us a measure of the ability to carry out an interaction. Now with this definition, the variation of the state of the body over time gives a measure of the intensity of this interaction. From this variation in time, we can establish Newton's second law. The approach described above can be used with students in pre-university and university.

K1.00040 Obtaining the Thermal Efficiency of a Steam Railroad Machine Toy According Dale's Cone of Learning , OMAR TOMAS BAUTISTA-HERNANDEZ, GREGORIO RUIZ-CHAVARRIA, Universidad Autonoma Chapingo — Physics is crucial to understanding the world around us, the world inside us, and the world beyond us. It is the most basic and fundamental science, hence, our interest in developing innovative strategies supported by the imagination and knowledge to make the learning process funny, attractive and interesting to people, so, we can help to change the general idea that Physics is an abstract and complicated science. We all know this instinctively, however, turn-of-the-century educationist Edgar Dale illustrated this with research when he developed the Cone of Learning - which states that after two weeks we remember only 10% of what we read, but we remember 90% of what we do. Based on that theory, we obtain the thermal efficiency of a steam railroad machine -this is a toy train that could be bought at any department store-, and show you the great percentage of energy lost when moving this railroad machine, just as the real life is. While doing this practice we don't focus on the results itself, instead, we try to demostrate that physics is funny and it is not difficult to learn. We must stress that this practice was done with pre-universitary and univesitary students, however, can be shown to the community in general.

K1.00041 Statistical evidence of predation by theropods , SCOTT LEE, University of Toledo — Dinosaurs hold a great fascination for everyone and provide an interesting venue for teaching many elementary concepts of kinematics. Dinosaur trackways provide interesting information about the locomotion of these extinct animals. A statistical analysis of the known trackways made by theropods (carnivorous dinosaurs) shows that they usually moved by walking with an average speed of 2.4 $\pm$ 1.5 m/s. Fast running, determined by the relative stride length greater than 3, is observed in about 10% of the trackways, with speeds on the order of 10 m/s. These trackways are believed to have been formed during predation.

K1.00042 Surveying Students' Understanding of Quantum Mechanics[1] , CHANDRALEKHA SINGH, GUANGTIAN ZHU, University of Pittsburgh — Development of research-based multiple-choice tests about quantum mechanics is important for assessing students' difficulties and for evaluating curricula and pedagogies that strive to reduce the difficulties. We explore the difficulties that the undergraduate and graduate students have with non-relativistic quantum mechanics of one particle in one spatial dimension. We developed a research-based conceptual multiple-choice survey that targets these issues to obtain information about the common difficulties and administered it to more than a hundred students from seven different institutions. The issues targeted in the survey include the set of possible wavefunctions, bound and scattering states, quantum measurement, expectation values, the role of the Hamiltonian, time-dependence of wavefunction and time-dependence of expectation value. We find that the advanced undergraduate and graduate students have many common difficulties with these concepts and that research-based tutorials and peer-instruction tools can significantly reduce these difficulties. The survey can be administered to assess the effectiveness of various instructional strategies.

[1]Supported by the National Science Foundation.

K1.00043 Theoretical model to explain the problem-solving process in physics[1] , CARLOS LOPEZ, Universidad del Valle ee Mexico — This work reports a theoretical model developed with the aim to explain the mental mechanisms of knowledge building during the problem-solving process in physics using a hybrid approach of assimilation- formation of concepts. The model has been termed conceptual chains and represents graphic diagrams of conceptual dependency, which have yielded information about the background knowledge required during the learning process, as well as about the formation of diverse structures that correspond to distinct forms of networking concepts Additionally, the conceptual constructs of the model have been classified according to five types of knowledge. Evidence was found about the influence of these structures, as well as of the distinct types of knowledge about the degree of difficulty of the problems.

[1]I want to be grateful to Laureate International Universities, Baltimore M.D., USA, for the financing granted for the accomplishment of this work.

K1.00044 Graphical representation of the process of solving problems in statics , CARLOS LOPEZ, Instituto Tecnologico de Queretaro — It is presented a method of construction to a graphical representation technique of knowledge called Conceptual Chains. Especially, this tool has been focused to the representation of processes and applied to solving problems in physics, mathematics and engineering. The method is described in ten steps and is illustrated with its development in a particular topic of statics. Various possible didactic applications of this technique are showed.

K1.00045 Physics Education at University of Houston Clear Lake , SAMINA MASOOD, Univ. of Houston Clear Lake — We are developing a physics education program to prepare teachers to teach Physics in High Schools. The science teachers training needs to be brought to the level where they can motivate children and young adults in their classrooms to take interest in science learning to adopt science and engineering career. The early selection of career path helps the better preparation for the career.

K1.00046 GENERAL THEORY (THEORETICAL METHODS) –

K1.00047 Variational Study of a Finite Heisenberg Chain , ERIC ASHENDORF, JOE WEINER, JAY D. MANCINI, Kingsborough College of CUNY, VASSILIOS FESSATIDIS, Fordham University, SAMUEL P. BOWEN, Chicago State University — Here we wish to study the ground-state of the $1D$ Heisenberg chain

$$H=-\frac{1}{2}J\sum_{l=1}^{N}\left[2\left(\sigma_l^+\sigma_{l+1}^+ + \sigma_l^-\sigma_{l+1}^-\right)+\sigma_l^z\sigma_{l+1}^z\right],$$

where the σ's are the usual Pauli spin matrices and J is the strength of the spin-spin interaction. The purpose of our revisiting such a well known system is to use it as a benchmark for our variational ansatz in which a trial vector is chosen $|\psi_0(\alpha)\rangle=\exp\left(\alpha\sum_{l=1}^{N}\sigma_l^+\sigma_{l+1}^z\right)|0\rangle_N$, where α is the variational parameter and $|0\rangle_N$ is an appropriately chosen initial array of spins. We then construct a basis according to the prescription $|\psi_m\rangle=\partial_\alpha^m|\psi_0(\alpha)\rangle$ creating an energy matrix with elements $h_{ij}=h_{ij}(\alpha,J)$ whose eigenvalues are then evaluated.

K1.00048 Anharmonic Energy Spectrum for $V(x)=\pm x^4,\pm x^6,\pm x^8$, SAMUEL P. BOWEN, Chicago State University, JAY D. MANCINI, Kingsborough College of CUNY, VASSILIOS FESSATIDIS, Fordham University — In this work we wish to revisit the energy spectrum for the anharmonic potentials

$$H=\frac{p^2}{2m}\pm x^N,$$

where $N=4,6,8$. Using the second quantized operator formalism of Dirac, we have evaluated matrix truncations of up to 100×100. Our results for the energy spectrum are in disagreement with the work of Bender and Boettcher (PRL 80, 5243). They studied a *PT* symmetric Hamiltonian whose potential is given by $V(x)=-(ix)^N$ and who maintain that "when $N\geq2$, the spectrum is infinite, discrete and entirely real and positive". We find, for the potentials with $N=4,6,8$ that the spectrum is not completely positive and in fact has no lower bound.

K1.00049 Moments based calculations of PT-symmetric Hamiltonians , ROBERT MURAWSKI, Drew University, JAY MANCINI, Kingsborough College of CUNY, VASSILIOS FESSATIDIS, Fordham University — PT-symmetric Hamiltonians have gained recent interest in optics and particle physics [Phys. Rev. A **82**, 031801 (2010), Phys. Rev. Lett. **105**, 031601 (2010)] . These Hamiltonians remain invariant under the reflection of parity and time. What makes them surprisingly interesting is that PT-Hamiltonians have real positive spectra. In this paper, we calculate the moments of the PT Hamiltonian H=p^2+x^2 (ix)^r with r>0. We will use these moments to compute the ground state energy by the generalized moments expansion (GMX) and the canonical sequence method (CSM). Comparisons will be made to the Lanczos tridiagonalization scheme as well as to other published results.

K1.00050 Ab initio approach to magnon-electron coupling , PAWEL BUCZEK, ARTHUR ERNST, LEONID M. SANDRATSKII, HARDY GROSS, Max Planck Institute of Microstructure Physics, Weinberg 2, Halle/S., Germany — The electronic properties of magnets and exchange-enhanced paramagnets are strongly influenced by the spin-flip fluctuations. In particular, their important role in the pnictide high-temperature superconductivity is has been conjectured [Mazin & Johannes, *Nat. Phys.* **5**, 141 (2009)]. To formulate a parameter free model of electron-electron interaction involving emission and absorption of magnons we combine our recently developed implementation of the linear response time dependent density functional theory for spin fluctuations [Buczek *et al.*, *Phys. Rev. Lett.* **105**, 097205 (2010)] with the methods of many body perturbation theory [Vignale & Singwi, *Phys. Rev. B* **32**, 2156 (1985); Zhukov *et al.*, *Phys. Rev. Lett.* **93**, 096401 (2004)]. This theoretical toolbox is applied to the description of recent inelastic tunneling spectroscopy experiments [Balashov *et al.*, *Phys. Rev. Lett.* **97**, 187201 (2006)], which have shown that the emission of magnons by electrons can open additional tunneling channels and increase conductivity. As second application, we discuss a scheme of the magnon mediated Cooper pair formation in PdH_x and LaFeAsO.

K1.00051 Classification of Gapped Symmetric Phases in 1D Spin Systems , XIE CHEN, Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA, ZHENG-CHENG GU, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106, USA, XIAO-GANG WEN, Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA — Topological phases exist in quantum many-body systems beyond the usual symmetry breaking understanding of phase and phase transition. The question of what kind of topological phases exist seems hard especially for strongly interacting systems. Here we make an attempt to answer this question for gapped interacting quantum spin systems whose ground states are short-range correlated. Based on the local unitary equivalence relation between short-range correlated states in the same phase, we classify possible quantum phases for 1D matrix product states, which represent well the class of 1D gapped ground states. We find that in the absence of any symmetry all states are equivalent to trivial product states, which means that there is no topological order in 1D. However, if certain symmetry is required, many phases exist with different symmetry protected topological orders. Understanding about topological order and symmetry breaking order in spin systems also allows us to obtain a classification of 1D fermion topological phases.

K1.00052 Effective equilibrium theory of non-equilibrium quantum transport , PRASENJIT DUTT, Yale University, New Haven, CT., JENS KOCH, Northwestern University, Evanston, IL., JONG HAN, SUNY Buffalo, Buffalo, NY., KARYN LE HUR, Yale University, New Haven, CT. — We establish a rigorous theoretical foundation for an effective equilibrium description of electronic transport through quantum impurity models out of equilibrium. An imaginary time framework involving the Lippmann-Schwinger operators of the system is proposed and expounded. This forms the basis for the implementation of standard equilibrium many body techniques, effectively avoiding the complexities of the Keldysh contour, and is used to compute transport observables. We present a novel perturbative scheme for treating interactions, which we use to study the Anderson impurity model out of equilibrium. Generalizations to non-perturbative methods are also explored. We use this formalism to investigate the effect of voltage bias, temperature and a magnetic field on the fate of the Abrikosov-Suhl resonance and make a comparison with numerics and experimental results.

K1.00053 Magnetic properties of $CuZrTiO_5$, H.M. ALYAHYAEI, Department of Physics and Astronomy, University of California, Riverside, Riverside, California 92521, USA, R.A. JISHI, D.M. GUZMAN, Department of Physics, California State University, Los Angeles, California 90032, USA, O. TA, A.A. SHARIF, Department of Mechanical Engineering, California State University, Los Angeles, California 90032, USA — $CuZrTiO_5$ is a newly synthesized crystal that contains copper oxide planes [1]. We have carried out first-principles calculations using density functional theory in order to determine the ground state of this crystal. We considered various nonmagnetic and magnetic phases and calculated the corresponding total energies. We found that in the ground state, the magnetic moments on the copper ions adopt an antiferromagnetic arrangement. The effects of doping on the electronic properties of this crystal are investigated.

[1] U. Troitzsch et al., Journal of Solid State Chemistry 183, 668(2010).

K1.00054 Vacillation in density of correlated electron-electron pair confined in 2D quantum dot , TAKUMA OKUNISHI, ATSUSHI TSUBAKI, TOMOKI TAGAWA, KYOZABURO TAKEDA, Waseda University, WASEDA UNIV. TAKEDA LABORATORY TEAM — We studied an electronic structure of charged particles confined in a 2D quantum dot (QD), taking into account an electron correlation through a configuration interaction (CI) by employing resonating unrestricted Hartree-Fock (res-UHF) approach. The UHF solutions for the QD are nonorthogonal mutually but are appropriate for a basis functions of a res-UHF CI calculation because they represent a conceivable electron- spin configurations rationally. Consequently, the res-UHF CI provides intuitive understandings for an electron correlation with narrowing down the number of employed Slater bases, although at an expense of orthogonality among the Slater bases. We further embedded this res-UHF CI approach to solve a time- dependent (TD) Schroedinger equation, and studied the TD features caused by an electron correlation computationally. We found that the electron correlation induces the characteristic vacillation in the total charge density. We then employed a projection analysis and investigated the change in the vacillation frequencies by varying the confinement length and also the initial charge distribution.

K1.00055 Ground state instability in spin polarization for electrons confined in 2D square quantum dots , KYOZABURO TAKEDA, MASAMU ISHIZUKI, TAKUMA OKUNISHI, YHUKI NEGISHI, Waseda University — We present a theoretical study of the ground state electronic structure and the spin polarization for four electrons confined in 2D square quantum dots (2D SQDs). We employ standard mean field theory (MFT) approaches using the unrestricted Hartree-Fock (UHF) and density functional theory (DFT) calculations. The resonant UHF configuration interaction (res-UHF CI) calculation was also performed in order to understand the electron correlation more intuitively. The MFT ground state is expected to be fully spin-polarized when square SQDs have a small confinement length L or aspect ratio, in agreement with Hund's rule. In contrast, the spin-unpolarized ground state singlet is expected in all in other SQDs, the MFT anti-Hund state is produced by the spin-density wave having the zero total spin. The res-UHF CI calculation restores the geometrical symmetry in the resulting ground state, but the res- UHF CI ground state maintains the zero total spin. Thus, ground state instability is expected in the spin-polarization of the SQD system, which eventually violates Hund's rule in accordance with the Coulomb interaction.

K1.00056 Real-space Green's function calculations of valence Compton profiles for Nonresonant Inelastic X-ray Scattering[1] , BRIAN MATTERN, JOSHUA KAS, JOHN REHR, U. Washington — Nonresonant inelastic x-ray scattering (NIXS) from core- and semi-core shells at 50-1000 eV binding energies is an emerging field of synchrotron light source science, with applications in high pressure science, electrical energy storage, f-electron materials, and catalysis, etc. In such experiments, the Compton scattering of x-rays by valence electrons produces a significant background signal that spans the energy loss range of interest for NIXS. Thus, first-principles theoretical calculations of the double-differential cross-section for Compton scattering in the energy loss and momentum transfer ranges of interest are needed to account for this background. Here, we report an approach using a real space Green's function method to calculate the valence Compton profile in the impulse approximation. Illustrative calculations are presented and compared with experiment.

[1]This research is supported by a grant from the US Department of Energy Office of Basic Energy Sciences.

K1.00057 Exchange-correlation energy functionals for low-dimensional electronic nanostructures: Recent developments and applications[1] , STEFANO PITTALIS, University of Missouri-Columbia, U.S.A., E. RÄSÄNEN, Nanoscience Center, University of Jyvaskyla, Finland, C.A. ROZZI, University of Modena, Italy, G. VIGNALE, University of Missouri-Columbia, U.S.A. — In the analysis of low-dimensional electronic nanostructures, the evaluation of the consequence of the electron-electron interaction is a challenging task. In particular, an accurate determination of the exchange-correlation energy in two-dimensional systems is of great importance in understanding the many-body physics of modern electronic devices. Here we review several approaches within density functional theory, spanning from the bottom to the top of the ladder of functional approximations. Considering applications to quantum dots, rings, slabs, and periodic systems, we conclude that the presented approaches form a valuable first-principle toolkit for dealing with the many-body physics of such devices.

[1]S.P. and G.V. are supported by DOE grant DE-FG02-05ER46203.

K1.00058 Exchange energy and potential using the Laplacian of the density , CHRIS WAGNER, ANTONIO CANCIO, Ball State University — abstract- The challenge of density functional theory is the useful approximation of the exchange correlation energy. This energy can be approximated with the local electron density and the gradient of the density. Many different GGA's have been made recently and there is controversy over the best overall functional. Recent Monte Carlo simulations give evidence that the Laplacian of the density might be a better starting place than the gradient to correct the local density approximation. It also gives a better representation of the exchange potential at the nuclear cusp and of bonding between atoms. We have tested several Laplacian based GGA models for exchange for small atoms. We use known constraints on the exchange energy used in current GGA's. In many models unphysical oscillations occur in the potential, and understanding and eliminating them is part of the focus of this research. Preliminary results suggest that smaller values for short and long range constraints in the literature give more physically reasonable results in the Laplacian models.

K1.00059 Hybrid Density Functional Studies of a Promising Photovoltaic Material: Zinc Phosphide , STEVEN DEMERS, AXEL VAN DE WALLE, Dept. of Applied Physics and Materials Science, California Institute of Technology — Although Zinc phosphide is a semiconductor which has high absorption in the visible spectrum that is made from abundant elements, its use as a low-cost photovoltaic is limited by difficulties in n-doping the material. We study this compound via Density Functional Theory calculations based upon recently developed hybrid functionals designed to accurately describes band gaps. We explore the effects of various point defects with energy levels near the fermi energy on the electronic band structure in an effort to identify suitable dopants in this system. The thermodynamic stability of these defects is also assessed.

K1.00060 Mass-Energy Relationship Must Include Factors For Vibrational and Rotational Kinetic Energies as Well as Various Potential Energies , STEWART BREKKE, Northeastern Illinois University (former grad student) — Einstein proposed that at low speeds $E = M_0c^2 + 1/2M_0v^2$. However, a mass may also have vibrating and rotating kinetic energies and may also have various potential energies such as gravitational, electric and magnetic potential energies which must be part of the total mass-energy equivalence. Therefore, the basic equation for the mass-energy equivalence should be $E = M_0c^2+1/2M_0v^2+1/2I\omega^2+1/2kx^2+(GM_0M_2)/r+(KQ_0Q_2)/r+(Um_0m_2)/r$ where the last three terms are the gravitational, electrostatic and magnetic potential energies of the mass and the second, third and fourth terms are the linear, rotational and vibrational kinetic energies of the mass.Also, Einstein did not include the rotational and vibrational kinetic energies in his relationship for relativistic kinetic energy and therefore the kinetic energy T cannot equal $(E - E_0) = 1/2M_0v^2$, but rather must equal $T = 1/2M_0v^2 + 1/2I\omega^2 + 1/2kx^2$ including the vibrational and rotational kinetic energies besides the linear kinetic energy alone.

K1.00061 A Theory of Frozen Light According to the General Theory of Relativity , DMITRI RABOUNSKI, LARISSA BORISSOVA — We suggest a theory to frozen light, which was first registered in 2000 by Lene Hau. Frozen light is explained here as a new state of matter. The explanation is given through space-time terms of the General Theory of Relativity. We consider a fully degenerate region of space (space-time), which is the ultimate case of the isotropic region (home of photons), where the metric is particularly degenerate. Both the space-time interval, the observable time interval, and the observable three-dimensional interval are zero in a fully degenerate region. Therefore, we refer to such a region and particles which inhabit it as zero-space and zero-particles. Moving to the coordinate quantities inside zero-space shows that real speed therein is that of light, depending on the gravitational potential and the rotation of space. It is shown that the eikonal equation for zero-particles is a standing wave equation: zero-particles are standing light waves, while zero-space is filled with a system of standing light waves (light-like hologram). With these, zero-particles appear to a regular (external) observer as mere stopped light. This paper has been submitted to The Abraham Zelmanov Journal.

K1.00062 Symplectic Integrator and its Applications , HIROTO KOBAYASHI, Chubu University — The first- and the second-order symplectic integrators for the one-dimensional harmonic oscillator are reconstructed on the basis of effective Liouville operators, which can be defined only within the convergence radius. The first-order one for the q^4-potential system breaks down for different time steps depending on the initial condition, which indicates that no conservation value exists for the system in the first- order symplectic integrator.

K1.00063 Interacting many-body simulations including contacts using graphics processing units (GPU) , TOBIAS KRAMER, University of Regensburg, Germany — Already the solution of the interacting classical many-body problem is difficult to achieve, since the integration of the equations of motions couples all positions of the particles contained in the system. Transport calculations require to include the contacts within the simulation and to study the effect of interactions there. Classical and quantum-mechanical equations of motions can be related by the time-dependent variational principle for Coulombic interacting electrons in a magnetic field [1]. Interacting systems require to carefully consider the questions of self-consistency. The emergence of an mean-field potential out of a large (10000 electrons!) many-body calculation is shown in [2]. The calculation is only possible due to our usage of graphics processing units, which are ideal tools to study interacting systems.

[1] Two interacting electrons in a magnetic field: comparison of semiclassical, quantum, and variational solutions, T. Kramer, AIP in press (2010), arxiv:1009.6051
[2] Self-consistent calculation of electric potentials in Hall devices, T. Kramer, V. Krueckl, E. Heller, and R. Parrott Phys. Rev. B, 81, 205306 (2010)

K1.00065 Mesoscale simulation of the rheology of high molecular weight polymer gels , YELENA SLIOZBERG, JOHN BRENNAN, TIMOTHY SIRK, JAN ANDZELM, U. S. Army Research Laboratory — Polymer gels are comprised of physically or chemically cross-linked polymers that are highly swollen with solvent. The rheology of these gels depends on their morphological properties, such as the number of bridging chains and trapped entanglements. The prediction of structural and mechanical properties of gels using computational approaches is challenging and requires advanced particle-based mesoscale methodologies. Recently, we have implemented an approach to predict mechanical properties of high molecular weight block copolymers by allowing for chain entanglement behavior within the dissipative particle dynamics (DPD) methodology. Diffusion coefficients have been evaluated to locate the crossover from the Rouse to reptation dynamics. In this talk, we will demonstrate that including a segmental repulsive potential in addition to the usual DPD framework can prevent chain crossings and leads to an improved representation of mechanical and structural properties of polymer gels.

K1.00066 Resiliency of the Mixed-State Wigner Function , TOMAS MATERDEY, University of Massachusetts Boston — Numerical solution of the quantum Vlasov equation showed details of the phase-space dynamics of the Wigner function. Resiliency of the mixed-state Wigner function over changes of external electric and magnetic fields will be discussed.

K1.00067 Perhaps Gravitational Waves do not Exist , ORVIN WAGNER, Wagner Research Laboratory — I have recently been working with waves that appear to penetrate everything including mountains. I call these waves "waves in dark matter" because of their penetrating qualities. These waves seem to indicate that dark matter interacts more than just with gravity and may be important in supporting life, for example. These waves may dissipate energy in binary orbitting systems, such as paired pulsars, and explain their orbital decay. Many authors, including Einstein, provide supporting evidence that gravitational waves do not exist. Recent experiments indicate the same. See the website: "Darkmatterwaves.com"

K1.00068 The mass, energy, space and time systemic theory-MEST-energy balance system of wave-particle duality , DAYONG CAO, Beijing Natural Providence Science & Technology Development Co., Ltd — The paper suppose that the probability of displacement is the space and the probability of cycle is the time. And accroding to the quantum mechanics, the paper get the equation of the space : $S = P(r) = f^2$, (1) Among it, S: the space, f: the amplitude of wave, r: the displacement, P(r): probability function of displacement. Accroding to the Benford's law, the paper get the equation of the time equation: $T = P(2\pi t) = ln(1 + \frac{1}{2\pi t}) = \nu$, (2) Among it, T: the real time, t: date of clock, ν: the frequence of wave, P(t): probability function of date of the clock. $E = h\nu$, (3) $m = \frac{h}{\lambda c}$, (4) Among it, E: the energy of particle, m: the mass of particle, c: the velocity of particle, ν: the frequence of particle, λ: the wavelengh, h: the Planck constant. $E'\psi = i\hbar\frac{\partial\psi}{\partial t}$, (5) $m'\psi = -i\hbar\frac{\partial\psi\partial t}{(\partial x)^2}$, (6) Among it, $E'\psi$: the energy of wave, $m'\psi$: the mass of wave, c′: the velocity of wave, ψ: the Wave Functions. The paper give new idea that unlike mass repel each other, like mass attract; And like energy repel each other, unlike energy attract. So there is a mass-energy duality too. The energy radiate the repulsive (energy) wave and the mass absorb the absorptive (mass) wave. And there is a balance system between the energy wave and mass wave. $E + E'\psi = mc^2 + m'\psi c'^2, (c'^2 = -\frac{(\partial x)^2}{(\partial t)^2})$, (7)

K1.00069 Computational study on ionic diffusion and dynamic properties in silicate and bioactive glasses

, YE XIANG, JINCHENG DU, University of North Texas — Ionic diffusion and dynamic properties in silicate glasses have been extensively studied experimentally due to its importance in understanding ion conduction and glass dissolution. In this study, computational study on ionic diffusion and dynamic properties was carried out using molecular dynamics simulations with effective partial charge potentials. The simulated structure models were validated by comparing with experimental data and systematic discussions on effects of system size, simulation thermal ensemble and temperature range were carried out. The dynamic properties were also related to structural changes with the glass. Finally, investigation of SrO/CaO substitution effect on the diffusion behaviors in 45S glasses is provided.

K1.00070 ENERGY RESEARCH AND APPLICATIONS –

K1.00071 Optimization of open circuit voltage in parallel solar cell tandems[1]

, ALEXANDER KUZNETSOV, ANVAR ZAKHIDOV, Nanotech Institute, University of Texas at Dallas — Significant improvement of the solar cell efficiency is achieved by combining solar cells into tandems. Matching of the open circuit voltages (V_{oc}) of individual cells is required in order to maximize the efficiency of the parallel tandem. However practically it is hard to achieve because usually individual cells of the tandem absorb light at different wavelengths and produce very different V_{oc}. Mismatch of open circuit voltages results in deteriorated performance of a parallel tandem. In this work we use circuit analysis to determine parameters of parallel tandem's individual cells that guarantee its most efficient operation. The results of our calculations can be used for optimization of individual solar cells when designing a parallel tandem.

[1]This work is supported by Robert A. Welch Foundation Grant AT-1617, AFRL/Rice grant via CONTACT consortium

K1.00072 Degradation of CIGS Devices Studied using Controlled Moisture Ingress

, RAJALAKSHMI SUNDARAMOORTHY, JOHN PERN, JIAN LI, TIM GESSERT, National Renewable Energy Laboratory, NATIONAL CENTRE FOR PHOTOVOLTAICS TEAM — The damp heat (DH) study at 85˚C and 85% relative humidity of unencapsulated standard CIGS devices fabricated at NREL exhibited various degradation modes. In the initial 20 h of exposure there is a steep decrease in efficiency, followed by a gradual decrease until 1000 h. The devices in this study were subjected to controlled moisture ingress. Periodic light and dark current-voltage (JV), capacitance-voltage (CV) measurements were carried out before, during, and after the course of exposure. Initial trends in CV and JV data show that the decrease in the device performance correlates to the degree of degradation of the TCO and the buffer layer during the first 20 h of exposure. However, from 20-100 h of exposure the abrupt changes in CV and decrease in Voc suggest the moisture penetration deeper into the junction which might alter junction interface. This paper attempts to correlate the JV and the CV data to understand the degradation mechanism during the initial hours of DH exposure in CIGS devices.

K1.00073 Tunable Surface Energy Morphologies of P3HT-PCBM Bulk Heterojunction OPV's[1]

, ABUL M.A. HUQ, ALAMGIR KARIM, Department of Polymer Engineering, University of Akron, USA — In this study we used the commonly studied blend of Phenyl-C61-butyric acid methyl ester (PCBM) and Poly(3-Hexylthiophene) (P3HT) and studied their morphological development (1:1 ratio) under different substrate surface energy conditions. Confined and tunable surface energy can direct the morphology of immiscible blends which can be successfully utilized to gain desired properties of the semiconducting organic materials. We first show that solvent and temperature of film casting have equally dominant effect on the final P3HT:PCBM morphology. We observe that P3HT crystal size and size distribution depend upon the nature of substrate, thickness of the film, temperature of casting solution, and overall blend concentration in solvent. We can also tune P3HT:PCBM morphology by sandwiching the blend films between two PDMS films with well defined surface energies. These studies offer insights for development of highly controlled bulk heterojunction morphology for improving the efficiency of organic photovoltaics (OPVs).

[1]Funding from Department of Energy Grant # DE-SC0005364.

K1.00074 Markedly Enhanced Performance of Dye Sensitized TiO_2 Nanoparticle Solar Cells via Rational Surface Treatment

, MARGARET SCHEINER[1], Cornell University, XUKAI XIN, Iowa State University, ZHIQUN LIN, Iowa State Univeristy — Dye sensitized solar cell (DSSC) was fabricated with the P-25 TiO_2 nanoparticle film sensitized with N719 dye. $TiCl_4$ treatment was found to increase the power conversion efficiency of DSSC. More importantly, subsequent treatment with O_2 plasma further enhanced the efficiency, while the O_2 plasma processing of an untreated TiO_2 photoanode resulted in a lower efficiency. With $TiCl_4$ and O_2 plasma treatments, dye sensitized TiO_2 nanoparticle solar cell with 21 μm thick active layer illuminated under 100 mW/cm^2 exhibited a markedly enhanced power conversion efficiency of 8.35% as compared to 3.86% for untreated cells.

[1]This work was done in Iowa State University.

K1.00075 Structural and Electrical Characterization of Pulsed Laser Deposited CdS/CdTe Thin Films

, MICHAEL NEWBY, M. ALPER SAHINER, SAMUEL EMERY, MICHELLE JAMER, JEFFREY SERFASS, Seton Hall University, MARK CROFT, Rutgers University — The thin films of CdS/CdTe were deposited on ITO coated glass substrates using pulsed laser deposition (PLD). The film growth conditions were systematically varied and the thin film structural properties were determined using a x-ray diffraction (XRD) x-ray absorption spectroscopy (XAS). The effect of the thicknesses of the CdS and CdTe layers, laser energy and the deposition temperature on the film quality and structure were investigated. The photovoltaic properties of the film were then tested using a Keithley sourcemeter and an accompanying Labview program. The results of variation of thickness and growth conditions on the photovoltaic output of the films will be presented.

K1.00076 Monte Carlo Simulations for Charge Transport in Bulk-Heterojunction Solar Cells: Effect of Morphology on Charge Carrier Mobility

, YOUNG MIN NAM, WON HO JO, Department of Materials Science and Engineering, Seoul National University, Seoul, Republic of Korea — Although it is well understood that the nano-scaled morphology of active layer is critical for determining the efficiency of bulk-heterojunction solar cells, the effect of the variation in morphology upon the local mobility of charge carriers and the performance of solar cell has largely been unknown. Since the computer simulation is a powerful method to provide important information for the relationship between mobility and morphology, we use a Monte Carlo to reveal the dependence of mobility upon the morphology. As the domain size and the blend composition of morphology across the active layer are systematically varied, the mobility of charge carriers and the solar cell performance are calculated. The result of simulation reveals that the charge carrier mobility and the performance of solar cell improved largely due to the efficient extraction of charge carriers at the electrodes, when the domain size is optimized and the blend composition becomes donor-rich at the anode and acceptor-rich at the cathode.

K1.00077 Exciton Energy Transfer from Halide Terminated Nanocrystals to Graphene in Solar Photovoltaics

, OBAFUNSO AJAYI, JUSTIN ABRAMSON, NICHOLAS ANDERSON, JONATHAN OWEN, YUE ZHAO, PHILLIP KIM, FELICE GESUELE, CHEE WEI WONG, Columbia University — Graphene, a zero-gap semiconductor, has been identified as an ideal electrode for nanocrystal solar cell photovoltaic applications due to its high carrier mobility. Further advances in efficient current extraction are required towards this end. We investigate the resonant energy transfer dynamics between photoexcited nanocrystals and graphene, where the energy transfer rate is characterized by the fluorescent quenching of the quantum dots in the presence of graphene. Energy transfer has been shown to have a d^{-4} dependence on the nanocrystal distance from the graphene surface, with a correction due to blinking statistics. We investigate this relationship with single and few layer graphene. We study halide-terminated CdSe quantum dots; where the absence of the insulating outershell improves the electronic coupling of the donor-acceptor system leads to improved electron transfer. We observe quenching of the halide terminated nanocrystals on graphene, with the quenching factor ρ defined asI^Q/I^G (the relative intensities on quartz and graphene).

K1.00078 ABSTRACT WITHDRAWN –

K1.00079 Electrical and Optical Properties of ITO thin films prepared by Dual Ion Beam Sputtering[1]

, ALAN WOODALL, WIM GEERTS, ANUP BANDYOPADHYAY, Department of Physics, Texas State University, San Marcos, TX 78666 — Indium Tin Oxide (ITO) thin films find application as transparent electrodes in photodetectors and solar cell devices. We prepared ITO thin films by dual ion beam sputtering from an ITO target on glass microscope slides. During the deposition the substrate was exposed to an atomic oxygen beam. We investigated the influence of the oxygen flow and RF power on the optical and electrical properties of the thin films. The substrates were cleaned ultrasonically in IPA prior to being loaded in the vacuum system (background pressure in 1E-7 torr range). The argon sputtering pressure as well as the beam and acceleration voltages were kept constant during deposition. The RF power of the assist beam was kept at 200 Watt. The oxygen atomic beam was varied by varying the oxygen flow from 0 to 5 sccm. The RF power of the main gun was varied from 64 to 110 Watt. The resistivity of the samples were measured by linear 4pp. The optical properties of the samples were measured by transmission spectroscopy and ellipsometry. The resistivity and the absorption of the films appeared to be minimum at 5 sccm and 86 Watt.

[1]This work was supported by an MI-CCSA grant from Research Corporation

K1.00080 DNA-Templated Synthesis of Pt Nanoparticles on Single-Walled Carbon Nanotubes and their Electrocatalytic Properties

, QIANQIAN LIU, LIFENG DONG[1], Missouri State University — Platinum (Pt) supported on single-walled carbon nanotubes is one of the most efficient catalysts for both methanol and ethanol electroxidations. However, there is lack of a facile and environmental method to synthesize Pt nanoparticles on SWCNTs. In this study, we investigated a novel method to synthesize Pt nanoparticles on SWCNTs using DNA molecules as dispersing agent for nanotubes and templates for Pt nanoparticles. Morphology and structure of Pt nanoparticles and their distributions along SWCNTs as well as interactions between SWCNTs and DNA molecules were studied with the use of scanning electron microscopy, transmission electron microscopy, UV-vis spectroscopy, and X-ray diffraction spectrometer. Electrocatalytic activities of Pt nanoparticles for methanol and ethanol oxidations were characterized using cyclic voltammetry and impedance spectroscopy. With this study, we conclude effects of DNA molecules on synthesis of Pt nanoparticles on SWCNTs and electrocatalytic activity of Pt nanoparticles supported on SWCNTs for methanol and ethanol oxidations.

[1]Qingdao University of Science and Technology

K1.00082 First-Principles Study of LiPON Solid Electrolyte

, SANTOSH K.C., Department of Physics, University of Texas at Dallas, Richardson, Tx 75080, KA XIONG, KYEONGJAE CHO, Department of Material Science & Engineering, University of Texas at Dallas, Richardson, Tx 75080 — There has been much interest in the thin-film solid electrolyte for solid state battery and ionics applications. LiPON is a representative material developed by Oak Ridge National Laboratory [1]. In this work, we use first principles calculations based on the density functional theory to investigate the Li- ion migration mechanisms of LiPON family materials [2]. We investigate atomic structures, electronic structures and defect formation energies of these materials. To determine the migration path of Li diffusion, the activation energies are calculated. This study helps us to understand fundamental mechanisms of Li-ion migration and to improve Li ion conductivity in the solid electrolytes.

[1] Patil et al, Material Research Bulletin, 43 (2008) 1913-1942.
[2] Yaojun A. Du and N. A. W. Holzwarth, Physical Review B, 81 (2010).

K1.00083 Electrical and electrochemical characterization of nano-sized $LiFePO_4$ cathode materials synthesized by a lauric acid-based sol–gel method

, KHADIJE BAZZI, AMBESH DIXIT, M. B. SAHANA, C. SUDAKAR, Wayne State University, M. NAZRI, Applied Sciences Inc., Cedarville, Ohio, P. P. VAISHNAVA, Kettering University, Flint, Michigan, V. NAIK, University of Michigan-Dearborn, G. A. NAZRI, R. NAIK, Wayne State University — We synthesized pure $LiFePO_4$ and C-$LiFePO_4$ nanoparticles by sol-gel technique. Carbon coating was accomplished by including Lauric acid in the sol-gel precursor solution. Three C-$LiFePO_4$ samples of particle sizes 29, 27, 23 nm, were prepared by varying lauric acid concentration in the precursor solution. All the samples were characterized by X-ray diffraction, Raman, conductivity, and electrochemical measurements. The micro-Raman measurements showed two major bands at $\sim$1585 cm^{-1} (G) and at $\sim$1345 cm^{-1} (D) in all the C-$LiFePO_4$ samples. The 23 nm particle size sample showed minimum (D/G) band ratio and the maximum electrical conductivity among the three samples. The measured value of the capacity for 23 nm sized sample, $\sim$170 mAh/g, approached the theoretical capacity limit value for $LiFePO_4$

K1.00084 Templated electrodeposition of nanoporous silicon for battery applications

, STEPHANIE LIM, Bryn Mawr College, PA, USA, KARINE NAMUR, FLORIE MARTINEAU, JEREMY MALLET, Universite de Reims, France, JIABIN LIU, QIAN WU, HAN-CHANG YANG, X. M. CHENG, Bryn Mawr College, PA, USA — While battery technology has improved greatly in the last several years, the ability of batteries to store energy is still small compared to that of fossil fuels. In lithium ion batteries, the key issue is insufficient energy density, which is related to the interfacial surface area of the battery electrode. There is an urgent need to develop high capacity electrode materials and among the most promising candidates are Si based anode materials with specific energy capacities up to ten times greater than those of conventional graphite-based materials. We report the fabrication of nanoporous Si using templated electrochemical deposition method. The fabrication involves the following steps: self-assembly of monodispersed polystyrene spheres, electrochemical deposition of Si into the self-assembled template, and sphere removal by a dissolution process. The pore size of the nanoporous Si was tuned by using various sizes of template polystyrene spheres. Scanning electron microscopy images confirmed the high porosity of the samples. The templated electrochemical deposition technique provides a promising alternative approach to preparing highly porous anode materials for battery applications.

K1.00085 Li ion migration of lithium thiophosphate solid electrolyte materials[1] , ROBERTO LONGO PAZOS, KA XIONG, WEICHAO WANG, KYEONGJAE CHO, Materials Science & Engineering Dept, The University of Texas at Dallas, Richardson, TX 75080 — Li_2S-P_2S_5-based glasses are of great interest to be used as electrolytes in solid-state batteries. However, a detailed understanding on their structures and diffusion mechanisms is still missing. In this work, we investigate the atomic structures and ion diffusion mechanisms of various thiophosphate composites. These materials show intriguing structural similarities to their analogous Li phosphates. As a high ion conductivity battery material, interstitial and vacancy Li point defects should be reasonably stable within the host system. Besides, system with charged defect must be insulating to prevent electronic conduct which may low the ion conductivity. Our results show that interstitial Li has lower formation energy than Li vacancy, thus indicating that the ion conductivity may arise from the migration of interstitial Li. We propose possible solutions to optimize it. This study will help us to gain fundamental understanding on the Li ion diffusion process.

[1]This work is supported by DOE Energy Storage project.

K1.00086 Simulating Dendritic Formation and Possible Prevention Within Lithium-ion Batteries , JOSEPH ORTIZ, Stony Brook University, ARPON RAKSIT, Commack High School, NING SUN, DILIP GERSAPPE, Stony Brook University — As technology advances and becomes more dependent on lithium-ion batteries for power, the formation and subsequent separation of dendrites along the cathode may shorten the lifespan and efficiency of these batteries. However, not much is known about the mechanisms that cause dendrite formation within the battery or how to prevent their occurrence. Using a three-dimensional lattice-Boltzmann simulation, a lithium-ion battery was simulated that would allow for dendritic formation and separation. The simulation was carried out using several pre-existing cathode morphologies, and the hindrance and prevention effects of these changes were examined.

K1.00087 Luminescent Properties of $Ca_3Sc_2Si_3O_{12}$: Mn^{2+} and Ce^{3+} for a White LED , WILLIAM COGGINS, JESSICA LANG, LI MA, Physics Department Georgia Southern Univ. — In this experiment, we studied the excitation and emission properties, as well as the fluorescence decay of the doubly doped $Ca_3Sc_2Si_3O_{12}$: Mn^{2+} and Ce^{3+} phosphor. The phosphor is coated on a GaN LED chip, and the Mn^{2+} and Ce^{3+} centers give red and green emissions, respectively, subject to the blue excitation from the chip. Together with the transmitted blue light from the LED chip, the system yields an ideal white light, with a potential application for lighting. The red emission from Mn^{2+} ions has a longer decay time than that of the green emission from the Ce^{3+}. The color composition and stability along with the input power have also been studied.

K1.00089 Introduction to SC-Potential , FLORENTIN SMARANDACHE, University of New Mexico, Gallup, VICTOR CHRISTIANTO — A new type of potential for nucleus, which is different from Coulomb potential or Yukawa potential, is introduced. This new called Smarandache-Christianto potential may have effect for radius range within r = 5-10 fm. For experimental verification of this potential, we find possible applications in the context of Condensed Matter Nuclear reaction. According to Takahashi's research, it is more likely to get condensed matter nuclear reaction using cluster of deuterium (4D) rather than using D+D reaction (as in hot-fusion, in this process Coulomb barrier is very high). In recent work, Takahashi shows that in the TSC framework it is also possible to do CMNS reaction not only with DDDD, but also with DDDH, DDHH, DHHH, or HHHH, where the reaction can be different. In other words, TSC can be a mixture of heavy and light water (as in neutrosophic logic). More interestingly, his EQPET/TSC (*tetrahedra symmetric condensate*) model, Takahashi can predict a new potential called STTBA (*sudden-tall thin barrier approximate*) which includes negative potential (reverse potential) and differs from Coulomb potential. The SC-potential, which has sinusoidal form, can be viewed as a generalization of Takahashi's TSC/STTBA potential.

K1.00090 "Force Field" for Plasma Confinement[1] , CARLOS ORDONEZ, University of North Texas — Theoretical research associated with producing an electromagnetic field referred to as a "force field" is reported. A force field is defined at present as a static electromagnetic field that has the following characteristics: (1) It has an effective range that is much smaller than the dimensions of a cloud, plasma or beam of charged particles that is confined by the field. (2) It can simultaneously reflect incident charged particles of either sign of charge. A force field could consist of a spatially periodic sequence of magnetic cusps that are electrostatically plugged using applied electrostatic potential variations similar to that found in nested Penning traps. For plasma confinement, a possible configuration consists of a sequence of coaxial ring cusps. The diameter of the ring cusps varies axially, with the smallest rings located near the axial ends of the confinement volume. Two point cusps that are coaxial with the ring cusps are located at the axial ends of the confinement volumes. A current-carrying wire placed along the axis of symmetry could be used to produce a minimum-B configuration. In the work reported, a theoretical understanding is developed of the single-particle reflection properties of a force field that confines a non-drifting, isotropic plasma.

[1]This material is based upon work supported by the Department of Energy under Grant No. DE-FG02-06ER54883.

K1.00091 Charged Particle Interactions with a Static Electromagnetic "Force Field"[1] , JOSE PACHECO, DUNCAN WEATHERS, CARLOS ORDONEZ — Experimental research associated with producing an electromagnetic field referred to as a "force field" is reported. A force field is defined at present as a short-range static electromagnetic field that can simultaneously reflect incident charged particles of either sign of charge. The charged particles can originate from a cloud, plasma or beam. A force field consisting of a spatially periodic sequence of magnetic cusps is investigated, where the magnetic cusps are electrostatically plugged using applied electrostatic potential variations similar to those found in nested Penning traps. Such a configuration could in principle be utilized to trap an effectively unmagnetized or minimum-B configuration plasma. The aim of the work reported is to understand the plasma-particle reflection properties of a planar force field created with straight, parallel line cusps. Initial experimental results are presented.

[1]This material is based upon work supported by the Department of Energy under Grant No. DE-FG02-06ER54883.

K1.00092 Energy Transfer Between Antiprotons and Leptons Within a Strong Magnetic Field[1] , JOSE CORREA, JONATHAN WURTELE, CARLOS ORDONEZ — Some experiments conducted at the CERN Antiproton Decelerator are aimed at creating and confining antihydrogen. In many of the experiments, energetic antiprotons are cooled by collisions with electrons within a strong magnetic field. The cold antiprotons are subsequently made to interact with positrons under a strong magnetic field leading to some recombination. In the work to be reported, an analytical model for strongly magnetized collisions is developed and applied to investigate the energy loss of antiprotons interacting with cold and warm leptons under a strong magnetic field. In this model, the strong magnetization constrains the momentum transfer to one dimension, which is parallel to the magnetic field. Thus, collisional energy transfer is dominated by short-range collisions. The result is remarkably different from the unmagnetized case. The theoretical expectations are compared with prior and new computer simulations. The agreement found reveals that the model captures important features of the interaction of electrical charges of disparate masses such as antiprotons and leptons within a strong magnetic field.

[1]This material is based upon work supported by the Department of Energy under Grant No. DE-FG02-06ER54883.

K1.00093 Isothermal Expansion of a Solid-Particle-Entrained Gas and Plasma-Based Energy Conversion

, ERIC LESSMANN, MATTHEW TRAUM, DUNCAN WEATHERS, CARLOS ORDONEZ — Experimental and theoretical research is reported on the expansion of a two-phase fluid consisting of a mixture of compressed gas and solid particles. Experimental temperature measurements indicate that the expansion is describable as isothermal for the conditions studied. During the expansion, the energy of the compressed gas is converted into kinetic energy of the solid particles. The solid particles travel at a subsonic speed, serve as a heat exchange medium, and are recycled. In the experiment, the gas-solid two-phase fluid travels through a nozzle during the isothermal expansion. Conversion of the energy of a compressed gas has been demonstrated experimentally using a turbine to convert the kinetic energy of the solid particles into other forms. A second method is also being studied for converting the kinetic energy of the solid particles after the gas expansion. The second method, which would replace the turbine, would convert the kinetic energy of the solid particles into electrical energy by charging the solid particles (e.g., by passing them through an electron plasma or by reflection off one plate of a capacitor). The charged solid particles would then carry a current across a change in electric potential inertially (without collisions with a wall) and then be discharged (e.g., by passing them through an ion plasma or by reflection off one plate of a second capacitor).

K1.00094 Nanostructure Control of P3HT:PCBM Bulk Hetero-junction Polymer Solar Cells[1]

, J. SEOK, E. GANN, C.M. BALIK, H. ADE, NCSU, B. OCKO, X. LU, H. HLAING, BNL — Highly regioregular Poly(3-hexyl thiophene) (P3HT) and [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) are a widely used model system for Bulk hetero-junction (BHJ) solar cells. For optimized P3HT:PCBM BHJ solar cells, not only is a small domain size on the order to the exciton diffusion length ($\sim$10nm) required, but the orientation of P3HT crystallites should be optimized as well. Small domains result in effective charge separation and minimize charge recombination at the interface between P3HT and PCBM. Additionally, face-on crystalline orientation of P3HT in which the $\pi - \pi$ stacking direction is parallel to the electric field enhances the hole charge carrier mobility. We are presenting a new strategy to achieve somewhat increased face-on P3HT crystalline orientation and smaller domain size in P3HT/PCBM BHJ solar cells than what is readily achievable with thermal annealing alone. This improved nanostructure control is achieved by in-situ polymerization of 2,5-dibromothiophene present in the thin films after short vapor annealing. Improvements in power conversion efficiency of approx. 30% relative to thermal annealing alone were achieved.

[1]DOE DE-FG02-98ER45737

K1.00095 First-Principles Studies on Lattice Dynamical Properties of Zn_4Sb_3 Compounds[1]

, YI ZHANG, CHANGFENG CHEN, Physics Department and HiPSEC, University of Nevada, Las Vegas, JIHUI YANG, Electrochemical Energy Research Lab, GM R&D Center — The origin of extremely low lattice thermal conductivity in Zn_4Sb_3 compound has attracted great interests but remains not fully understood due to its complex crystal structure. We have performed extensive first-principles calculations on the lattice vibration modes and thermodynamics of Zn_4Sb_3 based on its experimental crystal structure. The low frequency modes and structural inhomogeneity that could be responsible for the low thermal conductivity have been discussed.

[1]This work is supproted by DOE Agreements DE-FC52-06NA26274 and DE-FC26-04NT42278 and by GM. Computation resource in NCCS is supported by DOE.

K1.00096 Impact of impurities on the electronic structures of thermoelectric material Mg_2Si[1]

, KA XIONG, SABINA SOBHANNI, RAHUL GUPTA, WEICHAO WANG, BRUCE GNADE, KYEONGJAE CHO, University of Texas at Dallas — Thermoelectric (TE) materials have attracted a lot of attention because of its capability of converting heat into electricity or vice versa. In this work, we investigate the effects of dopants in Mg_2Si, which is a promising TE material candidate. We calculate the electronic structures and stability of various dopants (Al, In, P, As, Sb, Bi, Ag, Cu, Zn, and Cd) in Mg_2Si with different charge states, using density functional theory (DFT) method with HSE functional which gives accurate band gap prediction. This DFT study helps us to gain insights on the defect states of these dopants in Mg_2Si and the mechanisms which cause the modulation of the Mg_2Si TE efficiency.

[1]This work is supported by the II-VI Foundation, a private foundation.

K1.00097 Neutron Scattering Measurements of Temperature-Dependent Phonon Spectra in Thermoelectric Materials PbTe and (Ag,Sb)Te_2[1]

, JIE MA, OLIVIER DELAIRE, BRIAN SALES, KAROL MARTY, DOUGLAS ABERNATHY, MATTHEW STONE, GEORG EHLERS, ORNL COLLABORATION — The thermoelectric materials PbTe and (Ag,Sb)Te_2, which both crystallize in the rocksalt structure, have attracted much attention due to their high zT values. Prior theoretical and experimental studies have investigated the phonon dispersions of PbTe, and the importance of the electron-phonon and phonon-phonon couplings has been recognized. However, phonons have not been investigated in details in (Ag,Sb)Te_2. Also, little is known about the phonon linewidths, which directly correlate with the lattice thermal conductivity. In order to better understand the microscopic origins of the lattice thermal conductivity, time-of-flight and triple-axis inelastic neutron scattering measurements were performed as a function of temperature in both compounds. The results of phonon linewidths and their systematic dependence on temperature are presented, providing a direct measurement of the contribution of phonons to the total thermal conductivity.

[1]O.D. acknowledges funding from US DOE/BES as part of an Energy Frontier Research Center, DOE DE-SC0001299.

K1.00098 $Gd_{116}Co_{49}Sn_{118}$: A Complex Intermetallic Phonon-Glass/Electron-Crystal[1]

, DEVIN SCHMITT, NEEL HALDOLAARACHCHIGE, YIMIN XIONG, RONGYING JIN, DAVID YOUNG, JULIA CHAN, Louisiana State University — State-of-the art thermoelectric devices today operate at very low efficiencies and are expensive to produce. However, the growing need for alternate energy sources based on novel technologies has brought thermoelectrics to the forefront of applied materials research. Thermoelectrics could have a significant impact in this area, if their performance is significantly enhanced to a figure of merit (ZT) above 1.5. Our research focuses on the growth and structure-property relationships of intermetallics, specifically crystal structures with large lattice parameters that contain heavy atoms. These materials may be good thermoelectric candidates due to their potentially low lattice thermal conductivities and enhanced Seebeck values resulting from polar intermetallic properties. We have recently grown $Gd_{116}Co_{49}Sn_{118}$ (*Fm-3m*, $a \cong 30.2$ Å), a compound related to the $Dy_{117}Co_{57}Sn_{112}$ structure type. Physical property measurements indicate that this is an ambipolar semiconductor with an exceptionally low lattice thermal conductivity ($\kappa_l \cong 0.5$ W/m-K). The observed phonon-glass/electron-crystal properties make $Gd_{116}Co_{49}Sn_{118}$ and its analogues potential thermoelectric candidates.

[1]We acknowledge NSF-DMR0756281 and NSF-DMR0449022.

K1.00099 Bipolar Membranes for Acid Base Flow Batteries , MITCHELL ANTHAMATTEN, SUPACHAREE RODDECHA, JACOB JORNÉ, ANNA COUGHLAN, University of Rochester — Rechargeable batteries can provide grid-scale electricity storage to match power generation with consumption and promote renewable energy sources. Flow batteries offer modular and flexible design, low cost per kWh and high efficiencies. A novel flow battery concept will be presented based on acid-base neutralization where protons (H+) and hydroxyl (OH-) ions react electrochemically to produce water. The large free energy of this highly reversible reaction can be stored chemically, and, upon discharge, can be harvested as usable electricity. The acid-base flow battery concept avoids the use of a sluggish oxygen electrode and utilizes the highly reversible hydrogen electrode, thus eliminating the need for expensive noble metal catalysts. The proposed flow battery is a hybrid of a battery and a fuel cell—hydrogen gas storing chemical energy is produced at one electrode and is immediately consumed at the other electrode. The two electrodes are exposed to low and high pH solutions, and these solutions are separated by a hybrid membrane containing a hybrid cation and anion exchange membrane (CEM/AEM). Membrane design will be discussed, along with ion-transport data for synthesized membranes.

K1.00100 ATOMIC, MOLECULAR AND OPTICAL (AMO) PHYSICS –

K1.00101 Universal contact of strongly interacting Fermi gases , MARK DELLOSTRITTO, THEJA DE SILVA, Binghamton University — We study strongly interacting two component Fermi gas near a Feshbach resonance. By using a ground state energy functional constructed based on asymptotic limits and Monte Carlo calculations, we calculate the contact, structure factor, and collective oscillation frequencies in the BCS-BEC crossover region. The calculated contact and structure factor show excellent agreement with recent experiments. We show that the upper bounds of the collective modes have universal form in the sense that they depend only on the contact and the homogenous energy. In other words, the collective modes of the Fermi atoms trapped near Feshbach resonance can be calculated without the explicit knowledge of trapping potential.

K1.00102 Spin-charge separation in one-dimensional fermion systems beyond Luttinger liquid theory , THOMAS SCHMIDT, Yale University, ADILET IMAMBEKOV, Rice University, LEONID GLAZMAN, Yale University — We develop a nonperturbative zero-temperature theory for the dynamic response functions of interacting one-dimensional spin-1/2 fermions. In contrast to the conventional Luttinger liquid theory, we take into account the nonlinearity of the fermion dispersion exactly. We calculate the power-law singularities of the spectral function and the charge- and spin-density structure factors for arbitrary momenta and interaction strengths. The exponents characterizing the singularities are functions of momenta and differ significantly from the predictions of the linear Luttinger liquid theory. We generalize the notion of the spin-charge separation to the nonlinear spectrum. This generalization leads to phenomenological relations between threshold exponents and the threshold energy.

K1.00103 Control the spin coherence of a spin-1 Bose-Einstein Condensate with dynamical decoupling approach , BOYUAN NING, JUN ZHUANG, WENXIAN ZHANG, Department of Optical Science and Engineering, Fudan University, Shanghai 200433, China, J.Q. YOU, Department of Physics, Fudan University, Shanghai 200433, China — The coherence of spinor Bose-Einstein condensates (BECs) is determined by the dynamically unstable collective modes. Recently, Uhrig Dynamical Decoupling (UDD), a sequence containing n π-pulses, has been applied to eliminate the decoherence of a qubit in the spin-boson (SB) model up to the order of $\mathcal{O}(t^{n+1})$ and proved to be a universal method. Stimulated by its promising power, we conjecture whether the UDD sequence could also preserve the coherence of a spinor BEC by modulating the spin exchange interaction through optical Feshbach resonance. In this work, we theoretically analyze the effect of UDD, periodic DD (PDD) and concatenated DD (CDD) to maintain the coherence of a ^{87}Rb spin-1 BEC and a scalar BEC. Our numerical results show that the CDD, as n increases, suppresses the decoherence more than the other two DD sequences in both the spinor and the scalar BECs. However, it is interesting that all three sequences only remove the decoherence up to the same order $\mathcal{O}(t)$. We further carry out analytical works for the scalar BEC, which confirms our numerical results that UDD, compared to the case of SB model, is not as superior as expected at coherence control in BECs.

K1.00104 Bosonic matter inside a periodic array of tubes , P. SALAS, UNAM, F.J. SEVILLA, M. FORTES, M.A. SOLIS, Instituto de Fisica, UNAM — We report the Bose-Einstein Condensation critical temperature, internal energy and specific heat per particle of an ideal boson gas in periodically trapping channels. These are simulated by two perpendicular external Kronig-Penney delta potentials applied on the x-y plane and allowing the particles to move freely in the remaining direction. We obtain the Bose-Einstein condensation critical temperature of the system as a function of the separation between deltas and as a function of their intensity which models the penetrability of the tube walls. It is shown that T_c decreases monotonically, from the 3D ideal boson gas T_0 for vanishing delta strenght, down to 0 as the intensity grows to infinity while keeping the channel's cross section constant. The quotient T_c/T_0 as a function of the width of the tubes starts at 1, reaches a minimum value that depends on the permeability and returns to 1 as the widths vary from infinity to 0. We observe that the specific heat as a function of the temperature is modified by the tubular structure, showing a set of maxima and minima for different values of permeability of the walls and widths of the tubes. In particular, when half the wave-length of the boson gas is the same as the tubes' square cross section, the system clearly exhibits the trapping effect due to the tubes. In this case the specific heat has a minimum very similar to that of the one- dimensional case.

K1.00105 Specific heat of bosons in periodical bilayers , O.A. RODRIGUEZ, P. SALAS, UNAM, M.A. SOLIS, Instituto de Fisica, UNAM — We report the specific heat at constant volume of an ideal boson gas inside a periodical bilayer structure modeled with a generalized Kronig-Penney (KP) delta potential in the z-direction while the particles are free in the other two directions. The generalized KP potential has two different strength delta potentials by unit cell, and they are separated βa, where a is the unit cell length and $0 \leq \beta \leq 1$. After calculating the energy band structure we use it to obtain the Bose-Einstein condensation critical temperature besides the chemical potential, the internal energy and the specific heat, as functions of the temperature, for different values of the parameters a, β and the delta strengths. For any parameter set we observe a Bose-Einstein condensation at a lower temperature than that of an infinite ideal Bose gas in the thermodynamic limit and with the same particle density. From the specific heat we distinguish at least four characteristic lengths. They are associated to the thermal wave length values at: the BEC critical temperature where the specific heat shows a peak and a discontinuity in their derivative; two minima of the specific heat where the thermal wave lengths are equal to two times the plane separations βa and $(a - \beta a)$; and about 0.7 times the minimum plane separation, where the specific heat behavior returns to that of an ideal Bose gas. Also the delta strength effects on the specific heat are discussed.

K1.00106 Probing and Manipulating Fermi Gases Using Classical Impurities[1] , LEI JIANG, LESLIE O. BAKSMATY, HAN PU, Department of Physics and Astronomy, and RQI, Rice University, Houston, TX, USA, HUI HU, ARC Centre of Excellence for Quantum-Atom Optics, Swinburne University of Technology, Melbourne, Australia, YAN CHEN, Laboratory of Advanced Materials and Department of Physics, Fudan University, Shanghai, China — Impurities can be used as probes to detect material properties and to understand quantum phenomena. Here we study the effect of a single classical impurity in ultracold s-wave Fermi superfluids. We use T-matrix and B-dG method to study both 1D and 3D cases to mean-field level. A magnetic impurity can induce a mid-gap bound state located inside the pairing gap. In addition, magnetic impurity can locally induce population imbalance in the system, potentially providing a method to realize FFLO-like state in a controlled way. We further extend the 1D impurity case to strong correlated region using DMRG. We also propose a modified RF spectroscopy to measure the local density of states, as a cold-atom analog of STM.

[1]This work is supported by the NSF, the Welch Foundation and the DARPA OLE Program

K1.00107 Generating sodium Bose-Einstein condensates in hybrid magnetic quadrupole and optical traps

, ZONGKAI TIAN, JIE JIANG, JARED AUSTIN, JOHN JEPSON, YINGMEI LIU, Department of Physics, Oklahoma State University, Stillwater, OK 74078 — We present the design and construction of a novel apparatus to rapidly and simply generate ^{23}Na Bose-Einstein condensates in hybrid magnetic and optical traps. Sodium atoms are collected in a magnetic-optical trap, captured in a magnetic quadrupole trap, and then cooled through forced radio-frequency evaporation. To avoid Majorana spin-flip losses at the center of the magnetic quadrupole trap, the cold dense atomic cloud is transferred to a crossed red-detuned optical dipole trap. By reducing the optical trap depth, sodium Bose-Einstein condensates are generated from forced evaporation and rethermalization in the crossed optical trap. This hybrid approach combines the advantages of both magnetic quadrupole and optical traps.

K1.00108 Construction and Implementation of a Low-Cost Rubidium Magneto-Optical Trap[1]

, JUDITH OLSON, Ithaca College — A low-cost magneto-optical trap (MOT) for ultra-cold atoms is a wonderful tool for undergraduate research and teaching laboratories that highlights many topics in modern physics. We researched and created such a MOT using two external-cavity diode lasers, two laser locking systems, optics, magnetic coils, and Rubidium vapor cells. At our undergraduate institution, we chose a combination of equipment that we fabricated ourselves together with some purchased items as an optimum balance between cost and building time. However, an emphasis was placed upon self-construction of components, such as machining the laser cavities and constructing the majority of the circuitry within the institution. The total cost of our MOT was about $25,000. We were successfully able to trap more than 10 million Rubidium atoms in 1 cubic centimeter. Such a MOT is a feasible addition to any undergraduate course of study. The theory of operation and construction methods of our MOT will be presented along with our first measurement results.

[1]Many thanks to Ithaca College and the Ithaca College Department of Physics.

K1.00109 Ultracold Realization of AntiFerromagenteic Order[1]

, UTTAM SHRESTHA, University of California, Irvine — We investigate numerically the experimental feasibility of observing the antiferromagnetic (AF) order in the bosonic mixtures of rubidium (^{87}Rb) and potassium (^{41}K) in a two-dimensional optical lattice with external trapping potential. Within the mean-field approximation we have found the ground states which, for a specific range of parameters such as inter-species interactions and lattice height, interpolate from phase separation to the AF order. For the moderate lattice heights the coexistence of the Mott and AF phase is possible for rubidium atoms while the potassium atoms remain superfluid with overlapped AF phase. In our view there has not been any study on AF order in two-component systems when one component remains in the superfluid phase while the other is in the Mott phase. Therefore, this observation may provide a novel regime for studying quantum magnetism in ultracold systems.

[1]This work was supported by the EU Contract EU STREP NAMEQUAM.

K1.00110 FFLO phase on an optical lattice: a quantum Monte Carlo study[1]

, CHIA-CHEN CHANG, SHIWEI ZHANG, Department of Physics, College of William and Mary — Recent experimental progress in cold Fermi gases has demonstrated the possibility of realizing exotic quantum phases in optical lattices. One example is the Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) state arising from pairing across the Fermi surfaces in a spin-imbalanced system with attractive interaction. We study ground state magnetic properties in 2D and 3D repulsive Hubbard models at intermediate interaction strengths by means of a highly accurate auxiliary-field quantum Monte Carlo method [1] coupled with Twist-averaged boundary conditions. The sign problem is controlled by a generalized constrained path approximation. It is found that the ground state shows incommensurate spin density wave order with periodic spatial modulation when the model is slightly doped away from $n = 1$. We present our results in 2D [2] and 3D, and discuss their implications, through a particle-hole transformation, on the FFLO phase on an optical lattice of spin-imbalanced fermions with an attractive interaction. This work is supported by ARO. Reference: [1] Chia-Chen Chang and Shiwei Zhang, Phys. Rev. B 78, 165101 (2008) [2] Chia-Chen Chang and Shiwei Zhang, Phys. Rev. Lett. 104, 116402 (2010).

[1]This work is supported by ARO.

K1.00111 Progress toward realization of antiferromagnetic ordering of cold atoms in an optical lattice[1]

, P.M. DUARTE, R. HART, T.L. YANG, J.M. HITCHCOCK, T.A. CORCOVILOS, R.G. HULET, Department of Physics and Astronomy and Rice Quantum Institute, Rice University, Houston, TX 77005 — We present progress toward the observation of antiferromagnetic (AFM) ordering of fermionic atoms in an optical lattice using Bragg scattering of light. We first laser cool ^{6}Li atoms using the $2S_{1/2} \rightarrow 2P_{3/2}$ transition and then further cool using the $2S_{1/2} \rightarrow 3P_{3/2}$ transition to T $\sim$ 65 μK, leading to enhanced loading into a far detuned optical dipole trap. After forced evaporative cooling, an incoherent spin mixture of the two lowest magnetic sublevels of the ground state is adiabatically loaded into a 3D optical lattice. By adjusting the s-wave scattering length and the depth of the lattice, we tune the interaction and hopping terms of the Hubbard Hamiltonian. Bragg scattering of light from the lattice planes can be used to detect sample ordering such as in the Mott insulator state. At low temperatures and weak interactions, a phase transition to AFM ordering of the two spin states is predicted to occur. The increased symmetry of the AFM state allows for Bragg scattering of light from the ordered spin planes, $\pm(^1/_2\,^1/_2\,^1/_2)$, and hence unambiguous detection of the AFM state. We present our progress in detecting the Mott insulator and AFM states.

[1]Supported by NSF, ONR, DARPA/ARO, and the Welch and Keck Foundations

K1.00112 A Qauntum Theory of Ultracold Atoms in Spatially Inhomogenoues Optical Lattices

, DAGIM TILAHUN, BYOUNGHAK LEE — Ultracold atoms in optical lattices undergo a quantum phase transition from a superfluid to a Mott insulator as the potential depth is increased. But the interpretations of most cold atoms experiments are complicated by the fact that the experimental systems are inhomogeneous, for example due to the harmonic trapping potential that is always present. Or the focus of the study itself could be what causes the non-uniformity, such as disorder. Here We apply a theory developed by one of the authors and a collaborator to these inhomogeneous systems to discuss their ground state and elementary excitations.

K1.00113 Geometric Unitary Gates in Cold Atom Ensembles on an Atom Chip

, YICONG ZHENG, TODD BRUN, University of Southern California, QUANTUM COMMUNICATION TEAM — We propose a feasible scheme to achieve quantum computation based on geometric manipulation of ensembles of atoms, and analyze it for neutral rubidium atoms magnetically trapped in planoconcave microcavities on an atom chip. The geometric operations are accomplished by optical excitation of a single atom into a Rydberg state in a constant electric field. Strong dipole-dipole interactions and incident lasers drive the dark state of the atom ensembles to undergo some specified cyclic evolutions that realize a universal set of quantum gates. Such geometric manipulation turns out naturally to protect the qubits from the errors induced by non-uniform laser illumination as well as cavity loss. The gate performance and decoherence processes are analyzed by numerical simulation.

K1.00114 A closed-cycle dilution refrigerator with free-space and fiber optical access for quantum optomechanics experiments at 25mK , SIMON GROEBLACHER, WITLEF WIECZOREK, University of Vienna, Austria, PETER CHRIST, MATTHIAS BUEHLER, Oxford Instruments, Munich, Germany, DOREEN WERNICKE, Entropy GmbH, Munich, Germany, JENS HOEHNE, Oxford Instruments, Munich, Germany, MARKUS ASPELMEYER, University of Vienna, Austria — We report on the operation of a closed-cycle dilution refrigerator for quantum optomechanics experiments at 25mK. The dilution fridge is accessible both via free-space as well as fiber coupling, allowing us to perform a variety of optical experiments at low temperatures. It is designed to vibrationally isolate the experiment allowing for stable operation of a high-finesse optical cavity. This enables us to perform cavity-optomechanics experiments at ultra-low temperatures.

K1.00115 Correlation energy of a homogeneous dipolar Fermi gas[1] , BO LIU, LAN YIN, School of Physics, Peking University, Beijing 100871, China — We study the normal state of a 3-D homogeneous dipolar Fermi gas beyond the Hartree-Fock approximation. The correlation energy is found of the same order as the Fock energy, unusually strong for a Fermi-liquid system. As a result, the critical density of mechanical collapse is smaller than that in the Hartree-Fock approximation. An new energy functional including the correlation energy is constructed to describe inhomogeneous cases, and its properties are explored.

[1]This work is supported by NSFC under Grant No. 10974004,and by Chinese MOST under grant number 2006CB921402.

K1.00116 Quantum Phases of Fermionic Cold Atoms Through Pairing and Dissociation , NICOLAS LOPEZ, SHAN-WEN TSAI, UCR, E. TIMMERMANS, LANL, CHI-YONG LIN, National Dong Hwa University, Taiwan — Cold atom experiments have realized molecule creation consisting of paired fermions and dissociation of weakly bound molecules into correlated fermions by tuning of the interactions with external fields [1,2]. We study many-body correlations in such system where molecules are weakly bound and therefore pairs of fermionic atoms convert into and dissociate from the bound molecule state. This exchange mediates a long-range interaction between the fermions. We consider a simple many-body Hamiltonian that includes the destruction of fermionic atom pairs to form single bosonic molecules and vice versa [3]. We employ a functional renormalization-group approach to search for instabilities from the disordered quantum liquid phase that may arise from a boson mediated fermion-fermion interaction. We calculate the renormalized frequency-dependent fermion interactions vertices and renormalized molecular binding energy.

[1] M. Greiner, C. A. Regal, and D. S. Jin, Nature **426**, 537 (2003).
[2] M. Greiner, C. A. Regal, J. T. Stewart, and D. S. Jin, Phys. Rev. Lett. **94**, 110401 (2005).
[3] E. Timmermans, K. Furuya, P. W. Milonni, and A. K. Kerman, Phys. Lett. A **285**, 228 (2001).

K1.00117 Influence of Non-Linear Interactions on the Propagation of Electromagnetic Fields in Moving Many-Electron Atomic Systems[1] , VERNE JACOBS, Naval Research Labortory — Reduced-density-matrix descriptions are developed for the propagation of electromagnetic fields in moving many-electron atomic systems, taking into account the center-of-mass motions, atomic collision processes, and applied magnetic fields. The time-domain (equation-of-motion) and the frequency-domain (resolvent- operator) formulations are developed in a unified manner. A semiclassical perturbative treatment of the electromagnetic interaction is employed to derive compact Liouville- space operator expressions for the general n'th-order non-linear macroscopic electromagnetic-response tensors. Coherent atomic excitations and the full tetradic- matrix form of the collision-radiative self-energy operator in the Markov approximation are taken into account.

[1]Work supported by the Office of Naval Research.

K1.00118 Analysis of two simultaneous EITs in a four-level atomic system in a W-scheme using a dressed-state representation , CRISTIAN BAHRIM, Department of Physics, Lamar University — A four-level atomic system in a W-scheme is used for slowing down *simultaneously* two circularly polarized optical fields using a linearly polarized coupling field. Our four-level atomic system is composed by the $^1S_0$ ground state and three Zeeman levels of the $^1P_1$ excited state of any alkali-metal atom introduced in a weak magnetic field. When the coupling field is stronger than both probe fields, the electromagnetic induced transparency (EIT) is observed in the coherences associated to the two probes, while the coherence associated to the coupling field shows opacity. We calculate the quantum coherences from the steady-state solutions of the density matrix master equation, in which we neglect the collisional dephasing (we consider ultra-cold atoms), but we include the radiative decays from each Zeeman state to the ground state. The coupling mechanism between the atomic states and the optical fields in our W-system and the evolution of the EIT features with the intensity of the coupling field is done using an intuitive dressed state representation. We also analyze the transit time from the normal dispersive region to the EIT region: when a weak probe field is used, the transit time is the shortest and the width of the Autler-Townes doublet equals the lifetime of the excited atomic state which experiences EIT, but it increases rapidly as the intensity of the probe field increase.

K1.00119 Infrared Spectrum of the Astrophysical Molecule SiC_5 , T.H. LE, W.R.M. GRAHAM, Texas Christian University — An infrared spectrum of SiC_5, one of many Si-C molecular species expected to play roles in the atmospheres of late carbon stars and in the interstellar medium, has been observed for the first time. The Fourier transform infrared spectrum (FTIR) was recorded for SiC_5 produced by trapping, in solid Ar, the products of the Nd:YAG laser ablation of a sintered, silicon-carbon rod enriched with ^{13}C. Based on excellent agreement between measured frequencies of ^{13}C and $^{29,30}Si$ isotopomers and the predictions of DFT (density functional theory) B3LYP/cc-pVDZ calculations, the linear geometry of SiC_5 has been confirmed and the $\nu_4(\sigma_u)$ asymmetric stretching fundamental of SiC_5 has been identified at 936.9 $\pm$ 0.2 cm $^{-1}$.

K1.00120 Vibrational Spectroscopy and Structures of Novel Metal-Carbon Species of Astrophysical Interest , MICHELINE BEJJANI, WILLIAM GRAHAM, MAGNUS RITTBY, Texas Christian University — This study on metal-carbon molecules is part of an ongoing investigation of the structures and vibrational frequencies of small metal carbide clusters using Fourier transform infrared spectroscopy (FTIR) and density functional theory (DFT). These studies are motivated by the potential presence of small metal carbide molecules in astrophysical environments. Binary carbon compounds containing silicon and sulfur, including SiC_2, SiC_3, and SC_3, have been observed in interstellar space and circumstellar shells. In addition several metal-containing molecules, such as MgCN and MgNC have also been detected. Hence, metal carbides have been suggested as possible interstellar molecules although a lack of information on their spectral properties may so far have prevented their detection. Recent studies by this laboratory on the infrared spectroscopy of matrix-isolated metal tricarbide clusters, such as fanlike TiC_3 and ScC_3, linear CrC_3 and CoC_3 and floppy NiC_3Ni have begun to provide some of this information. Here, we report the structures and vibrational spectra of MnC_3, ZnC_3 and MgC_3^-.

K1.00121 The two-dimensional and three dimensional confinement of the hydrogen molecular ion, inside ellipses and spheroids, respectively[1] , MARTIN MOLINAR, GERMAN CAMPOY-GÜEREÑA, DIFUS, Universidad de Sonora — The Schrödinger equation for the confinement of the hydrogen molecular ion in the Born – Oppenheimer is solved. The molecule is confined by rigid and non-rigid ellipses and spheroids. The energies for the ground state and the first excited states are determined.

[1]Martin Molinar-Tabares acknowledge to Universidad de Sonora for supporting the attendance.

K1.00122 Variational wave function approach to quantum quenches in bosonic systems , FEDERICO BECCA, GIUSEPPE CARLEO, STEFANO BARONI, CNR, Istituto Officina dei Materiali and SISSA, Trieste — Recent experiments with ultracold atomic gases have opened the possibility for studying non-equilibrium quantum dynamics of many-body systems. In particular, the high degree of tunability allows one to rapidly change system parameters and observe the subsequent quantum evolution. We present a new variational approach to deal with time-dependent problems where quantum quenches of the microscopic parameters induce a highly non-trivial dynamics. We show to what extent a generalization of the Jastrow wave function may accomplish this task, even for two-dimensional models, where standard Lanczos or density-matrix renormalization group methods are highly limited. Examples for interacting hard-core and soft-core bosons are shown. The generalization to fermionic models is also discussed.

K1.00123 Phase diagram of a population-imbalanced attractive Fermi gas in the 1D-3D crossover regime , SATYAN BHONGALE, George Mason University, LESLIE BAKSMATY, LEI JIANG, HAN PU, Rice University — Phase diagram of a population imbalanced attractive Fermi gas in the 1D-3D dimensional crossover regime is obtained via deriving a multi-channel inter-atomic scattering pseudopotential. Such a phase diagram has strong implications for the observation of FFLO superfluidity within trapped fermions. Recent experiment with ultra-cold Li6 have mapped the phase diagram for 1D attractive fermions [Nature 467, 567 (2010)], however the superfluid property is yet to be confirmed. While the signature of FFLO in 1D is predicted to coincide with micro-phase separated domains, the feasibility of direct experimental identification of the domain walls remains questionable due to strong fluctuations. On the other hand, in 3D, fluctuations may be neglected, but the FFLO corresponds to just a tiny sliver of the phase diagram. Moreover, the topology of the phase diagram is drastically different in the two extreme dimensional limits. We show how the 1D and 3D dimensional limits are connected and indicate the possible new physics in the crossover regime.

K1.00124 Controllable optical switch using a Bose-Einstein condensate in an optical cavity , SHUAI YANG, Institute for Quantum Studies and Department of Physics, Texas A&M University, College Station, Texas 77843, USA, M. AL-AMRI, The National Center for Mathematics and Physics, KACST, P.O. Box 6086, Riyadh 11442, Saudi, JÖRG EVERS, Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, D-69117 Heidelberg, Germany, M. SUHAIL ZUBAIRY, Institute for Quantum Studies and Department of Physics, Texas A&M University, College Station, Texas 77843, USA — The optical bistability of an ultra cold atomic ensemble located in a small volume ultra-high finesse optical cavity is investigated. We find that the transverse pumping field can be used to control the bistable behavior of the intra cavity photons induced by the input pumping along the cavity axis. This phenomenon can be used as a controllable optical switch.

K1.00125 QUANTUM INFORMATION, CONCEPTS AND COMPUTATION –

K1.00126 Quantum Mechanics as Dualism , ROBERT JONES, Emporia State University — I do not agree with mind-body dualism. Today the consensus view is that thought and mind is a combination of processes like memory, generalization, comparison, deduction, organization, induction, classification, feature detection, analogy, etc. performed by computational machinery. (R. Jones, Trans. of the Kansas Acad. Sci., vol. 109, # 3/4, 2006 and www.robert-w-jones.com, philosopher, theory of thought) But I believe that quantum mechanics is a more plausible dualist theory of reality. The quantum mechanical wave function is nonphysical, it exists in a 3N space (for an N body system) not in (x,y,z,t) 4-space, and does not possess physical properties. But real physical things like energy (which do exist in our 4-space world) influence the wave function and the wave function, in its turn, influences real physical things, like where a particle can be found in 4-space. The coupling between the spirit-like wave function and things found in the real (4-space) world (like energy) is via mathematical equations like the Schrodinger equation and Born normalization.

K1.00127 Some Statistical Measures and Analytical Results of Quantum Walks under Weak Measurement and Weak Values Regime , DEBABRATA GHOSHAL, George Mason University, MARCO LANZAGORTA, ITT Corportation, SALVADOR VENEGAS-ANDRACA, Tecnológico de Monterrey Campus Estado de México (ITESM-CEM) — Motivated by experimental results on quantum weak measurements and weak values as well as by the need to develop new insights for quantum algorithm development, we study the behavior of quantum walks under the regime of quantum weak measurements and weak values of pre- and post-selected measurements (QWWM hereinafter). In particular, we investigate the limiting position probability distribution and several statistical measures (such as standard deviation) of a QWWM on an infinite line, and compare such results with corresponding classical and quantum walks position probability distributions and statistical measures, stressing the differences provided by weak measurements and weak values with respect to results computed by using canonical observables. We start by producing a concise introduction to quantum weak values and quantum weak measurements. We then introduce definitions as well as both analytical and numerical results for a QWWM under Hadamard evolution and extend our analysis to quantum evolution ruled by general unitary operators. Moreover, we define a 2-walker QWWM on an infinite 2D lattice and explore its behavior on limiting probability distribution, standard deviation and degree of entanglement between walkers.

K1.00128 Generating Entangled States With Hybrid Parity Gates[1] , ZHI-MING ZHANG, FENG MEI, YA-FEI YU, XUN-LI FENG, South China Normal University — We propose a scheme for generating entangled states among different single atoms trapped in separated cavities. In our scheme, by reflecting an input coherent optical pulse from a cavity with a single trapped atom, a controlled phase-shift gate between the atom and the coherent optical pulse can be achieved. Based on this gate and homodyne detection, we construct an n-qubit parity gate and show its use for distribution of a large class of entangled states, including the GHZ states, the W states, the Dicke states, and certain sums of the Dicke states. We also show that such distribution can be performed with high success probability and high fidelity even in the presence of channel loss.

[1]This work was supported by the National Natural Science Foundation of China (No. 60978009), and the National Basic Research Program of China (Nos. 2007CB925204 and 2009CB929604).

K1.00129 Optical Engineering for Quantum Computing Over the Optical Frequency Comb , MORAN CHEN, OLIVIER PFISTER, University of Virginia — The optical frequency comb (OFC) of a single optical parametric oscillator (OPO) has shown a spectacular, if theoretical, scalability potential as a continuous-variable one-way quantum register. Indeed, an arbitrarily large, square-grid cluster state, suitable for universal quantum computing, can in principle be generated in one fell swoop in the OPO, by use of a triply concurrent nonlinear crystal (already demonstrated) and a 15-mode pump. Here we present a precise and feasible implementation plan for this complex pump spectrum, using single-sideband, suppressed-carrier (SSB-SC) electrooptic modulation. Another requirement is the proper termination of the set of interacting entangled modes within the OFC. We show that OFC dispersion can be realistically managed, by use of microcavity OPO mirrors, so as to shift the frontier modes out of resonance and essentially annihilate their interaction. Solving these two "optical engineering" problems paves the way to the experimental realization of scalable cluster-state entanglement "over the rainbow."

K1.00130 Implementing quantum phase gates with Ising anyons , DAVID J. CLARKE, KIRILL SHTENGEL, University of California, Riverside — Non-Abelian anyons of Ising type are likely to occur in a number of physical systems, including quantum Hall systems, where recent experiments support their existence. In general, non-Abelian anyons may be utilized to provide a topologically error-protected medium for quantum information processing. However, the topologically protected operations that may be obtained by braiding and measuring topological charge of Ising anyons are not computationally universal. Nevertheless they can be made universal when supplemented with a single-qubit phase gate. We propose a method of implementing arbitrary single qubit phase gates for Ising anyons by utilizing interference of auxiliary anyons around computational anyons. While this gate is not topologically protected, our estimates show that its error rate can be made lower than the threshold for error correction. The error rate for systems with neutral Ising anyons (e.g. topological insulator) is inherently lower than that for systems in which the anyons carry charge (e.g. quantum Hall systems).

K1.00131 Finding edge permutations in a graph using quantum walks , ZLATKO DIMCOVIC, Department of Physics, YEVGENIY KOVCHEGOV, Department of Mathematics, Oregon State University — The problem of graph structure discovery is important in many fields of science. Quantum walks are expected to bring significant algorithmic improvements to quantum computing. More generally, random walks (Markov chains on graphs) can be very useful as a different approach to problems. We use a specific quantum walk to address unknown permutations in a graph. Consider two matching graphs, with unknown permutations of edges that connect them. For example: a vertex on the left is connected to a set of vertices to its right; on the far right is another vertex, connected to another set of nodes, to its left. These two sets of nodes are connected in the middle, but we do not know which left nodes connect to which right ones. We construct a quantum walk on such a graph structure that allows us to gain a surprising amount of information, or completely determine permutations, often in a single pass over the graph. We detect classes of interesting properties of our walk on such unknown graphs. Classical walks cannot resolve some cases at all, implying a formally "infinite" speed up. This walk is an example of use of our recent framework for building quantum walks, based on classical walks with memory. The framework contains all major known walks, while it can also build walks on structures prohibitively difficult for current techniques.

K1.00132 Decoherence in a Dynamical Quantum Phase Transition , SARAH MOSTAME, Harvard University, GERNOT SCHALLER, TU Berlin, RALF SCHUETZHOLD, University of Duisburg-Essen — Motivated by the similarity between adiabatic quantum algorithms and quantum phase transitions, we study the impact of decoherence on the sweep through a second-order quantum phase transition for the prototypical example of the Ising chain in a transverse field. For site-independent and site-dependent coupling strengths as well as different operator couplings, the results show that (in contrast to first-order transitions) the impact of decoherence caused by a weak coupling to a rather general environment increases with system size which might limit the scalability of the corresponding adiabatic quantum algorithm. We also propose a physical setup that can be used to simulate the quantum dynamics of the Ising model.

K1.00133 Quantum Phase Transitions in Cavity Coupled Dot systems , VIJAY KASISOMAYAJULA, ONOFRIO RUSSO, New Jersey Institute of Technology — We investigate a Quantum Dot System, in which the transconductance, in part, is due to spin coupling, with each dot subjected to a biasing voltage. When this system is housed in a QED cavity, the cavity dot coupling alters the spin coupling of the coupled dots significantly via the Purcell Effect. In this paper we show the extent to which one can control the various coupling parameters: the inter dot coupling, the individual dots coupling with the cavity and the coupled dots coupling with the cavity as a single entity. We show that the dots coupled to each other and to the cavity, the spin transport can be controlled selectively.[1] We derive the conditions for such control explicitly. Further, we discuss the Quantum phase transition effects due to the charge and spin transport through the dots.[2] The electron transport through the dots, electron-electron spin interaction and the electron-photon interaction are treated using the Non-equilibrium Green's Function Formalism.

[1]http://publish.aps.org/search/field/author/Trif_Mircea (Trif Mircea), http://publish.aps.org/search/field/author/Golovach_Vitaly_N (Vitaly N. Golovach), and http://publish.aps.org/search/field/author/Loss_Daniel (Daniel Loss), Phys. Rev. B 75, 085307 (2007)
[2]Michal Grochol, PRB 79, 205306 2009

K1.00134 Efficient control of the NV center spin in diamond[1] , ZHI-HUI WANG, Ames Laboratory US DOE, DOMENICO D'ALESSANDRO, Iowa State University, Dept. of Mathematics, VIATCHESLAV DOBROVITSKI, Ames Laboratory, US DOE — Fast and accurate control of the spin of a nitrogen-vacancy (NV) center in diamond is a key for realization of diamond-based quantum information processing. We investigate time-optimal rotation [1] of a qubit implemented with the spin of a NV center. We examine performance of the control, and show that one can achieve a gain of 25% in rotation time compared to the broadly used rotating wave approximation. At certain values of the bias field, noticeable population accumulates on the third energy level and the fidelity of the control is degraded. We show that this is due to the transitions induced by the higher-order harmonics in the control field, which can be suppressed by frequency filtering of the control field at the expense of increased rotation time.

[1] U. Boscain, P. Mason, J. Math. Phys. 47, 062101 (2006).

[1]Work at Ames Laboratory was supported by the Department of Energy - Basic Energy Sciences under Contract No. DE-AC02-07CH11358

K1.00135 Observation of σ_x coupling signal in a gap-tunable flux qubit , XIAOBO ZHU, NTT Basic Research Laboratories, ALEXANDER KEMP, SHIRO SAITO, HAYATO NAKANO, KOUICHI SEMBA — We experimentally demonstrate the *in situ* tunability of the gap of a superconducting flux qubit, which was achieved by replacing the smallest Josephson junction of the qubit with a dc-SQUID. We observe different gaps as a function of the external magnetic pre-biasing field and the local magnetic field through the dc-SQUID controlled by high-bandwidth on chip control lines. The persistent current and gap behavior agree well with the numerical simulation results. We set the sensitivity of the gap on the control lines during the sample design stage. With a tuning range of several gigahertz on a qubit dynamics timescale, we observe coherent system dynamics at the degeneracy point [1]. We measured the microwave amplitude dependence of Rabi frequency at the same resonant frequency but at different flux bias of the gap-tunable flux qubit. It showed a systematical deviation between these two set of data, which indicated we observed σ_x coupling signal between the flux qubit and the microwave-line. Different from conventional σ_z coupling, this σ_x coupling has a remarkable merit toward realization of idea QND measurement.

[1] Xiaobo Zhu, Alexander Kemp, Shiro Saito, and Kouichi Semba, APPLIED PHYSICS LETTERS 97, 102503 (2010).

K1.00136 Characterization of flux-driven Josephson parametric amplifiers[1] , A. BAUST, E.P. MENZEL, T. NIEMCZYK, E. HOFFMANN, M. HAEBERLEIN, F. DEPPE, A. MARX, R. GROSS, Walther-Meissner-Institut and TU Muenchen, Garching, Germany, E. SOLANO, Universidad del Pais Vasco and IKERBASQUE Foundation, Bilbao, Spain, K. INOMATA, RIKEN, Wako, Japan, T. YAMAMOTO, Y. NAKAMURA, NEC, Tsukuba and RIKEN, Wako, Japan — Phase sensitive linear amplifiers receive increasing interest for applications in the field of circuit QED as they allow for the amplification of one signal quadrature without, in principle, adding noise. The flux-driven Josephson parametric amplifier characterized in this work is formed by a SQUID- terminated transmission line resonator with resonant frequency that can be varied by applying an ac magnetic flux signal through the SQUID. We have characterized two Josephson parametric amplifiers with different design parameters with respect to the center frequency and quality factor of the resonator, phase-dependent and phase-independent gains, as well as compression points and bandwidths.

[1]This work is supported by SFB 631, NIM, Basque Government IT4720-10, Spanish MICINN FIS2009-12773-C02-01, and EU project SOLID.

K1.00137 Towards ultrastrong coupling of superconducting transmission line resonators[1] , F. DEPPE, T. WEISSL, E. HOFFMANN, M. HAEBERLEIN, A. BAUST, Walther-Meissner-Institut and TU Muenchen, Garching, Germany, E. MENZEL, M. SCHWARZ, T. NIEMCZYK, A. MARX, Walther-Meissner-Institut, Garching, Germany, D. ZUECO, CSIC-Universidad de Zaragoza, Zaragoza, Spain, J. J. GARCIA RIPOLL, Instituto de Fisica Fundamental, CSIC, Madrid, Spain, R. GROSS, Walther-Meissner-Institut and TU Muenchen, Garching, Germany — Coupled superconducting transmission line resonators have potential applications in quantum information processing and fundamental quantum mechanics. Experimentally, high coupling strengths are desirable for a clear demonstration of quantum effects. We achieve coupling strengths of 10% of the resonator frequency (ultrastrong coupling) by distributed coupling. We find that, differently from the case of point-like coupling, the normal modes are no longer arranged symmetrically with respect to the single resonator frequency. Nevertheless, a detailed theoretical analysis shows that the system can still be described by a beam splitter Hamiltonian for two effective resonators. We expect that this result will allow for straightforward experimental access to exciting effects such as thermal entanglement in our samples.

[1]Support by: DFG via SFB 631; German Excellence Initiative via NIM; FIS2008-01240 and FIS2009-13364-C02-0 (MICINN).

K1.00138 Observation of 0.2 ms Lifetime in a Cooper-pair Box , Z. KIM, B. SURI, V. ZARETSKEY, Dept. of Physics, Univ. of Maryland, S. NOVIKOV, K. OSBORN, A. MIZEL, Lab. for Physical Sciences, F. WELLSTOOD, JQI, CNAM, Dept. of Physics, University of Maryland, B. PALMER, Lab. for Physical Sciences — We have coupled a quasi-lumped element superconducting microwave resonator with a resonant frequency of 5.44 GHz to an Al/AlO_X/Al Cooper-pair box (CPB) charge qubit. The resonator is in turn weakly coupled to a transmission line and shows no higher resonant modes up to 20 GHz. By monitoring perturbations of the resonant frequency, we have measured the spectrum and lifetime (T_1) of the CPB at the charge degeneracy point while the CPB was detuned from the resonator by up to 3.5 GHz. The maximum T_1 of the CPB was 200 μs for $f = 4$ to 4.5 GHz, while T_1 decreased to 4 μs around 8 GHz. Our measured T_1's imply that the loss tangent in the AlO_X junction barrier must be less than about 4×10^{-8} at 4.5 GHz, about 4 orders of magnitude less than reported in larger area Al/AlO_X/Al tunnel junctions.

K1.00139 ABSTRACT WITHDRAWN —

K1.00140 "Quantum-Computing"(Q-C) = Simple-Arithmetic Since Digits = Quanta/Bosons Via Algebraic-INVERSION 1881(<1901-05-25) of Digits On-Average Logarithmic-Law = ONLY BEQS!!! , E. I. PI, EDWARD CARL-LUDWIG SIEGEL, FUZZYICS=CATEGORYICS(SON OF TRIZ) — Digits'(On Average) Newcomb(1881)-Weyl(1914)-Benford(1938) "NeWBe" Logarithmic-Law <P> = log{base=10}(1 + 1/d) = log{base=10}([d + 1]/d) Siegel [Abs.973-60-124, AMS Nat.Mtg.(2002)] INVERSION to ONLY Bose-Einstein quantum-statistics(BEQS) d = 1/[10^(<P>)-1] ~ 1/[exp(<P>)-1]~ 1/[exp(<w>)-1] ~ {1/[1+(<w>)+...]-1] ~ "1"/<w>^1.000...Archimedes' Zipf-law HYPERBOLICITY ("noise" ~ "generalized-susceptibility") power-spectrum INEVITABILITY with gapFUL BEC to digit d = 0, <P(0)> = oo, GAP = [<P(0)>=oo]-[<P(1)>=0.32]=oo has deep meaning for (so called) Q-C. Identification of digits(BCE) as quanta(1901-05 ACE) because quanta are/always were digits: energy-levels: ground-state d=0, first excited-state d=1,..., with no intermediate/fractional-levels, separated by quantum: Q = (d=1)-(d=0) = 1 means (on average any/all simple arithmetic computations with digits are ab initio by definition Q-C. Example: a blank-check is a BEC of digits d=0; writing some non-zero digits d>0, then signing check, is quantum-excitation from d=0 to d>0. Thus (so called) Q-C has existed since man learned to count/manipulate hand's digits. Simple arithmetic(except for: division; factoring with remainders) is/has been from time immemorial (on average) "Q-C"!!!

K1.00141 DichotomY IdentitY: Euler-Bernoulli Numbers, Sets-Multisets, FD-BE Quantum-Statistics, 1/f\^{0}-1/f\^{1} Power-Spectra, Ellipse-Hyperbola Conic-Sections, Local-Global Extent: "Category-Semantics" , G.-C. ROTA, EDWARD CARL-LUDWIG SIEGEL, FUZZYICS=CATEGORYICS(SON OF TRIZ) — Seminal Apostol[Math.Mag.81,3,178(08);Am.Math.Month.115,9,795(08)]-Rota[Intro.Prob. Thy.(95)-p.50-55] DichotomY equivalence-class: set-theory: sets V multisets; closed V open; to Abromowitz-Stegun[Hdbk.Math.Fns.(64)]-ch.23,p.803!]: numbers/polynomials generating-functions: Euler V Bernoulli; to Siegel[Schrodinger Cent.Symp.(87); Symp.Fractals, MRS Fall Mtg.,(1989)-5-papers!] power-spectrum: 1/f\^{0}-White V 1/f\^{1}-Zipf/Pink (Archimedes) HYPERBOLICITY INEVITABILITY; to analytic-geometry Conic-Sections: Ellipse V (via Parabola) V Hyperbola; to Extent/Scale/Radius: Locality V Globality, Root-Causes/Ultimate-Origins: Dimensionality: odd-Z V (via fractal) V even-Z, to Symmetries/(Noether's-theorem connected)/Conservation-Laws Dichotomy: restored/conservation/convergence=0- V broken/non-conservation/divergence=/=0: with asymptotic-limit antipodes morphisms/ crossovers: Eureka!!!; "FUZZYICS"="CATEGORYICS"!!! Connection to Kummer(1850) Bernoulli-numbers proof of FLT is via Siegel(CCNY;1964) < (1994)[AMS Joint Mtg. (2002)-Abs.973-60-124] short succinct physics proof: FLT = Least-Action Principle!!!

K1.00142 NON-Shor Factorization Via BEQS BEC: Watkins Number-Theory "Pure"-Mathematics U With Statistical-Physics; Benford Log-Law Inversion to ONLY BEQS digit d=0 BEC!!! , M. LYONS, EDWARD CARL-LUDWIG SIEGEL, FUZZYICS=CATEGORYICS(SON OF TRIZ) — Weiss-Page-Holthaus[Physica A,341,586(04); http://arxiv.org/abs/cond-mat/0403295] number-FACTORIZATION VIA BEQS BEC VS.(?) Shor-algorithm, strongly-supporting Watkins' [www.secamlocal.ex.ac.uk/people/staff/mrwatkin/] Intersection of number-theory "pure"-maths WITH (Statistical)-Physics, as Siegel[AMS Joint.Mtg.(02)-Abs.973-60-124] Benford logarithmic-law algebraic-INVERSION to ONLY BEQS with d=0 digit <P(d=0)>=oo gapFUL BEC!!! Siegel Riemann-hypothesis proof via Rayleigh[Phil.Trans.CLXI(1870)]-Polya[Math.Ann.(21)]-[Random-Walks & Electric-Nets., MAA(81)]-"Anderson"[PRL(58)]-localization-Siegel[Symp.Fractals,MRS Fall Mtg.(89)-5-papers!!!] FUZZYICS=CATEGORYICS: [LOCALITY]–MORPHISM/CROSSOVER/ AUTMATHCAT/DIM-CAT/ ANTONYM–>(GLOBALITY) FUNCTOR/SYNONYM/ concomitance to "noise"<=/Fluct.-Dissip. theorem/ FUNCTOR/SYNONYM/ equivalence/proportionality to => "generalized-susceptibility" power-spectrum [FLAT/FUNCTIONLESS/WHITE]–MORPHISM/ CROSSOVER/AUTMATHCAT/DIM-CAT/ANTONYM–> HYPERBOLICITY/ZIPF-law INEVITABILITY) intersection with ONLY BEQS BEC).

K1.00143 Number-Theory in Nuclear-Physics in Number-Theory: Non-Primality Factorization As Fission VS. Primality As Fusion; Composites' Islands of INstability: Feshbach-Resonances? , A. SMITH, EDWARD CARL-LUDWIG SIEGEL, FUZZYICS=CATEGORYICS(SON OF TRIZ) — Numbers: primality/indivisibility/non-factorization versus compositeness/divisibility/ factorization, often in tandem but not always, provocatively close analogy to nuclear-physics: (2 + 1)=(fusion)=3; (3+1)=(fission)=4[=2 x 2]; (4+1)=(fusion)=5; (5 +1)=(fission)=6[=2 x 3]; (6 + 1)=(fusion)=7; (7+1)=(fission)=8[= 2 x 4 = 2 x 2 x 2]; (8 + 1) =(non: fission nor fusion)= 9[=3 x 3]; then ONLY composites' Islands of fusion-INstability: 8, 9, 10; then 14, 15, 16, ... Could inter-digit Feshbach-resonances exist??? Possible applications to: quantum-information/ computing non-Shore factorization, millennium-problem Riemann-hypotheses proof as Goodkin BEC intersection with graph-theory "short-cut" method: Rayleigh(1870)-Polya(1922)-"Anderson"(1958)-localization, Goldbach-conjecture, financial auditing/accounting as quantum-statistical-physics; ... abound!!! Watkins [www.secamlocal.ex.ac.uk/people/staff/mrwatkin/] "Number-Theory in Physics" many interconnections: "pure"-maths number-theory to physics including Siegel [AMS Joint Mtg.(2002)-Abs.# 973-60-124] inversion of statistics on-average digits' Newcomb(1881)-Weyl(14-16)-Benford(38)-law to reveal both the quantum and BEQS (digits = bosons = digits:"spinEless-boZos"). 1881 < 1885 < 1901 < 1905 < 1925 < 1927, altering quantum-theory history!!!

K1.00144 Physics Proofs of Four Millennium-Problems(MP) via CATEGORY-SEMANTICS(C-S)/F=C Aristotle SQUARE-of-OPPOSITION(SoO) DEduction-LOGIC DichotomY , LONDON CLAY, FUZZYICS=CATEGORYICS(SON OF TRIZ)/Brookline, EDWARD CARL-LUDWIG SIEGEL, FUZZYICS=CATEGORYICS(SON OF TRIZ)/La Jolla/Las Vegas — Siegel-Baez Cognitive-Category-Semantics"(C-C-S) tabular list-format matrix truth-table analytics SoO jargonial-obfuscation elimination query WHAT? yields four "pure"-maths MP "Feet of Clay!!!" proofs: (1) Siegel [AMS Natl.Mtg.(02)-Abs.973-03-126: (CCNY;64)!!!<<<(94;Wiles)] Fermat's: Last-Thm. = Least-Action Ppl.; (2) P=/=NP TRIVIAL simple Euclid geometry/dimensions: NO computer anything"Feet of Clay!!!"; (3) Birch-Swinnerton-Dyer conjecture; (4) Riemann-hypotheses via COMBO.: Siegel[AMS Natl.Mtg.(02)-Abs.973-60-124] digits log-law inversion to ONLY BEQS with ONLY zero-digit BEC, AND Rayleigh[1870;graph-thy."short-CUT method"[Doyle-Snell, Random-Walks & Electric-Nets,MAA(81)]-"Anderson"[(58)] critical-strip C-localization!!! SoO DichotomY ("V") IdentitY: #s:(Euler v Bernoulli) = (Sets v Multisets) = Quantum-Statistics(FD v BE) = Power-Spectra(1/f^(0) v 1/f^(1)) = Conic-Sections(Ellipse v Hyperbola) = Extent(Locality v Globality);Siegel[(89)] (so MIScalled) "complexity" as UTTER-SIMPLICITY(!!!) v COMPLICATEDNESS MEASURE(S) definition.

K1.00146 Algorithmic-Reducibility = Renormalization-Group Fixed-Points; "Noise"-Induced Phase-Transitions (NITs) to Accelerate Algorithmics ("NIT-Picking") Replacing CRUTCHES!!!: Gauss Modular/Clock-Arithmetic Congruences = Signal X Noise PRODUCTS. . , J. SIEGEL, EDWARD CARL-LUDWIG SIEGEL, FUZZYICS=CATEGORYICS(SON OF TRIZ) — Cook-Levin computational-"complexity"(C-C) algorithmic-equivalence reduction-theorem reducibility equivalence to renormalization-(semi)-group phase-transitions critical-phenomena statistical-physics universality-classes fixed-points, is exploited with Gauss modular/clock-arithmetic/model congruences = signal X noise PRODUCT reinterpretation. Siegel-Baez FUZZYICS=CATEGORYICS(SON of "TRIZ"): Category-Semantics(C-S) tabular list-format truth-table matrix analytics predicts and implements "noise"-induced phase-transitions (NITs) to accelerate versus to decelerate Harel [Algorithmics(1987)]-Sipser[Intro. Theory Computation(1997) algorithmic C-C: "NIT-picking" to optimize optimization-problems optimally(OOPO). Versus iso-"noise" power-spectrum quantitative-only amplitude/magnitude-only variation stochastic-resonance, this "NIT-picking" is "noise" power-spectrum QUALitative-type variation via quantitative critical-exponents variation. Computer-"science" algorithmic C-C models: Turing-machine, finite-state-models/automata, are identified as early-days once-workable but NOW ONLY LIMITING CRUTCHES IMPEDING latter-days new-insights!!!

K1.00147 MAGNETISM (EXPERIMENT, THEORY, APPLICATIONS) –

K1.00148 Impurity effects in excitonic insulators[1] , JIAN LI, Texas Center for Superconductivity, University of Houston, Houston, Texas 77204, NINGNING HAO, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, PR China, BEIJING NATIONAL LABORATORY FOR CONDENSED MATTER PHYSICS TEAM — Both nonmagnetic and magnetic impurity effects in spin singlet and triplet excitonic insulators were investigated. The bound state energies caused by single impurity were given. The different compositions of the bound states can be used to detect the symmetry of the excitonic insulators. In finite concentration problems, nonmagnetic impurities showed same pair-breaking effect in singlet and triplet excitonic insulators while magnetic impurities showed weaker pair-breaking effect in triplet excitonic insulators than in singlet ones. The pair-breaking effects suppressed the ferromagnetic range via doping and gave a natural explaination for experimental results.

[1]This work was financially supported by NSFC, CAS and 973-project of MOST of China.

K1.00149 Origins of Asymmetric Magnetization Reversal in Exchange Biased Multilayers[1] , YANG LIU, SHUOGUO WANG, YANG LI, NING CHEN, SHUAI LIU, MINGHUA LI, GUANGHUA YU, DEPARTMENT OF MATERIALS PHYSICS AND CHEMISTRY, UNIVERSITY OF SCIENCE AND TECHNOLOGY BEIJING TEAM, STATE KEY LABORATORY OF MAGNETISM, BEIJING NATIONAL LABORATORY FOR CONDENSED MATTER PHYSICS, INSTITU TEAM, UNIVERSITY OF PUERTO RICO AT MAYAGUEZ TEAM — Novel asymmetric magnetization reversal behaviors (ARBs) as well as positive exchange bias (EB) are observed by using the alternating gradient force magnetometer (AGM) in both Co/FeMn bilayer with an oblique out-of-plane exchange anisotropy and the Co/FeMn bilayer in which Co layer has a quite heavy thickness. There are two different ARBs, arised from the ferromagnetic and the antiferromagnetic layer respectively under the perpendicular magnetization. Our results show that two intrinsic origins of the ARBs (i.e. the competing anisotropy and the inhomogeneity of the magnetic structure) coexist. Both of them are indispensable for the development of the ARBs in our Co/FeMn multilayers.

[1]This work was supported by the National Science Foundation under Grant no. DMR-0821284, NASA under Grant Nos. NNX10AM80H and NNX07AO30A.

K1.00150 Magnetic properties of $FeCl_3$ investigated by ^{57}Fe NMR , BYEONGKI KANG, SOONCHIL LEE, KAIST — $FeCl_3$ crystallizes in a hexagonal layered structure and has a spiral antiferromagnetic phase below $T_N = 8.8K$, where the spins are spirally ordered with $2\pi/15$ period along [140] direction. It is reported that the magnetic phase changes to an order with two sublattices above $1.5T$ and there is a spin-flop transition above $4.0T$. We observed ^{57}Fe ferromagnetic nuclear magnetic resonance(NMR) signal for $FeCl_3$ for the first time at low temperature. The sublattice magnetization $M(T)$ obtained from the temperature dependence of the NMR frequency is well fit by the Bloch's T^2 law for antiferromagnets. The spectral change with external field provided a microscopic evidence for the spin-flop transition. The transition was not abrupt but progressive with increasing field.

K1.00151 Investigations of Exchange and Magnetic Anisotropic Interactions of Magnetic Ions in Antiferromagnetic Materials , ALEXANDER BAZHAN, P.L.Kapitza Institute for Physical Problems, RAS, ul. Kosygina 2, 119334 Moscow, Russia — Investigations of exchange and magnetic anisotropic interactions of magnetic ions, which determine antiferromagnetic orderings in materials, used in HTS, are of interest due to investigations of transformations of antiferromagnetic orderings, when additional two dimensional systems of correlated electrons, holes carriers are introduced. Discussions of states, which can appear before HTS, are of interest in such investigations. In experimental investigations of, determined by exchange and magnetic anisotropic interactions, magnetic phase transitions, investigations of separate components of samples magnetic moments, which determine orientations of samples magnetic moments, are useful. Investigations of, determined by orientations of ordered magnetic moments, magnetic phase transitions in antiferromagnetic materials and states with weak ferromagnetism at selected orientations of ordered magnetic moments in antiferromagnetic materials using vector vibrating sample magnetometer with horizontal magnetic field, up to 90kOe, and liquid helium temperatures, which can investigate separately magnetic field dependencies of three perpendicular components of samples magnetic moments, demonstrate possibilities of such magnetometers in investigations of exchange and magnetic anisotropic interactions of magnetic ions.

K1.00152 Kinetic properties of small one-dimensional Ising magnetic , VLADIMIR UDODOV, DMITRIY SPIRIN, Katanov Khakas State University, KATANOV KHAKAS STATE UNIVERSITY TEAM — Within the framework of a generalized Ising model, a one-dimensional magnetic of a finite length with free ends is considered. The correlation length critical exponent ν and kinetic critical exponent z of the magnet is calculated taking into account the next nearest neighbor interactions and the external field. Of special interest are non-equilibrium processes taking place within the critical temperature interval, which are characterized critical exponent y and dynamic critical index z. Due to significant difficulties encountered in the experimental investigations (e.g., measurement of z), a natural solution to this complex problem would be modeling of those non-eqilibrium processes. This work addresses non-equilibrium processes in one-dimensional magnetics. Using the Monte Carlo method, an equilibrium critical exponent of the correlation length ν and the dynamic critical index z are calculated for a finite-size magnetic.

K1.00153 On the critical behaviour of two-dimensional liquid crystals , ANA I. FARIÑAS-SÁNCHEZ, Departamento de Fisica, Universidad Simon Bolivar, Venezuela, ROBERT BOTET, Laboratoire de Physique des Solides, Universite Paris-Sud, France, BERTRAND BERCHE, Groupe de Physique Statistique, Institut Jean Lamour, France, RICARDO PAREDES, Laboratorio de Simulacion, Instituto de Matematicas. Unidad Cuernavaca. UNAM, Mexico — The Lebwohl-Lasher (LL) model is the traditional model used to describe the nematic-isotropic transition of real liquid crystals. In this paper, we develop a numerical study of the temperature behaviour and of finite-size scaling of the two-dimensional (2D) LL-model. We discuss two possible scenarios. In the first one, the 2D LL-model presents a phase transition similar to the topological transition appearing in the 2D XY-model. In the second one, the 2D LL-model does not exhibit any critical transition, but its low temperature behaviour is rather characterized by a crossover from a disordered phase to an ordered phase at zero temperature. We realize and discuss various comparisons with the 2D XY-model and the 2D Heisenberg model. Having added finite-size scaling behaviour of the order parameter and conformal mapping of order parameter profile to previous studies, we analyze the critical scaling of the probability distribution function; hyperscaling relations and stiffness order parameter and conclude that the second scenario (no critical transition) is the most plausible.

K1.00154 Re-entrant spin glass state in $(Ce_{1-x}Tb_x)Fe_2$ compounds , A. HALDAR, K.G. SURESH, Department of Physics, Indian Institute of Technology Bombay, Mumbai- 400076, India, A.K. NIGAM, Tata Institute of Fundamental Research, Homi Bhabha Road, Mumbai- 400005, India — Doped $CeFe_2$ compounds are well known for their unique features like first order magneto-structural transition, metastability, supercooling/superheating effects, phase co-existence, glassiness etc. $4f$ band magnetism and the antiferromagnetic ground state as a consequence of this are the interesting features of this system Though doping at the Fe site has been studied extensively, the effect of rare earth (R) substitution at the Ce site is not investigated in detail. We have recently shown that Er substitution causes a spin glass state below its ordering temperature. In this paper, we show that a similar re-entrant spin glass (RSG) phase can be achieved with Tb substitution as well. Characteristic experimental evidences, like large thermo-magnetic irreversibility and strong frequency dependence of ac-susceptibility have been observed. Spin freezing temperature has been found to obey critical slowing down mechanism with relaxation time of the order of 10^{-6}s. The relaxation behavior is also investigated using time variation of dc magnetization. Theoretical fitting of the relaxation data suggests that that the RSG state is made of clusters and not of atomic moments. The RSG state is attributed to the random substitution of Tb in the nearly nonmagnetic Ce sublattice and the modulation of the R-Fe exchange.

K1.00155 The first-Order phase transition in β-MnO_2 studied by ^{55}Mn Nuclear Magnetic Resonance , CHANGSOO KIM, EUNA JO, SOONCHIL LEE, Korea Advanced Institute of Science and Technology — β-MnO_2 has a conductivity due to negative charge carriers generated from slight off-stoichiometry of oxygens. We obtained 55Mn antiferromagnetic nuclear magnetic resonance (NMR) signal for β-MnO_2 at low temperature for the first time. The resonance frequency of the main peak centered at 254 MHz is nearly unchanged from 4.2 K to 130 K though it is known that the magnetic phase changes near 94 K from the antiferromagnetic state to the paramagnetic state. This suggests that the magnetic phase transition is a first order transition and the mixed phases coexist both below and above the phase transition temperature. Side peaks were found at 161 MHz, 181 MHz and 297 MHz. Through annealing β-MnO_2, which generates oxygen defects, we investigated whether these peaks originate from manganese ions with their valence other than 4+. However, the NMR spectra of the annealed β- MnO_2 showed no difference in side peaks.

K1.00156 ^{55}Mn NMR for Antiferromagnetic α-Mn_2O_3 , EUNA JO, KAIST, CHANGSOO KIM, SOONCHIL LEE, KAIST — The zero-field ^{55}Mn NMR spectrum for antiferromagnetic α-Mn_2O_3 was measured at low temperatures. Manganese sesquioxide (Mn_2O_3) is used in combustion catalysis, a method of reducing the emissions of organic compounds and nitrous oxide from waste gas, as an environmentally - friendly and inexpensive catalyzer instead of Pt and Pd. The magnetic moment estimated from the resonance frequency was $2.6\mu_B$ per Mn^{3+} ion. The temperature dependence of the sublattice magnetization fits not Bloch's T^2 law well but the exponential form applicable because there is an initial energy gap in the dispersion relation of the spin wave. From the fitting, an energy gap of 1.82 meV and an anisotropy energy of 0.22 meV were obtained. The spin-spin relaxation rate was measured as a function of the frequency and the Suhl-Nakamura interaction is suppressed by this energy gap.

K1.00157 Hysteresis in weak ferromagnets[1] , YA. B. BAZALIY[2], University of South Carolina, L.T. TSYMBAL, O. Galkin Donetsk Physics and Technology Institute, G.N. KAKAZEI[3], Universidade do Porto, S.V. VASILIEV, O. Galkin Donetsk Physics and Technology Institute — Magnetic hysteresis is studied in the orthoferrites ErFeO3 and TmFeO3 using the single crystal samples of millimeter dimensions. It is shown that in both materials one observes a temperature transition manifesting itself through the temperature hysteresis of the magnetic moment and a peculiar temperature evolution of the field hysteresis loop shapes near this transition. Experiments rule out the hypothesis that the ordering of the orthoferrite's rare earth magnetic moments plays an important role in these phenomena. The hysteresis curves can be explained by a few-domain magnetic state of the samples that results from the weak ferromagnetism of the orthoferrites. The phenomenon is generic for weak ferromagnets with temperature dependent magnetization. A large characteristic magnetic length makes the behavior of the relatively big samples analogous to that observed in the nano-size samples of strong ferromagnets.

[1]Supported by NSF DMR-0847159, Ukrainian DFFD F28/456-2009, Portuguese FCT "Ciencia 2007."

[2]also at the Institute of Magnetism, Kyiv, Ukraine

[3]also at the Institute of Magnetism, Kyiv, Ukraine

K1.00158 Measurements of charge localization effects in uranium and plutonium intermetallic compounds from $L_{\rm III}$ X-ray absorption spectroscopy , YU JIANG, C.H. BOOTH, Lawrence Berkeley National Laboratory, E.D. BAUER, J.N. MITCHELL, P.H. TOBASH, J.D. THOMPSON, J.L. SARRAO, Los Alamos National Laboratory, M.A. WALL, P.G. ALLEN, Lawrence Livermore National Laboratory, D. NORDLUND, Stanford Synchrotron Radiation Lightsource — At the heart of the complex behavior of $5f$-electrons in uranium and plutonium is the variable localization of the $5f$ orbital. Plutonium, in particular, can behave like a localized lanthanide system or a delocalized transition-metal system, depending on its coordination environment. This behavior gives rise to a variety of novel physical properties in U and Pu compounds: unexpected magnetic susceptibilities, non-Fermi-liquid behavior, superconductivity, etc. To understand the dual nature of U and Pu $5f$ orbitals, we report measurements of the actinide $L_{\rm III}$-edge X-ray absorption spectra, including high-resolution partial fluorescence yield measurements, for a wide variety of intermetallics, including α-U, $UCoGa_5$, UCd_{11}, $\alpha-$ and $\delta-$Pu, $PuCoGa_5$, and $PuCoIn_5$. A systematic shift of the $L_{\rm III}$-edge energy is observed, and is correlated to the Sommerfeld coefficient from heat capacity measurements. Based on these results, we argue that this type of experiment is a direct measure of the degree of $5f$ orbital localization for U and Pu.

K1.00159 Anisotropic magnetic behavior of single crystalline CeGe , SUDESH DHAR, PRANAB KUMAR DAS, NEERAJ KUMAR, ARUMUGAM THAMIZHAVEL, RUTA KULKARNI, Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Mumbai — We report the anisotropic magnetic properties of a Czochralski grown single crystal of CeGe, which crystallizes in the orthorhombic structure with the space group Pnma (#63). The compound orders antiferromagnetically at TN = 10.9 K, in agreement with the value reported previously on a polycrystalline sample. A metamagnetic transition at $\sim$ 6.5 T followed by saturation at higher fields is observed along [010], the easy axis of magnetization. The heat capacity data confirm the bulk nature of magnetic ordering with a peak of nearly 13 J/mol K at 10.9 K. The peak decreases in height and shifts to lower temperatures in applied magnetic field, consistent with the antiferromagnetic ordering of Ce ions. Subtraction of phonon heat capacity, as measured for LaGe, reveals a broad hump around 30 K, suggesting the existence of low lying crystal electric field levels, which is well reproduced by two doublets located at 45 and 152 K, respectively. The electrical resistivity shows normal metallic behavior indicating the absence of Kondo interaction. At TN the resistivity measured along the three principal directions shows an upturn which is tentatively attributed to the gaps opened in the antiferromagnetic state. A magnetic phase diagram has been constructed based on the magnetization data.

K1.00160 Spin-polarization and transmission properties in heterostructures with magnetic nano elements , ARMEN KOCHARIAN, Department of Physics, California State University, AVAG SAHAKYAN, RUZAN MOVSESYAN, The State Engineering University of Armenia — The problem of electron resonant and non-resonant scatterings on two magnetized barriers is studied in the one-dimension. The transfer-matrix is built up to exactly calculate the coefficient of the electron transmittance through the system of two magnetic barriers with non-collinear magnetizations. The polarization of the transmitted electron wave for resonance and non-resonance transmittances is calculated [Kocharian, et al, JMMM 322, L42, 2010]. The transmittance coefficient and spin polarization can be drastically enhanced and controlled by the angle between the barrier magnetizations. Our result for spin transmission is analogous to Malus's law for passing light polarization through crossed polarizers. This provides efficient control of spin polarization via the applied magnetic field which is an apparent manifestation of the spin- valve effect. The strong dependence of magnetoconductance on the non-colinearity angle in two magnetized barriers resembles the corresponding effects in noncollinear spintronics for a number of other magnetic multilayer heterostructured systems and layered magnetic nanostructures.

K1.00161 Nb doped TiN as a superconducting electrode for spin polarization measurements of oxides , DIPANJAN MAZUMDAR, MANJIT PATHAK, XING ZHONG, VIJAY KARTIK, ARUNAVA GUPTA, PATRICK LECLAIR, Center for Materials for Information Technology, University of Alabama, Tuscaloosa, AL 35487, MINT ALABAMA SPINTRONICS TEAM — Spin Polarized tunneling (SPT) measurements are an unambiguous way of measuring the interface spin polarization (SP) of oxide thin films and interfaces. SPT uses a superconducting electrode as a spin detector, probing within $\sim$1 meV of the Fermi level. However the commonly used superconductor, namely Al, is not suitable for oxides due to its strong chemical affinity for oxygen. Nitrides like TiN and NbN alleviates this problem. Here we propose the use of Nb doped TiN. The critical temperature (T_c) and magnetic field (H_c) for TiN are too low for practical SPT measurements. While NbN has a higher T_c and H_c, its high spin-orbit scattering rate makes it less ideal for SPT [1]. TiNbN should provide a sufficiently high H_c and T_c while maintaining a sufficiently low spin-orbit scattering rate for high-resolution SPT measurements. We present measurements of known high SP oxides ($LaSrMnO_3$) and of all-oxide spin-filter devices (LSMO/STO/NFO).

[1] Hyunsoo Yang *et al.* Appl. Phys. Lett. **88**, 182501 (2006)

K1.00162 DIFFUSIVE-Magnetoresistance(DMR) Proton(PMR)/Hydrogen-ion WATER: PRE-"Fert"/"Grunberg" GMR[and CMR]: Quo-Vadis "Honesty"???: PLAGIARISM!!!
, ALBART FART, PETER GRUNTBUG, EDWARD SIEGEL, EMET/TRUTH-in-the-"SEANCES" — Proton/Hydrogen-ion *Diffusive*-Magnetoresistance(DMR) of Siegel[APS March-Mtgs.(70s)] based upon Siegel[Int'l. Conf. Mag.-Alloys and Oxides("ICMAO"), The Technion(77); J. Mag. Mag. Mtls. 7, 312(78)] FIRST experimental-discovery of GMR and FIRST theoretical prediction of CMR[ibid. 7, 338 (78)], facilitates NEW water production in global-warming exacerbated dry arid/semi-arid regions: Only HYDROGEN is/can be "FLYING-WATER"!!! (aka "chemical-rain-in-pipelines"). EMET/TRUTH-in-the-"SEANCES", would-be "Sciences": C. Perelman-Corredoira [Against the Tide(07)] featuring Martin-Bradshaw ["Healing the SHAME That BINDS You"(80s)] systemic sociological-dysfunctionality(S-D), and Grigory Perelman's HEROIC ETHICS (refusal of both pure-maths Poincare-conjecture proof 2007 Fields-medal and 2010 Clay-Institute so-called/media-hyped/P.Red/spin-doctored millennium-prize million-dollar would-be award, militates as well in the current "SEANCE" of physics/maths politics/media-hype/P.R /spin-doctoring VS. Siegel FIRST experimental GMR a never-acknowledged full decade PRE-"Fert"(88) /"Grunberg(89)" "Phales-GroPE"/Thompson-CSF/ KFZ-JEWlich 2007 physics Wolf/Japan/Nobel-prizes!!!

K1.00163 Investigation of spin torque driven magnetization reversal in elliptical elements[1] , ANGELIQUE MONTGOMERY, CLAUDIA K.A. MEWES, TIM MEWES, The Unversity of Alabama — Spin transfer torque [1, 2] can be utilized to switch the magnetization in small ferromagnetic elements, which can be used to implement a magnetic random access memory [3]. One crucial parameter for spin torque switching is the critical current required to achieve switching. To investigate spin transfer torque we simulate the magnetization dynamics using our Matlab based micromagnetic code (M^3), which uses a fast Fourier transform method to evaluate the longrange magnetostatic field, exchange interaction is implemented using 6, 12 or 26 neighbor methods [4] and also includes adiabatic and non-adiabatic spin torque terms. We have performed simulations using different mesh sizes to examine the influence of the cell size on the micromagnetic results. We have investigated the influence of the current density and pinned layer orientation on the magnetization dynamics and in particular on the switching time.

[1] J. Slonczewski, J. Mag. Mag. Mat. **159**, 1 (1996).
[2] L. Berger, Phys. Rev. B **54**, 9353 (1996).
[3] E. Chen et al., IEEE Trans. Mag. **46**, 1873-1878 (2010).
[4] M.J. Donahue, D.G. Porter, Physica B **343**, 177 (2004).

[1]This work was supported by REU supplement #1023069 for NSF DMR #0804243.

K1.00164 Demagnetization field distribution in paramagnetic materials , NEIL BAUMANN, MICHAEL MALLERNEE, ROSS DICKINSON, GUOQING WU, Physics Department, University of West Florida, Pensacola, FL 32514 — A general method for the calculation of distribution of demagnetization field in paramagnetic materials is described, and the demagnetization field is calculated for samples with rectangular geometries. The results show high non-uniformity for the demagnetization field inside the sample depending on the sample aspect ratio and the direction of the externally applied magnetic field. Application is made to the modeling of the NMR spectra, providing good fit to the measured NMR spectra.

K1.00165 Magnetic Damping in Individual Cobalt Nanoparticles[1] , WENCHAO JIANG, Georgia Tech, FELIPE TIJIWA BIRK, DRAGOMIR DAVIDOVIC — Magnetization precession in ferromagnets is subject to damping by means of coupling between the magnetization and the environment. In a ferromagnetic metallic particle, the damping changes in a fundamental way when the electron-in-a-box level spacing becomes larger than the magnetization precession energy. Damping has crucial significance in magnetic storage technology, so understanding its size dependence is important for the miniaturization of electronics. Here, we present an electron tunneling technique to study damping in single Cobalt nanoparticles tunnel coupled to non-magnetic leads. Injecting a tunnel current into the particle raises its magnon temperature and induces magnetization dynamics. Tunnel currents as low as a few pA are able to excite or even reverse the particle's magnetization. Using the magnetic switching field as a magnon thermometer, we obtain very low values (10^{-8}) for the dimensionless damping parameter, α, indicating weak dissipative coupling to the environment.

[1]This work has been supported by the Department of Energy (DE-FG02-06ER46281).

K1.00166 Thin Film Study of YFeO3 Deposited Via Pulsed Laser Deposition for Use in Spintronic Applications , ADAM HINCKLEY, RAM GUPTA, YESAPPA KOLEKAR, KARTIK GHOSH, PAWAN KAHOL, Missouri State University — Recently, rare-earth orthoferrites have received much attention. Their propensity for multiferroic capabilities could play a key role in the fabrication of an efficient spintronic system. Such materials as BiFeO3 and CeFeO3 have already shown promise for uses in microphotonics as well as acting as spin valves, where YFeO3 has been shown to exhibit weak ferromagnetic tendencies in bulk. However, research conducted on the magnetic and electrical properties of YFeO3 thin films are sparse and in need of further investigation. Hence we have developed bulk YFeO3 for the purpose of investigating these thin film properties. Films will be grown via KrF Pulsed Laser Deposition on LaAlO3 substrates due to their similar lattice constant values and characterized via X-Ray Diffraction, Hall Effect Analysis and SQUID Magnetometer examinations. Previous SQUID results from the bulk material display an inverted hysteresis loop, indicating the existence of differing magnetic phases in bulk. Our goal is to examine the effects from thin film construction on these magnetic phases and examine whether thin films of YFeO3 exhibit a coupling between magnetic and electrical phases. This work is supported by National Science Foundation (Award Number DMR- 0907037).

K1.00167 Quntum beat generated by an acoustic wave in single-molecule magnets , GWANG-HEE KIM, Sejong University, Seoul 143-747, South Korea — The Spin oscillation is studied for the case where a standing acoustic wave is delivered to two level states in single-molecule magnets. In order to obtain such states, we first saturate the sample in strong negative magnetic field and increase the field until it reaches zero. Maintaining zero field, we begin to apply the standing acousitc wave to the sample and see the change of the magnetization between the ground state and the excited state. Taking $\langle S_z \rangle$ averaged over the wavelength of the sound where $\langle S_z \rangle$ is the expectation value of the projection of the spin onto the easy anisotropy axis, we present the analytic form of $\langle S_z \rangle$ at $\hbar\omega = \Delta$ where ω is the frequency of sound and Δ the energy gap between two states. In addition, we find the optimal condition for quatnum beat strucuture and discuss the possibility of the future experiment.

K1.00168 Unusual Magnetic Behaviors with Large Anisotropy and 1/3 Magnetization Plateau in the CoV_2O_6 , S.-Y. PARK, T.-H. JANG, Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Korea, B.-G. PARK, Pohang Accelerator Laboratory, Pohang University of Science and Technology, Pohang 790-784, Korea, K.-P. HONG, Korea Atomic Energy Research Institute, Daejon 350-600, Korea, Y.-H. JEONG, Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Korea — The pseudo-one dimensional brannerite type CoV_2O_6 has been studied by magnetization measurement, heat capacity and neutron powder diffraction between 300 and 1.5K. CoV_2O_6 crystallizes in two modifications; a low-temperature γ- form of triclinic structure and high-temperature α-form of monoclinic structure. α-CoV_2O_6 of monoclinic structure shows a large magnetic anisotropy and an antiferromagnetic transition at T_N=14K. Furthermore, the magnetization measurement up to 9T shows 1/3 magnetization plateau below 10K and saturated magnetic moment $4.5\mu_B/Co^{2+}$, which is much larger than the spin-only value of $3.0\mu_B/Co^{2+}$ for the full moments of Co^{2+} ions. On the contrary, γ-CoV_2O_6 of triclinic structure shows saturated magnetic moment $3.0\mu_B/Co^{2+}$ with antiferromagnetic trantion at T_N=6.2K. We discuss the different magnetic behaviors of the α- and γ- phase of CoV_2O_6.

K1.00169 Magnetic Carbon Nanotubes Tethered with Maghemite Nanoparticles , IL TAE KIM, GRADY NUNNERY, KARL JACOB, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA, 30332, JUSTIN SCHWARTZ, XIAOTAO LIU, National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL, 32310, RINA TANNENBAUM, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA, 30332 — We describe a novel, facile method for the synthesis of magnetic carbon nanotubes (m-CNTs) decorated with monodisperse γ-Fe_2O_3 magnetic (maghemite) nanoparticles and their aligned feature in a magnetic field. The tethering of the nanoparticles was achieved by the initial activation of the surface of the CNTs with carboxylic acid groups, followed by the attachment of the γ-Fe_2O_3 nanoparticles via a modified sol-gel process. Sodium dodecylbenzene sulfonate (NaDDBS) was introduced into the suspension to prevent the formation of an iron oxide 3D network. Various characterization methods were used to confirm the formation of well-defined maghemite nanoparticles. The tethered nanoparticles imparted magnetic characteristics to the CNTs, which became superparamagnetic. The m-CNTs were oriented parallel to the direction of a magnetic field. This has the potential of enhancing various properties, e.g. mechanical and electrical properties, in composite materials.

K1.00170 The spin -1 anisotropic Heisenberg antiferromagnet on a square lattice at low temperatures[1] , ANTONIO PIRES, UFMG — In the last years the quantum two dimensional spin 1/2 Heisenberg antiferromangnet has been extensively studied. However, new physical features, such as quantum phase transitions, due to additional terms, as for instance single ion anisotropy, are possible when S = 1. Here we study the low temperature behavior of the quantum spin-1 Heisenberg antiferromagnet with exchange and single site anisotropies on the square lattice. The properties of the model change drastically as the single ions anisotropy D varies from very small to very large values. A quantum phase transition takes place at a critical value of D. Two techniques are used to study the model. In the low D region we use a self consistent harmonic approximation. For D above the critical value a bond operator formalism is used. We present the phase diagram for the model.

[1]This work was partially supported by CNPQ and FAPEMIG.

K1.00171 Critical theory of the topological quantum phase transition in the AKLT–SZH chain

, HONG-CHEN JIANG, Microsoft Research, Station Q, University of California, Santa Barbara, CA 93106, STEPHAN RACHEL, Yale University, Department of Physics, New Haven, CT 06520, ZHENG-YU WENG, Institute for Advanced Study, Tsinghua University, Beijing, 100084, P. R. China, SHOU-CHENG ZHANG, Department of Physics, McCullough Building, Stanford University, Stanford, CA 94305, ZHENGHAN WANG, Microsoft Research, Station Q, University of California, Santa Barbara, CA 93106 — We systematically study the phase diagram of $S = 2$ spin chain by means of density-matrix renormalization group and exact diagonalization. We find two gapped phases which are topologically distinct: the AKLT phase is characterized by $S = 1$ edge spins while the SZH phase by $S = 3/2$ edge spins. Except from a multicritical point where a direct topological quantum phase transition occurs, we identify a dimer phase between both gapped phases. The whole phase boundary between dimer and SZH phases, including the multicritical point, is a critical line with central charge $c = 5/2$. Finally, we propose and confirm that this line corresponds to $\mathrm{SO}(5)_1$ Wess–Zumino–Witten conformal field theory.

K1.00172 Deuterated vs Normal Hydrogen Magnetism of M (Mn,Co) Dichloride Monohydrate, and Crystal Structure

, S. PAGOLA, K.T. TROWELL, K.C. HAVAS, Z.D. REED, D.G. CHAN, G.C. DEFOTIS, College of William and Mary — Presented here are susceptibility data for fully deuterated forms of the title materials, and comparison with normal hydrogen forms. Also shown is the first structure determination for any monohydrate compound, for the Mn system with the simplest magnetic behavior to analyze. Interesting similarities and contrasts appear relative to normal hydrogen analogs. For the Co system the location of an enhanced susceptibility maximum, and its magnitude, match very well those of the normal hydrogen form. The deuterated Mn material shows a similar very broad susceptibility maximum as normal material, implying low-dimensional (probably d=1) magnetism, and with indication of a transition somewhat below T(max), presumably due to weak interchain interactions. But, the location of the maximum is at significantly lower temperature than in normal material, and the size is larger; both findings suggest a weaker intrachain interaction. Yet, the apparent transition, near 2.17 K, differs hardly at all in location from that in the normal material. The crystal structure determination for the normal Mn system provides the first evidence of a structural reason for the low dimensional magnetism observed, in that somewhat isolated magnetic chains are apparent.

K1.00173 Effects of Magnetic Correlation of Localized Spins in Graphene

, YURIY SEMENOV, JOHN ZAVADA, KOSTYANTYN BORYSENKO, KI WOOK KIM, Department of Electrical and Computer Engineering, North Carolina State University, Raleigh, NC 27695-7911 — Prior analysis of the indirect exchange interaction between localized spins (LS) in graphene reveals an alternate sign depending on whether two LS belong to the same graphene sublattice or not. Prompted by these findings, we explored the role of the carrier-impurity exchange interaction in formation of magnetic phase states in graphene with vacancies and modification in graphene-based composite structures. Analysis of free energy F shows the anti-ferromagnetic (AF) ordering with partial compensation of the magnetizations M_A and M_B in two graphene sublattices. The difference M_A-M_B is caused by difference of the number of LS randomly distributed over the sublattices A and B. This effect of weak ferromagnetism becomes significant in multi-domain structure, provided a mean domain size is around 2 μm; it can explain the available experimental results. The proximity to ferromagnetic dielectric layers in a sandwich configuration results in an indirect magnetic interaction that can be expressed in terms of exchange bias field. The latter strongly depends on vacancy concentration x and even can reverse the direction of exchange bias field with x increasing. At the temperature of AF ordering the minimum of F corresponds to a tilt of M_A and M_B and even a collapse of the AF vector.

K1.00174 Magnetic impurities in spin-spiral multiferroic materials

, TRINANJAN DATTA, Augusta State University — We investigate the effect of magnetic impurities in the magnetic-spiral-induced multiferroic phases using an effective multiferroic Hamiltonian. We model the impurities as a two- level system and consider the regimes when the impurity spins relax both slowly and fast. Using realistic material parameters we study the effect of impurities on ferroelectricity for varying impurity strength. We find that when the impurity strength is weak the electric polarization is not affected. However as the impurity strength is increased the amplitude of the host spin components is reduced and the ferroelectricity suppressed. We also discuss the role of impurities on a realistic multiferroic spin Hamiltonian for the rare-earth- metal Mn perovskites.

K1.00175 Magnetism of Co/Mn/Ni Dichloride Dihydrate[1]

, G.C. DEFOTIS, A.S. HAMPTON, J.M. POTHEN, T.J. WALLIN, E.A. WELSHHANS, K.C. HAVAS, K.T. TROWELL, College of William and Mary — Many unusual kinds of behavior have appeared in well selected binary magnetic mixtures. It is also of interest to explore suitable ternary mixtures. Surveyed here are magnetic susceptibility and magnetization measurements for a range of compositions of the title system. This is only the second ternary insulating mixed magnet to be examined with systematic composition variation. Intrachain exchange is ferromagnetic in the Co and Ni components and antiferromagnetic in the Mn (chemical/structural metal-dichloride...infinite chains). Interchain interactions are comparable in size to intrachain, and antiferromagnetic in each component. Competing interactions occur in mixtures, as well as different kinds of spin anisotropy. Remarkable variety appears in the form of susceptibility vs temperature plots for different compositions, reflecting effects of random mixing. Different compositions display a susceptibility maximum located differently from any pure component's, or two maxima, or no maximum. Magnetization vs field isotherms also display contrasting behavior for different compositions, and varying degrees of hysteresis.

[1]Supported by an ACS-PRF grant

K1.00176 Coercivity, Anisotropy, and Relaxation in Nanocrystalline $Gd_{1-x}Fe_x$ Alloys with $x \leq 0.3$[1]

, P.M. SHAND, A.L. MEYER, M.W. STREICHER, U. Northern Iowa, V.J. LITWINOWICZ, J.E. SHIELD, U. Nebraska, D.L. LESLIE-PELECKY, U. Texas at Dallas — We have performed extensive dc and ac magnetization measurements on nanocrystalline $Gd_{1-x}Fe_x$($x \leq 0.3$) alloys at temperatures below the ferromagnetic Curie temperature. The coercivity for all x values generally increases with decreasing temperature. The temperature variation is similar to that of unalloyed Gd; however, the size of the coercivity at a given temperature varies with x in a non-monotonic fashion. The anisotropy as a function of temperature was extracted by applying the random anisotropy model to magnetization vs. field data. The variation of the anisotropy with temperature was very similar to the behavior of the coercivity, indicating that anisotropy is the dominant mechanism that drives the coercivity. The imaginary part of the ac susceptibility exhibited a peak at low temperatures. The temperature T_p at which the peak occurred shifts with frequency in a manner analogous to a cluster glass. For a given frequency, T_p increases with x. These phenomena can be explained in terms of the microscopic structure of the $Gd_{1-x}Fe_x$ alloys, which consists of nanoscale grains of Gd surrounded by disordered grain-boundary regions where the Fe atoms preferentially locate.

[1]Supported by NSF Grants DMR 0504177 and DMR 0504706.

K1.00177 Suppressing local hot spots due to eddy currents in magnetic coil systems[1]

, ZHEN YAO, AARON SHOJINAGA, YONG WU, Case Western Reserve University, SHMARYU SHVARTSMAN, TIMOTHY EAGAN, THOMAS CHMIELEWSKI, ViewRay Inc., ROBERT BROWN, Case Western Reserve University — A particular goal in magnetic field applications is to avoid eddy current heating in coils and shields. It is important, in MRI, for example, to avoid hot spots near the patient to be imaged as well as in the vicinity of soldering joints. We develop effective analytical formulas for the eddy current behavior of sources close to surrounding conductors, we verify these via numerical simulations, and we make successful comparisons to corresponding experimental temperature distributions. Optimized patterns of incisions made in the conductors are discovered for addressing particularly troublesome heating locations. The criteria include the need to minimize the number and length of the cuts. Theory and experiment are in agreement on the efficacy of this method for reducing steady-state temperatures. An example of results in the practical design of commercial coils and shields is that a single cut parallel to the long edge of rectangular conductors reduces the temperatures much more than making multiple cuts parallel to the short edge.

[1]Supported by Ohio Third Frontier Program

K1.00178 Anomalous remanent magnetization dependence of exchange bias effect in Ni50Mn37In13[1] , BAOMIN WANG, YONG LIU, School of Mechanical and Aerospace Engineering, Nanyang Technological University, 639798, Singapore, LAN WANG, Division of Physics and Applied Physics, School of Physical and Mathematical Sciences, Nanyang Technological University, 637371, Singapore — Here, we report an anomalous remanent magnetization dependence of exchange bias effect in Ni50Mn37In13 alloy. Both the value of exchange bias field and its sign can be tuned by the amplitude of remanent magnetization without changing its sign. This tunability is strongly dependent on the direction of initial magnetizing field for the hysteresis loop measurements. These results can be explained well by our recent proposal of isothermal field-induced transition from superspin glass to superferromagnetic state in Ni50Mn37In13 alloy.

[1]Support for this work came from Singapore National Research Foundation (RCA-08/018) and MOE Tier 2 (T207B1217).

K1.00179 Indirect spin-spin interaction mediated by cavity photons , GUILLERMO QUINTEIRO, Univ de Buenos Aires — I theoretically investigate the spin-spin indirect interaction mediated by photons, and compare the results with previous work on the indirect interaction mediated by excitons and/or polaritons in bulk semiconductor and two-dimensional cavities. The systems consist of a cavity, either 0D or 2D, containing two QDs, each one coupled to a donor impurity. The neutral QDs are excited by a cavity photon, and the resulting exciton interacts with the impurity via exchange between the electron in the donor and the electron in the exciton. In the case of a 2D cavity, where the system is optically excited by an off-resonance monochromatic laser field, I deduce an effective Ising Hamiltonian for the spin-spin interaction using a perturbation theory approach. In the case of a 0D cavity, the exact eigenvalues and eigenvectors of the complete Hamiltonian involving the donors, excitons and cavity photons were determined by numerical diagonalization. The eigenvectors and energies were then used to calculate the spin-spin correlation and an effective donor-donor Hamiltonian was deduced. The numerical calculations performed for all admissible values of the physical constants revealed that the in-plane or xy correlation is zero; thus, I concluded that the effective interaction is of the Ising type. In addition, I found that the largest effective coupling J_{eff} corresponds to a situation where the excitons and the cavity photon are completely mixed, forming a polariton.

K1.00180 Characterizing Multiferroics: Analyses through X-Ray Diffraction , EVAN WOLFE, HARLEY HART, SHELDON BLACKSHIRE, SRINIVAS POLISETTY, DISHENG CHEN, JINLING ZHOU, CHARLES FRYE, MIKEL HOLCOMB — Theory and experiments support that magnetoelectric coupling (electrical control of magnetism and vice versa) can be enhanced by taking advantage of interfacial coupling between magnetic and ferroelectric films. The interface between ferroelectric PZT and ferromagnetic LSMO is a promising candidate for storage and magnetic sensing devices. For example, LSMO, when exposed to a magnetic field, will contract; while PZT when strained will produce a voltage. Combining properties, the PZT/LSMO composite can be utilized to detect magnetic fields, and also be used as an energy scavenging device. In order to maximize the coupling across this interface, proper measurements and characterizations must be taken to detail how the materials interact on the atomic level. X-ray diffraction allows us to determine thickness, composite, and strain of the samples used. By analyzing the peak shift in XRD scans along our samples we can detail the amount of strain placed on the sample, aiding in discovering of the mechanisms responsible for interfacial magnetoelectric coupling. Through analysis, we can ensure the quality of the interface, thus allowing further advances for increases in magnetic sensitivity and higher voltage output.

K1.00181 Effect of annealing on the local structure of Fe and Co in CoFeB/MgO based magnetic tunnel junction: An extended X-ray absorption fine structure study , ABDUL RUMAIZ, Brookhaven National Laboratory, JOSEPH WOICIK, NIST, WEIGANG WANG, Johns Hopkins University, CHERNO JAYE, NIST, HASSNAIN JAFFARI, C.L CHIEN, JEAN JORDAN-SWEET, IBM T.J. Watson Research Center, JOHN XIAO, University of Delaware — The evolution of the local structure of Fe and Co as a function of annealing time in CoFeB/MgO/CoFeB magnetic tunnel junctions was studied using extended x-ray-absorption fine structure (EXAFS). EXAFS indicates B depletion and crystallization of the CoFeB layers within a few seconds of the post growth high temperature anneal. The decrease in first-shell Debye–Waller factor and hence the increase in structural order during annealing explains the increase in tunnel magnetoresistance observed as a result of post deposition annealing. Although the diffusion of B has also been confirmed by several other experiments, there has not been much consensus on where the B diffuses after high temperature anneal. Recent results from B Near edge x-ray absorption fine structure (NEXAFS) will also be discussed.

K1.00182 Anisotropy Energy, Spin-Atomic Vibration Interaction, and Spin-Flip Hamiltonian of a Single Atomic Spin in a Crystal Field , SATOSHI KOKADO, Faculty of Engineering, Shizuoka University, Japan, KIKUO HARIGAYA, Nanosystem Research Institute, AIST, Japan, AKIMASA SAKUMA, Graduate School of Engineering, Tohoku University, Japan — We derive the anisotropy energy $V_{\rm A}$, the spin-atomic vibration interaction $V_{\rm SA}$, and the spin-flip Hamiltonian $V_{\rm SF}$ of a single atomic spin system, "Fe^{2+} ($3d^6$) in a crystal field of tetragonal symmetry" [1,2]. We here apply the perturbation theory to a model with the spin- orbit interaction and the kinetic and potential energies of electrons. The model also takes into account the difference in vibration displacement between an effective nucleus and electrons, Δr. We first find conditions to enhance a coefficient $|D|$ of $V_{\rm A}$=$-|D|S_Z^2$, where D is an anisotropy constant and S_Z is the Z component of a spin operator. Second, we show that $V_{\rm SA}$ appears for $\Delta r \neq 0$, while $V_{\rm SF}$ is present independently of Δr. Also, the magnitudes of the coefficients of $V_{\rm SA}$ can be larger than those of the conventional spin-phonon interaction depending on vibration frequency.

[1] S. Kokado *et al.*, J. Phys. Soc. Jpn. **79**, 114721 (2010).
[2] S. Kokado *et al.*, phys. stat. solidi (c) **7**, 2612 (2010).

K1.00183 Synthesis and Analysis of Rare-Earth Nanoparticles Gd and Nd , JOSE AMARAL, CARMIN LIANG, DULCE ROMERO, PEI-CHUN HO, Physics/California State Univ, Fresno, SAEED ATTAR, Chemistry/California State Univ, Fresno, DENNIS MARGOSAN, USDA/Agriculture Research Service — We have synthesized sub-micron gadolinium particles using sodium borohydride reduction of gadolinium chloride in an inverse micelle solution of the surfactant didodecyldimethylammonium bromide (DDAB) and toluene. Gadolinium and neodymium are paramagnetic rare earth metals at room temperature and become ferromagnetic and anti-ferromagnetic below 293K and 19K, respectively. A liquid-liquid extraction using two immiscible solvents can separate the magnetic nanoparticles from unwanted by-products of the reduction. SEM images show spherical Gadolinium clusters less than one micrometer were produced. Nd nanoparticles do not synthesize using toluene and water and results using methanol and hexane are on-going. Magnetic nanoparticles can have enhanced magnetization and increased density in a finite region compared to their bulk material. Possible applications include high-density magnetic storage, high-density recording media, contrast agents to improve medical magnetic resonance imaging, and magnetic refrigeration.

K1.00184 High-temperature performance of bulk nanocomposite $SmCo_5$/-Fe(Co) magnets , CHUANBING RONG, NARAYAN POUDYAL, J. PING LIU, Department of Physics, University of Texas at Arlington, Arlington, TX 76019, USA, YING ZHANG, M.J. KRAMER, Division of Materials Science and Engineering, Ames Laboratory, Iowa State University, Ames, IA 50011, USA — Permanent magnetic materials capable of operating at elevated temperatures are highly required for advanced power systems. In this work, a new processing technique has been adopted to produce $SmCo_5$-based bulk nanocomposite magnets with high thermal stability. The processing consists of severe plastic deformation and warm compaction. The structure and high-temperature magnetic property characterizations show that the microstructure does not change with heating temperature up to 500 °C which ensures effective inter-phase exchange coupling at elevated temperature. It was also found that the thermal stability of the bulk nanocomposite magnets can be significantly improved with increasing density (decreasing porosity). The room temperature energy product drops fast with heating temperature above 300 °C for the magnets with 80% density, and with minimum decrease for the magnets with full density. Energy product about 11.1 MGOe can be obtained at 300 °C in the fully dense isotropic bulk $SmCo_5$/Fe nanocomposite magnets.

K1.00185 Unusual Structure and Magnetism in MnO Nanoclusters[1]

SHREEMOYEE GANGULY, Ph.D. student, S. N. Bose National Center for Basic Sciences, Kolkata, India, MUKUL KABIR, Postdoctoral researcher, MIT, USA, BIPLAB SANYAL, Associate Professor, Uppsala University, Sweden, ABHIJIT MOOKERJEE, Professor, S. N. Bose National Center for Basic Sciences, Kolkata, India — We report an unusual structural and magnetic evolution in stoichiometric MnO nanoclusters by an extensive and unbiased search through the potential energy surface within density functional theory. The $(MnO)_n$ nanoclusters adopt two-dimensional structures in size ranges in which Mn_n nanoclusters are three-dimensional and regardless of the size of the nanocluster, the magnetic coupling is found to be antiferromagnetic, and is strikingly different from Mn-based molecular magnets. Both of these features are explained through the inherent electronic structures of the nanoclusters.

[1]We gratefully acknowledge financial support from Swedish Research Links program funded by VR/SIDA and Carl Tryggers Foundation, Sweden.

K1.00186 The Effect of Magnetic Anisotropy on Colossal Electroresistance in Manganites[1]

ALESSANDRA GALLASTEGUI, RAFIYA JAVED, HYOUNGJEEN JEEN, AMLAN BISWAS, Department of Physics, University of Florida, Gainesville, FL 32611 — The combined effect of long range strain interactions and disorder on a first order transition leads to micrometer scale phase separation in hole-doped manganese oxides (manganites). The coexisting phases are ferromagnetic metallic (FMM), charge ordered insulating (COI), and paramagnetic insulating (PMI) and at certain temperatures these phases behave like a fluid under the influence of magnetic and electric fields. We will present magnetotransport data on nano/micro-structures of the manganite $(La_{1-y}Pr_y)_{0.67}Ca_{0.33}MnO_3$ (LPCMO) which show that the FMM phase behaves like a fluid in an electric field. In fact, due to the magnetic anisotropy of our materials, the behavior of the coexisting phases is reminiscent of a ferrofluid.

[1]NSF DMR-0804452

K1.00187 Metal-terminated carbon based nanostructures[1]

SAHAR MIRSHAMSI, YAN WANG, HAI-PING CHENG, Dep of Physics and Quantum Theory Project. Uni. of Florida — Carbon based structures have attracted immense interest in many different fields and among them graphene has attracted more attention because of its unique physical properties. Hybrid metal-Carbon nanostructures are of interest because of their electronic and magnetic properties. We have studied magnetic correlations at zigzag edges of metal terminated graphene nanoribbons by calculating the transverse and longitudinal fluctuations of magnetic moments from first-principles. With inclusion of non-collinear spin-orbit coupling, we have investigated the continuous rotation of the electron spin which occurs along the ribbon edges (spin waves). Also, we report here effects of edge disorders and finite size effects. Finally, we extend our model to include multiple layers and studying the inter-layer magnetic coupling and the effect to the inter-edge magnetic coupling of the ribbon.

[1]Supported by DOE/BES-DE-FG02-02ER45995 and NSF/DMR-0804407 and computed at UF-HPC center.

K1.00188 Temperature-dependent properties of the magnetic order in single-crystal $BiFeO_3$

V. KIRYUKHIN, M. RAMAZANOGLU, S-W. CHEONG, Rutgers Univ., W. RATCLIFF, NIST, S. LEE, KAERI — Neutron scattering studies of the magnetic structure of multiferroic $BiFeO_3$ are presented. We report temperature dependence of the magnetic order parameter, the period of the cycloidal modulation of the antiferromagnetic order, and the populations of the equivalent magnetic domains in the monodomain ferroelectric state. No anomalies below room temperature are found, excluding the spin-reorientation transitions proposed elsewhere.

K1.00189 Polarized micro Raman spectroscopy of multiferroic $BiFeO_3$ single crystals

C. BEEKMAN, University of Toronto, SANG-WOOK CHEONG, Rutgers University, KENNETH BURCH, University of Toronto — In Bismuth ferrite ($BiFeO_3$) antiferromagnetic and ferroelectric order parameters coexist at room temperature, making this material an excellent candidate for new functionalities, such as electrical control of ferromagnetism. Despite extensive reports on Raman scattering experiments on single crystals and thin films, controversy still remains in the observation and assignment of the phonon modes. However, proper Raman mode assignment to describe the phonons critical for the multiferroic behavior is necessary. We present polarized micro Raman spectroscopy of single crystals with uniform ferroelectric polarization. Careful examination of the Raman spectra upon crystal rotation enables us to unambiguously assign several (A_1, E_x and E_y) modes.

K1.00190 Effect of doping and strain on Néel temperature of Cr_2O_3: An ab initio study

SAI MU, ALEKSANDER WYSOCKI, KIRILL BELASHCHENKO, Department of Physics and Astronomy, University of Nebraska-Lincoln — Cr_2O_3 is a promising material for applications involving electrically switchable exchange bias [1]. For practical purposes it is desirable to enhance its Néel temperature (308K). Here we employ first principles calculations to elucidate the effect of substitutional doping and epitaxial strain on electronic structure and magnetism of Cr_2O_3. We use the supercell method and consider both transition metal (V, Ti, Mn, Fe, Co, Ni) and anion (N, B) impurities. We deduce the effect of doping on Néel temperature (T_N) by calculating the total energy change when the local moment on a transition metal impurity or on the Cr atoms near the anion impurity is flipped. We found that the transition metal impurities and N are detrimental to T_N. On the other hand, B impurities are expected to increase the Neel temperature.

[1] X. He. *et. al.* Nature Matter. **9**, 579 (2010).

K1.00191 High-pressure synthesis and unusual metallic conductivity of the A-site-ordered perovskite $CaCu_3Ir_4O_{12}$[1]

J.-G. CHENG, J.-S. ZHOU, J.B. GOODENOUGH, University of Texas at Austin — Recently, much attention has been paid to the A-site-order perovskites $AA'_3B_4O_{12}$ due to the observation of a large variety of intriguing physical properties. We have prepared an A-site-ordered perovskites $CaCu_3Ir_4O_{12}$ under 9 GPa and 1250 °C with a Walker-type Multianvil module. Rietveld refinements to the room-temperature x-ray diffraction pattern confirmed the cubic structure with lattice parameter a = 7.47380(6) Å in the space group Im-3. Magnetic and transport properties measurements show that $CaCu_3Ir_4O_{12}$ is a paramagnetic metal with unusual temperature dependence. The inverse magnetic susceptibility χ^{-1}(T) above 80 K follows the Curie-Weiss law with μ_{eff} = 4.23 μ_B/f.u. and θ_W = –233 K, while an unusual should-like feature is observed below 80 K. At the same temperature, the resistivity ρ(T) deviates from a T-linear behavior and exhibits a strong downward temperature dependence down to 4 K.

[1]Supported by NSF-DMR-0904282.

K1.00192 Magnetoresistance measurements in Ferro – Antiferromagnetic bilayers based on the Ca-doped lanthanum manganite system[1]

, M.E. GOMEZ, L. MARIN, G. RAMIREZ, Physics Department Universidad del Valle Cali, Colombia , P. PRIETO, CENM Colombia — We studied the isothermal magnetic field dependence of the resistance behavior in ferromagnetic–antiferromagnetic interface based on the Ca-doped lanthanum manganite system at temperatures below Neel temperature of the antiferromagnetic layer. We studied the influence of the thickness of the AF-layer, t_{AF}, and F-layer, t_F, on the ZFC and FC magnetoresistance (MR) in $La_{2/3}Ca_{1/3}MnO_3(t_F)$/ $La_{1/3}Ca_{2(3}MnO_3(t_{AF})$ bilayers. H_{FC} was 400 Oe and the applied magnetic field, H. We systematically varied the t_F and t_{AF} thickness, maintaining constant the total bilayer thickness ($d = t_F + t_{AF}$). We found that MR has hysteretic behavior as observed in $[La_{2/3}Ca_{1/3}MnO_3(t_F)/La_{1/3}Ca_{2(3}MnO_3(t_{AF})]_N$ superlattices, but; MR increases with the increasing field from H=0 to a maximum and then decreases continuously. This behavior also appears for negative fields in both ZFC and FC loops. The position and magnitude of the maximum is not symmetric with respect to the axis H=0.

[1]Work supported by CENM-COLCIENCIAS contract RC-0043-(2005).

K1.00193 Characterization of EuO_{1-x} thin films grown by oxidation of metallic Eu[1]

, B. COLWELL, A. KINSEY, S. SCHLOTTER, M. EBLEN-ZAYAS, Carleton College — EuO_{1-x} is of interest due to the similarities between its magnetic and transport properties and those of the manganites, and it also holds potential for spintronics applications. We have grown polycrystalline EuO_{1-x} films by oxidizing metallic Eu films. The films are characterized by x-ray diffraction, as well as measuring the resistivity and magnetization responses as a function of temperature. We will report on the relationship between the growth conditions and the properties of these samples, including a description of how annealing impacts the film properties.

[1]This work has been supported by the Research Corporation and NSF DMR-0804715.

K1.00194 Composition Dependence of the Anomalous Hall Effect in L10 FePt Thin Films[1]

, M. ALLISON, T. GEORGE, P. KHAREL, D. SELLMYER, Y. HUH, Department of Physics, South Dakota State University — FePt multi-layered thin film systems were investigated as to its composition effect on the anomalous hall effect. Thin bilayers of FePt were sputter-deposited in series of variable thicknesses on to a thermally oxidized substrate of SiO2. The total thickness of samples was controlled to be 12 nm. XRD and SEM were used to confirm structure and composition of thin films for systematic characterization. Resistivity and Magnetization measurements were studied at room temperature and low temperature using SQUID magnetometer. The minimal resistivity exists near 54% of Fe concentration. The anomalous hall effect dominates as Fe concentration increases. Hall angles drop rapidly at the both high and low Fe concentration while it exhibits a plateau-like dip near 54% of Fe concentration.

[1]This research is supported by the NSF (CHE-1012366 and Nebraska MRSEC Grant DMR-0820521).

K1.00195 Imaging and Electric Control of Boundary Magnetization and Exchange Bias in Chromia and Chromia/CoPd

, XI HE, Univ. of Nebraska, Lincoln, NE, NING WU, Univ. of Nebraksa, Lincoln, NE, YI WANG, ALEKASANDER WYSOCKI, TAKASHI KOMESU, KIRILL BELASHCHENKO, PETER DOWBEN, CHRISTIAN BINEK, Univ. of Nebraska, Lincoln, NE, UDAY LANKE, Canadian Light Source Inc., Saskatoon, Canada, ANTHONY CARUSO, Univ. of Missouri, Kansas City, ELIO VESCOVO, Brookhaven National Lab. NY — Promising spintronic concepts utilize electric control of boundary magnetization. Symmetry arguments predict that the magnetoelectric antiferromagnet (AF) Cr_2O_3, has a roughness insensitive surface magnetization which is coupled to the bulk AF order parameter. We provide macroscopic and microscopic evidence for this surface magnetization and its electric control. The latter is exploited in perpendicular exchange bias heterostructures where a ferromagnetic Pd/Co multilayer is deposited on the (0001) surface of a Cr_2O_3 single crystal. These heterostructures show reversible, room-temperature voltage-controlled switching of the exchange-bias field between positive and negative values.[1] This work is supported by NSF Career, NSF MRSEC, NRI, and Research Corporation.

[1]Xi He, et al. Nature Materials **9**, 579 (2010)

K1.00196 Effect of carbon doping on optical constants of half-metallic ferromagnet Mn_5Ge_3

, N. STOJILOVIC, University of Wisconsin Oshkosh, RONGWEI HU, The Johns Hopkins University, C. PETROVIC, Brookhaven National Laboratory, S.V. DORDEVIC, The University of Akron — Mn_5Ge_3 is an intermetallic ferromagnetic compound with the high Curie temperature (T_C = 296 K), a high spin polarization (P = 42%), and a good lattice match to germanium. Doping of Mn_5Ge_3 with carbon increases T_C above room temperature and makes these compounds promising candidates for spin injectors for potential spintronics applications. In this study we employ optical spectroscopy to measure near-normal reflectance in the frequency range from far-infrared to ultraviolet (70 – 50000 cm^{-1}) at temperatures between 10 and 300 K. In particular, we study the effect of carbon doping on the optical constants to gain a better insight into how it affects the electronic properties of the parent compound.

K1.00197 Spin polarization measurements in Fe_4N/MgO/NbN tunnel junctions using quasiparticle tunneling spectroscopy

, TAKAYUKI HOHJO, KEITA SAKUMA, TETSUYA MIYAWAKI, KENJI UEDA, Department of Crystalline Materials Science, Nagoya University, HIDEFUMI ASANO, YOSUKE KOMASAKI, MASAKIYO TSUNODA, Department of Electronic Engineering, Tohoku University — In spintronic applications, it is thought that Fe_4N is useful because it has been theoretically expected to have high spin polarization. Fe_4N/MgO/CoFeB magnetic tunnel junctions (MTJs) were fabricated, and an inverse tunnel magnetoresistance (TMR) effect was reported by our groups. However, spin polarization of Fe_4N is yet incompletely understood. We investigated spin polarization of Fe_4N, using quasiparticle tunneling spectroscopy (QTS), and the measured spin polarization of Fe_4N was compared with that in Fe_4N/MgO/CoFeB MTJs. Spin polarization of ferromagnetic materials can be directly measured by QTS. By using NbN and MgO as superconducting electrode and barrier layers, respectively, Fe_4N/MgO/NbN tunnel junctions were fabricated by magnetron sputtering. The thickness of MgO barrier layer was varied from 1.0 to 1.5 nm. The areal resistances of the Fe_4N/MgO/NbN tunnel junctions were close to those of Fe_4N/MgO/CoFeB MTJs, which had the same thickness of MgO barrier layer as those Fe_4N/MgO/NbN tunnel junctions. In QTS, spin polarization of Fe_4N was estimated to be ~ -0.68. This value is larger than spin polarization in MTJs.

K1.00198 Temperature and temporal evolution of nonlocal spin signals[1]

, YI JI, HAN ZOU, University of Delaware — An unusual temperature evolution of spin signals has been previously reported by others for metallic nonlocal spin valves (NLSV): The spin signal increases as the temperature decreases from room temperature, reaches a maximum value around 50 K, and then decreases as the temperature approaches 4 K. This has been interpreted as due to a high surface spin-flip rate, but the origins of which are yet to be understood. In this work, we show that for an as fabricated Py-Cu NLSV device this temperature dependence is clearly observed. The device was then stored in the ambient environment for a period of 5 months. Afterwards, we found an increase of the spin signals, and more interestingly the spin signal levels off at 27 miliohms, instead of decreasing, below 50 K. Based on this and our other experiments, we conclude that the surface spin-flip scattering originates from the magnetic impurities embedded in the Cu channel near the side surfaces. Upon oxidizing the Cu, the surface impurities are buried in the copper oxide and become less accessible to the conduction electrons. Therefore the surface spin-flip rate is reduced over time.

[1]Work supported by DOE Grant No. DE-FG02-07ER46374.

K1.00199 Spin-transfer induced vortex dynamics with non-standard angular dependence torque , PAOLO BORTOLOTTI, NICOLAS LOCATELLI, VINCENT CROS, JULIE GROLLIER, CNRS/Thales, Palaiseau, France, RITA MACHEDO, RICARDO FERREIRA, SUSANA CARDOSO, INESC-MN, Lisbon, Portugal, ALBERT FERT, CNRS/Thales, Palaiseau, France — Microwave emissions driven by spin-transfer were firstly observed on FeNi/Cu/FeNi pillars (standard samples) characterized by uniform magnetization. Interestingly, by tuning the spin accumulation profile, i.e., choosing Co/Cu/FeNi pillars with opportune ratio of thickness/spin diffusion length (non-standard samples), it is possible to obtain strong modification of the torque angular dependence and, more generally, of the magnetization dynamics itself. Eventually, oscillations at zero applied field were observed for these non-standard pillars, again for uniform magnetization. However, when a large current density is applied, the uniform hypothesis is broken and vortex states are favoured. In this work we want to stress that non standard-angular dependence, obtained for such Co/Cu/FeNi samples, plays an important role also for vortex dynamics. By the combined study of static and dynamic response, we can discriminate among all possible combinations of vortex chiralities and polarities. The evolution with field and current of such configurations clearly differs from samples with standard spin-torque angular dependence, resulting in a different dynamics for such non-standard samples.

K1.00200 Size effect on $GdMn_2O_5$ nanoparticles , CHENG-YU WENG, CHUN CHUEN YANG, WEI-LUEN HUANG, ZHE-AN JIAN, Department of Physics, Chung Yuan Christian University, YANG YUAN CHEN, Institute of Physics, Academia Sinica, DEPARTMENT OF PHYSICS, CHUNG YUAN CHRISTIAN UNIVERSITY COLLABORATION, INSTITUTE OF PHYSICS, ACADEMIA SINICA COLLABORATION — We fabricated six difference sizes of $GdMn_2O_5$ nanoparticles/nanobrick by hydrothermal method. Purity and particle size were determinate by x-ray diffraction and TEM/SEM images. Two Mn antiferromagnetic ordering peaks at around 38 and 40 K were observed in ac magnetic susceptibility experiments, where as particle size is larger than 60 nm. Curie-Weiss fitting revealed that the Néel temperatures are increased with increasing size. Similar phenomena were also found in the saturate magnetic moments obtaind from M-H experiments at 5 K. No hysteresis loops were found in any particle size. We believe these magnetic behaviors are correlated with size confinement effects. The estimated magnetic correlation length of Mn is in between 60 and 84 nm.

K1.00201 Anisotropic paramagnetism in monoclinic $Nd_2Ti_2O_7$ single crystals[1] , HUI XING, Zhejiang University, GEN LONG, SUNY at Buffalo, HANJIE GUO, YOUMING ZOU, CHUNMU FENG, GUANGHAN CAO, Zhejiang University, HAO ZENG, SUNY at Buffalo, ZHUAN XU, Zhejiang University — The anisotropic paramagnetism and specific heat in Nd2Ti2O7 single crystals are investigated. Angular dependence of the magnetization and Weiss temperatures show the dominant role of the crystal field effect in the magnetization. By incorporating the results from the diluted samples, contributions to Weiss temperature from exchange interactions and crystal field interactions are isolated. The exchange interactions are found to be ferromagnetic, while the crystal field contributes a large negative part to the Weiss temperature, along all three crystallographic directions. The magnetic specific heat reveals a two-level Schottky ground state scheme, due to the Zeeman splitting of the ground state doublet, and the g-factors are thus determined. These observations provide solid foundations for further investigations of Nd2Ti2O7.

[1]Work supported by the NSFC (No. 10634030), NSF DMR-0547036 and National Basic Research Program.

K1.00202 Magnetic Order and Spin Dynamics in a Hexagonal Rare Earth Manganite , J.S. HELTON, D.K. SINGH, NIST Center for Neutron Research, S. ELIZABETH, S. HARIKRISHNAN, Indian Institute of Science, Bangalore, J.W. LYNN, NIST Center for Neutron Research — Hexagonal rare earth manganites, RMnO$_3$ (R = Dy, Ho, Er, Tm, Yb, Lu, Y, or Sc), have attracted a great deal of recent attention as magnetoelectric multiferroics as most of these systems are ferroelectric at room temperature and display magnetic order below $T_N \approx 100$ K. This magnetic order can be quite complex, as both the R and Mn ions lie on geometrically frustrated triangular lattices. DyMnO$_3$ is typically orthorhombic, but can also be grown in the hexagonal phase; $Dy_{0.5}Y_{0.5}MnO_3$ displays the hexagonal phase and is magnetically diluted at the rare earth site. We have used neutron scattering experiments to explore the magnetic structure and spin dynamics of $Dy_{0.5}Y_{0.5}MnO_3$.

K1.00203 Z_2 topological classification of the $S = 1/2$ Heisenberg model on the two dimensional pylochlore lattice , SHO TANAYA, MITSUHIRO ARIKAWA, University of Tsukuba, ISAO MARUYAMA, Osaka University, YASUHIRO HATSUGAI, University of Tsukuba — We have investigated the $S = 1/2$ Heisenberg model on the two dimensional pyrochlore lattice [1] by using the Z_2 Berry phase [2] which is quantized due to the time reversal invariance. Since these Z_2 Berry phases are adiabatic invariants against change of the physical parameters, one can distinguish ground states when the quantized values are different. By suitably choosing ways of local $U(1)$ twists to define the Berry phases, one can show that the ground state in this system is adiabatically connected to a direct product state of local singlets or plaquette singlets. We have described the basic formulation and demonstrate the validity for finite systems using a Lanczos diagonalization.

[1] J.-B. Fouet, M. Mambrini, P. Sindzingre, and C.Lhuillier, Phys. Rev. B 67 (2003) 054411.
[2] Y. Hatsugai, J.Phys Soc. Jpn. 73 (2004) 2604.

K1.00204 Chirality waves in two-dimensional magnets , DMITRY SOLENOV, DMITRY MOZYRSKY, IVAR MARTIN, Los Alamos National Laboratory — Electron, as a particle with spin 1/2, moving though a magnetic material with non-coplanar magnetization pattern accumulates quantum mechanical (Berry) phase, characterized by the degree of non-coplanarity of the magnetic texture, or chirality. Until now metallic chiral magnets were thought to be quite rare and require either a fine tuning of the electron spectrum (nesting) or spin-orbit interactions. We show that two-dimensional magnets within a simple model of magnetism – a Kondo lattice model – favor a non-coplanar order (a distorted skyrmionic lattice) with unidirectional modulated chirality. Unlike recently observed chiral triangular skyrmion lattices supported by spin-orbit interaction and finite magnetic field (e.g. in MnSi), the chirality-wave order emerge at small-to-intermediate Kondo coupling strength in the absence of magnetic field or spin-orbit coupling

K1.00205 Non-polar electromagnon in hexa-$YMnO_3$, J.R. SIMPSON, Towson University, A.B. SUSHKOV, H.D. DREW, University of Maryland, M. MOSTOVOY, University of Groningen, A. GOZAR, Brookhaven National Laboratory, G. BLUMBERG, N. LEE, S.-W. CHEONG, Rutgers University — Coupled magnon-phonon excitations in magnetic materials have been observed in multiferroic materials and involve the polar optical phonons. Such excitations may be more general, occurring in non-ferroelectric magnets and involving non-polar (Raman or silent) phonons. Temperature-dependent Raman spectra of low-frequency excitations in single-crystal h-YMnO$_3$ are measured using a triple-grating spectrometer. We compare the spectral intensity of magnons to changes in the Raman-active phonons above and below the Neel temperature. Raman and infrared experimental results on h-YMnO3 demonstrate that the 5 meV hybrid mode observed in neutron scattering is an example of a Raman electromagnon.

K1.00206 T1-limited Nitrogen-Vacancy magnetometry of fluctuating AC magnetic fields[1] , CARLOS MERILES, ABDELGHANI LARAOUI, Department of Physics, City College of New York - CUNY, JONATHAN HODGES, Department of Electrical Engineering, Columbia University — Nitrogen-Vacancy (NV) centers in diamond are being actively investigated as a platform for nanoscale magnetic field sensing. In many of the envisioned applications the target AC magnetic field fluctuates over time and cannot be triggered in synchrony with the pulse protocol controlling NV evolution. Here we introduce a scheme to characterize the time correlation of the unknown field over a time interval limited by the NV spin-lattice relaxation time. Our approach uses two consecutive Hahn-echo sequences separated by a time interval of variable duration. We present an initial experimental demonstration of the technique using an engineered AC field and discuss possible extensions to the monitoring of slowly fluctuating spin ensembles.

[1]We acknowledge support from the National Science Foundation.

K1.00207 SUPERCONDUCTIVITY —

K1.00208 ^{13}C NMR Study of Graphite Intercalated Superconductor CaC_6 Crystals in the Normal State , MOOHEE LEE, SUNG HOON KIM, KI HYEOK KANG, B. J. MEAN, B. NDIAYE, Konkuk University, Seoul, South Korea, JUN SUNG KIM, POSTECH, Pohang, South Korea — ^{13}C NMR(Nuclear Magnetic Resonance) measurements have been performed to investigate the local electronic structure of a superconducting graphite intercalation compound CaC_6 (T_c = 11.4 K). A large number of single crystals were packed and sealed in a quartz tube for naturally abundant ^{13}C NMR. Spectrum, Knight shift, linewidth, spin-lattice relaxation time T_1, and the spin-spin relaxation time T_2 were measured in the normal state as function of temperature down to 70 K at 4.8 T and 8.0 T. ^{13}C NMR spectrum shows a narrow peak with a very small Knight shift. Knight shift and linewidth of the ^{13}C NMR are almost temperature-independent around, respectively, 0.012% and 1.2 kHz. The spin-lattice relaxation rate $1/T_1$ is proportional to temperature confirming a Korringa behavior as for nonmagnetic metals. The Korringa product is measured to be T_1T= 210 s.K. From this value, the Korringa ratio is deduced to be $\xi = 0.73$, close to unity, which suggests that the independent-electron description works well for CaC_6, without complexity arising from correlation and many-body effects.

K1.00209 Oxygen staging in phase separated $La_{2-x}Sr_xCuO_{4+y}$, HASHINI MOHOTTALA, University of Hartford, 200, Bloomfield Ave. West-Hartford, CT-06117, LINDA UDBY, e-Science and Nanoscience Centres, Niels Bohr Institute, Universistetsparken 5, 2100, S. EMERY, B.O. WELLS, J.I. BUDNICK, University of Connecticut, 2152, Hillside road, Storrs, CHRISTOF NIDERMAYER, ETHZ & PSI, CH-5232 Villigen PSI, Switzerland, KIM LEFMANN, e-Science and Nanoscience Centres, Niels Bohr Institute, Universistetsparken 5, 2100, N.H. ANDERSON, Ris DTU, Frederiksborgvej 399, 4000 Roskilde, Denmark, F.C. CHOU, Center for Condensed Matter Sciences, National Taiwan University,Taipei 10617, Taiwan — We studied oxygen staging in a series of $La_{2-x}Sr_xCuO_4$ (LSCO) samples using neutron scattering. The samples were oxidized using electrochemistry. Electronic phase separation was previously reported in the oxygen rich LSCO system with two stable phases identified as optimally doped superconducting phase and a magnetic phase (1/8th like) with the same ordering temperatures at 40 K . Our present studies show staging in this system. Although staging was observed and extensively studied in the samples with no Sr, it has not been reported or systematically studied in the systems with both Sr and oxygen. We do find staging in the oxygenated LSCO system, but the staging peaks evolve as Sr concentration increases and excess oxygen concentration decreases.

K1.00210 Muon probing in optimal and under- doped GdBCO , C. BOEKEMA, San Jose State University, H. SIO, Harvey Mudd College, M.C. BROWNE, San Jose State University — By means of MaxEnt-Burg, transverse-field (TF) μSR data of underdoped (δ1; T_c= 81 K) and optimal doped (δ0; T_c= 93 K) $GdBa_2Cu_3O_{7-\delta}$ (GdBCO) are analyzed. Site search studies for RBCO generated plausible candidates for muon sites [1] called the Balmer and Lin sites. We wish to confirm the muon-probe sites in GdBCO. One of the two Balmer sites and the Lin site are located near O vacancies. These two sites become unstable in underdoped GdBCO(δ1). Positive muons are repelled by the positive O vacancies. This repulsion effects would be more pronounced as temperature increases. At 120 K, three signals are present in GdBCO(δ1), while at roomtemperature (RT), only one dominant signal remains. In contrast, three signals occur at 120 K and RT for GdBCO(δ0), which has much less O vacancies. These results support earlier studies [1] of muon-O sites. Thus, the muons probe away from the CuO_2 plane, allowing μSR to detect magnetic fields originating from potential loop currents in these planes. [2] By ME-μSR analysis, the Balmer & Lin sites in GdBCO are confirmed. Research supported by NSF-REU.
[1] WK Dawson et al, J Appl Phys 64 (1988) 5809 & Hpf Int 63 (1990) 219.
[2] CM Varma, PRL 83 (1999) 3538; T Songatikamas et al, J Superconductivity and Novel Magn 23 (2010) 793.

K1.00211 Strongly anisotropic flux pinning in superconducting PbBi thin films covered by periodic ferromagnet stripes , DONALD NAUGLE, ZYXIN YE, WENHAO WU, IGOR LYUKSYUTOV, Department of Physics and Astronomy, Texas A&M University — We have studied the vortex pinning via their magnetic interaction with a periodic structure of parallel magnetic stripes. Superconducting lead-bismuth (82% Pb and 18% Bi) alloy films were covered by an insulating Ge layer and periodic a Ni array of magnetic stripes fabricated on the top of the Ge layer by electron-beam lithography and thermal evaporation. The critical current density was significantly stronger when the current was applied parallel to the stripes than when the current was perpendicular to the stripes. This is attributed to the barrier to the vortex motion provided by the magnetic interaction with magnetic stripes. The enhancement in critical current was most significant at temperatures close to the superconducting transition temperature.

K1.00212 Effect of current on the dc I-V characteristic of polycrystalline $YBa_2Cu_3O_{7-X}$ near Tc , SNEHADRI OTA, Institute of Physics, Bhubaneswar, Orissa — The dc I-V characteristic of polycrystalline $YBa_2Cu_3O_{7-X}$ high temperature superconductors (HTSC) is measured near the transition temperature (T_c). The T_c was found to be 90 K with a width of 2 K. The voltage was measured at various current values and with reversing the current. A difference in voltage was found, for forward and reverse current direction near T_c. This can be understood qualitatively as due to the d-wave superconductivity as predicted by the RVB theory. This can also be understood qualitatively as due to the presence of proximity junctions, which is generally indicated by finite transition width in HTSC or A15 superconductors. The observed directionality of the I-V characteristic can be understood in terms of trapped flux by the self-field of the current and the proximity junctions in these materials.

K1.00213 Superconducting and transport properties of $Y_3Ba_5Cu_8O_X$ and $Y_3Ca_2Ba_5Cu_8O_x$ prepared by sol-gel method , ALI ER, Old Dominion University, YUKSEL UFUKTEPE, AHMET EKICIBIL, Cukurova University, ALI OSMAN AYAS, Adiyaman University, SELDA KILIC CETIN, KERIM KIYMAC, Cukurova University — The influence of substitution of Ca has been studied using electrical resistivity (ρ), X-ray diffraction (XRD), atomic force microscopy (AFM), energy dispersive analysis (EDX), differential thermal analysis (DTA), thermogravimetric analysis (TGA), Hall coefficient (R_H), Hall mobility (μ_H) and magnetoresistance measurements. The XRD spectra showed that they almost have the same crystal structure of $Y_3Ca_2Ba_5Cu_8O_x$ as $Y_3Ba_5Cu_8O_x$with some impurities peaks. The resistivity measurements were made by the four-probe method. The $Y_3Ba_5Cu_8O_x$ and $Y_3Ca_2Ba_5Cu_8O_x$ have the highest T_c-onset at about 92.7 and 86.6 K, respectively. The Hall coefficient R_H and Hall mobility μ_H are measurement between 10-300 K temperatures at magnetic field of 0.55 T. The sign of R_H and μ_H are positive for two samples which indicate that the conduction is p-type for the samples. A small change of normal state resistivity and superconducting transition are observed in the resistivity curve with the magnetic field.

K1.00214 Dynamical conductivity at the dirty superconductor-metal quantum phase transition[1] , J.A. HOYOS, Universidade de São Paulo, ADRIAN DEL MAESTRO, Johns Hopkins University, BERND ROSENOW, University of Leipzig, THOMAS VOJTA, Missouri University of Science and Technology — We study the transport properties of ultrathin disordered nanowires in the neighborhood of the superconductor-metal quantum phase transition. To this end we combine numerical calculations with analytical strong-disorder renormalization group results. The quantum critical conductivity at zero temperature diverges logarithmically as a function of frequency. In the metallic phase, it obeys activated scaling associated with an infinite-randomness quantum critical point. We extend the scaling theory to higher dimensions and discuss implications for experiments.

[1]Financial support: Fapesp, CNPq, NSF, and Research Corporation

K1.00215 Spatially resolved NMR spectra for the Swiss cheese model in heavy fermion $PuCoGa_5$ superconductor , TANMOY DAS, JIAN-XIN ZHU, A.V. BALATSKY, M.J. GRAF, Theoretical Division, Los Alamos National Laboratory — Spatially resolved NMR experiments, which probe the local electronic excitations, play a vital role for studying the pairing symmetry of unconventional superconductors. Here we calculate the spatial modulation of the NMR spin-lattice relaxation rate (1/T1) for the Swiss cheese model as a function of impurity concentration in PuCoGa5 superconductor. The local suppression of the superconducting order parameter due to impurities is related to the number of holes in the Swiss cheese model. Our results indicate that Friedel-like oscillations,as seen in the local-density of states near an impurity, are also present in the behavior of 1/T1 as one moves away from the impurity site. We demonstrate that the gap nodes, which are filled by disorder, can be probed by NMR through the local information encoded in the spectra. The advantage of spatially resolved NMR compared to STM measurements is that the former probe is not sensitive to surface states. Work is supported by US DOE.

K1.00216 Sun Oven Grown Cuprates Superconductivity and Periodic Lattice Distortions PLD[1] , JUANA V. ACRIVOS, San Jose State University, J.G. CHIDVINADZE, Andronikashvili Institute Tbilisi, D.D. GULANOVA, Sun Physics Acad Sci Uzbekistan, D. LOY, San Jose State University — $Bi_{1.7}Pb_{0.3}Sr_2Ca_{n-1}Cu_nO_{4+2n+\delta}$ identified by the layer heavy element composition with substitution, s (2_s:2:n-1:n$\geq$2) cuprates grown by green chemistry, transition temperatures to superconductivity T_c=87 to 150K are related to their structure. Enhanced XRD at energies near but below the Cu K, and Pb and Bi L3-edges for pure n=2, 3 phases show Darwin shaped preferred [HKL] reflections that identify the magnitude of the allowed transition moment from the core state to extended unoccupied states determined by the electron density symmetry in that plane, confirmed by XAS of 3μm thick films. Weak PLD are still detected, but the stability gained by substitution of Bi by Pb is the formation of nearly symmetric Pb_8 cubes in $(2_s$:2:1:2$)_{13}$and $(2_s$:2:2:3$)_{17}$ super-lattices. The preferred 2D [HKL] reflection planes play the same role in the chemical activity of 3D solids as the linear bonds do in molecular reactions, governed by scattering dependent on the electron density symmetry in their highest and lowest unoccupied states.

[1]Supported by US NSF, Dreyfus, DOE Laboratories SSRL-SLAC, STUC-Ukraine and Georgia NSF.

K1.00217 Distribution of Co-dopants in LaFe1-xCoxAsO single crystals , JIAQIANG YAN, Ames laboratory, US-DOE, Ames, IA 50010, R.W. MCCALLUM, T.A. LOGRASSO — LaFe1-xCoxAsO single crystals have been grown in NaAs flux under ambient pressure. The content and distribution of Co-dopants were studied with wavelength dispersive x-ray spectroscopy. The plate-like single crystals consisit of multilayers with the thickness about 2 μm. No variation of Co content was observed in one single layer. However, Co content was observed to change gradually along the thickness (or z-) direction, which suggests layer-by-layer growth mechanism. The relation between the Co-content in crystals and starting materials was developed and the distribution coefficient of Co-dopants was estimated to be around 0.60.

K1.00218 Epitaxial growth of the electron-doped $Sr_{1-x}La_xCuO_2$ by magnetron spattering , KEITA SAKUMA, HIROYUKI AKATSUKA, TETSUYA MIYAWAKI, KENJI UEDA, HIDEFUMI ASANO, Department of Crystalline Materials Science, Nagoya University — The electron-doped $Sr_{1-x}La_xCuO_2$ (SLCO) has the simplest structure among high temperature superconductors (HTS). In addition, transition temperature of SLCO is the highest among electron-doped HTS. Therefore, SLCO is suitable for fundamental researches and electronic applications. Several groups reported growth of c-axis oriented SLCO thin films on various substrates, however a-axis oriented SLCO thin films, which are useful for superconductor junctions, have not been obtained. In this study, we deposited SLCO thin films on various substrates [(001) $KTaO_3$(KTO), $SrTiO_3$(STO), MgO and $LaAlO_3$(LAO)] by magnetron sputtering. KTO and STO have better lattice matching to SLCO[100] compared with MgO and LAO. SLCO thin films on KTO and STO were c-axis obtained. On the other hand, SLCO thin films on MgO and LAO were (101) and$a$-axis oriented, respectively. We considered that the differences of crystal orientations in these films were caused by lattice matching to the substrates. These results indicated that we can control crystal orientation of SLCO thin films using substrates with various lattice constants.

K1.00219 Superconductivity in $Zr_2(Co_{1-x}M_x)$ (M = Cu, Ga)[1] , K.J. SYU, C.H. WU, H.H. WU, S.C. CHEN, H.H. SUNG, W.H. LEE, National Chung Cheng University, W.H. LEE TEAM — As revealed in the powder x-ray diffraction and crystallographic data, the body-centered tetragonal structure of the parent compound Zr_2Co is retained in both $Zr_2(Co_{1-x}Cu_x)$ and $Zr_2(Co_{1-x}Ga_x)$ systems with the solubility limit near $x = 0.3$. The refined lattice parameters indicate that there is a movement for c to decrease and a to increase, due to the doping with Cu or Ga in the compound. Since the percentage change in lattice parameters c and a is comparable, a prominent peak in the unit cell volume v versus x curve therefore appears around$x = 0.15$ and $x = 0.2$ for $Zr_2(Co_{1-x}Cu_x)$ and $Zr_2(Co_{1-x}Ga_x)$ systems, respectively. Magnetic and electrical measurements show that there is an explicit maximum T_c close to $x = 0.05$ for both systems. As compared with the $Zr_2(Co_{1-x}Ni_x)$ system[1], it may imply that the superconducting transition temperature in $Zr_2(Co_{1-x}Cu_x)$ and $Zr_2(Co_{1-x}Ga_x)$ relate more to the spin density fluctuations than to the density of states at the Fermi level. [1]M. Takekuni, H.Sugita and S. Wada, Phys. Rev. B **58**, 11698 (1998).

[1]Supported by the National Science Council of Republic of China under grant numbers NSC 99-2112-M-194-006-MY3 and NSC99-2811-M-194-021.

K1.00220 Plausible loop currents in the GdBCO pseudogap phase , C. BOEKEMA, San Jose State University, T. SONGATIKAMAS, Santa Clara University, M.C. BROWNE, San Jose State University — For the cuprate pseudogap phase, Varma [1] predicts loop currents above T_c. We search for fields near 100 Oe, created by such currents in $GdBa_2Cu_3O_{7-\delta}$ (GdBCO). Using MaxEnt-Burg (ME) we analyze zero-field (ZF) muon-spin-rotation (μSR) data of underdoped (δ1; T_c= 81 K) and optimal doped (δ0; T_c= 93 K) GdBCO. [2] ME-μSR applied to ZF-GdBCO data yields T-dependent signals at 0-MHz (f0) and 0.3-MHz (f1) and hints of 1.4-MHz signals. To cancel any systematic (f1) effect, we analyze DS(t,T) = S(t,T>T_c) - S(t,T'<<T_c). This ME-Burg analysis of GdBCO(δ0 & δ1) indicates weak signals near 1.4 MHz above T_c (and f1 disappears). These ME-peaks occur at $\sim$1.3 MHz (95 Oe) for GdBCO(δ1) and $\sim$1.5 MHz (110 Oe) for GdBCO(δ0). These μSR signals, plausibly due to fields created by loop currents, appear only above T_c. Below T_c, only ME background noise exist in DS(t,T) transforms. The $\sim$1.4-MHz peak intensity to background ratio at its maximum is $\sim$5 for GdBCO(δ1) and $\sim$4 for GdBCO(δ0) at $\sim$10 degrees above T_c. Validating predicted loop currents is essential for understanding the pseudogap phase. Research supported by REU NSF & DOE LANL. [1] CM Varma, Phys Rev Lett 83 (1999) 3538; [2] T Songatikamas et al, J Supercond & Novel Magn 23 (2010) 793.

K1.00221 Modeling Superconducting properties of an inhomogeneous mixture of doped metallic and semiconductor carbon nanotubes , ILYA GRIGORENKO, Penn State University, ANVAR ZAKHIDOV, The University of Texas at Dallas — We considered theoretically the superconducting properties of a bundle of boron-doped carbon nanotubes, which consists of two types of nanotubes: semiconducting and metallic. The tubes are assumed to be close-packed, making a hexagonal lattice in the transverse section of the bundle. The properly doped semiconducting nanotubes are assumed to have a higher transition temperature than metallic because of the lower lying Van Hove singularities in the DOS (proven in experimentally found Kataura plot). We used an inhomogeneous microscopic model to describe the proximity effects between the two different types of tubes, and calculated the averaged superconducting critical temperature for the bundle given a ratio between the metallic and semiconductor nanotubes. We found that the critical temperature scales approximately quadratically as a function of the ratio. We also discuss briefly the possible effect of metallic nanotubes on the suppression of the phase fluctuations in 1-D superconducting pairing in properly doped semiconducting nanotubes.

K1.00222 Study of Mini-Gap Regime in Au Nanowires[1] , BRIAN COOPER, The Pennsylvania State University, JIAN WANG[2], MOSES CHAN, MEENAKSHI SINGH, MINGLIANG TIAN, JAINENDRA JAIN, The Pennsylvania State University — The inducement of superconductivity in 70nm single crystal Au nanowires (AuNWs) via the Proximity Effect was reported in 2009 [Wang, J. et al. *Phys. Rev. Lett.* **2009**, 102, 247003]. This study, carried out on 3 AuNWs of different lengths (1.0, 1.2 and 1.9 μm), showed a precipitous drop in the resistance to a fully superconducting state of the 1.0um wire; while the 1.2μm wire made the transition in 2 steps, and the 1.9μm wire never fully transitioned to a zero resistance state. This behaviour lead to the coinage of the so-called "mini-gap" phase in proximity induced superconducting nanowires. We are currently investigating the robustness of this "mini-gap" regime by parametric variations to the gold nanowire system. Looking at features such as crystallinity, AuNW diameter, electrode material, and directional magnetic field dependence, we are attempting to further illuminate the nature of this new "mini-gap" state.

[1]Penn State MRSEC under NSF grant DMR-0820404
[2]The Pennsylvania State University

K1.00223 Coherent pairing and phase separation in small negative U Hubbard nanoclusters away from half filling , KALUM PALANDAGE, Trinity College, Hartford, GAYANATH FERNANDO, Department of Physics, University of Connecticut, Storrs, ARMEN KOCHARIAN, Department of Physics, California State University, Los Angeles — The similarities and differences in the mechanism of electron pairing instabilities, driven by attractive and repulsive electron interaction, are studied in the ensemble of small clusters for one hole off half filling under variation of interaction strength and temperature. These exact calculations of charge and spin collective excitations, and corresponding critical transition temperatures yield intriguing insights into the level crossing degeneracies, phase separation transitions, condensation and formation of spatial inhomogeneities in various cluster geometries [Ultramicroscopy 109, 1066 (2009)]. Separate condensation of electron charge and spin degrees in negative U model away of half filling offers a new route for the mechanism of superconductivity in inhomogeneous systems, different from the quasi-particle BCS scenario for electron condensation. Phase diagrams resemble a number of inhomogeneous, coherent and incoherent nanoscale phases seen in various positive Hubbard cluster geometries in high Tc cuprates, iron pnictides, and other transition metal oxides.

K1.00224 Dynamics of an RF-driven Josephson junction near the bifurcation point , AMRIT POUDEL, MAXIM VAVILOV, University of Wisconsin-Madison — We investigate the dynamics of an RF driven Josephson junction coupled to thermal heath bath. We present a stochastic semiclassical equation of motion for the junction, obtained from a microscopic Hamiltonian of the system. We discuss conditions when the Langevin forces in this equation can be approximated by Markovian white noise. For this case, we obtain the Fokker-Planck equation, which we numerically solve to describe the switching process between two stable states near the bifurcation point.

K1.00225 Effects of 3d magnetic metal substitutions (Fe, Co, Ni) for V on superconducting T_c of the ZrV_2 system[1] , WUN-HSIN LEE, D.H. CHEN, K.J. SYU, S.C. CHEN, H.H. SUNG, National Chung Cheng University, W.H. LEE TEAM — The effects of Fe, Co and Ni substitution on the crystallographic data and superconducting transition temperature (T_c) of ZrV_2 have been investigated through powder x-ray diffraction, static magnetization and electrical-resistivity measurements. Variation of the room temperature refined lattice parameters indicate that there is a movement for a and unit cell volume v to decrease, linearly with increasing x up to 0.4, for the $Zr(V_{2-x}T_x)$ (T = Fe, Co and Ni) alloys. Magnetic and electrical measurements show that the superconducting transition temperature (T_c) of ZrV_2 is reduced by the doping of Fe, Co and Ni with depression rate $dT_c/dx \sim$ -14, -17.5, and -15 K/atom %, respectively. The doping of Co has a larger effect than Fe and Ni on the decrease of T_c.

[1]Supported by the National Science Council of Republic of China under grant numbers NSC 99-2112-M-194-006-MY3 and NSC99-2811-M-194-021.

K1.00226 Superconducting Properties of Lead-Bismuth Films Controlled by Ferromagnetic Nanowire Arrays , ZUXIN YE, IGOR F. LYUKSYUTOV, WENHAO WU, DONALD G. NAUGLE, Department of Physics and Astronomy, Texas A&M University — Superconducting properties of lead-bismuth (82% Pb and 18% Bi) alloy films deposited on ferromagnetic nanowire arrays have been investigated. Ferromagnetic Co or Ni nanowires are first electroplated into the columnar pores of anodic aluminum oxide (AAO) membranes. Superconducting $Pb_{82}Bi_{18}$ films are then quench-condensed onto the polished surface of the AAO membranes filled with magnetic nanowires. A strong dependence of the $Pb_{82}Bi_{18}$superconducting properties on the ratio of the superconducting film thickness to the magnetic nanowire diameter and the material variety was observed.

K1.00227 Magnetic nanorod - superconductor hybrid near the superconducting transition temperature , K. KIM, I. LYUKSYUTOV, D.G. NAUGLE, Department of Physics, Texas A&M University, College Station, TX77843, USA — We report measurements of the magnetoresistance and phase diagram of a lead-bismuth (82% Pb and 18% Bi) superconducting film with an embedded square array of Ni nanorods near the superconducting transition temperature. Magnetoresistance above Tc demonstrates oscillations compatible with flux quantization through the unit cell of the magnetic nanorod array. Strong hysteresis of the superconducting properties and an apparent increase of the second critical field is found.

K1.00228 Description of a primitive valley scattering unit cell to understand anisotropic inter-valley scattering in AlAs quantum wells , S. PRABHU-GAUNKAR, M. GRAYSON, Northwestern University — Valley degenerate systems have an extra scattering channel not present in single valley systems, namely inter-valley scattering. To help classify anisotropic inter-valley scattering in degenerate multi-valley systems, such as AlAs quantum wells (QWs), we define a valley scattering primitive unit cell in momentum space which allows one to distinguish purely in-plane momentum scattering from scattering requiring an out-of-plane momentum component. The standard depiction of a 2D Brillouin zone of a quantum confined valley-degenerate system projects all valleys to a single plane and this depiction loses information about the momentum scattering component that was projected out. Because QW confinement potentials are inherently anisotropic, the disorder potential characteristic of quantum confinement can create anisotropic short-wavelength inter- valley scattering potentials favoring in-plane momentum scattering. We demonstrate that the valley scattering cell for AlAs QWs grown along various orientations is particularly useful in identifying relevant scattering vectors. Initial estimates will be shown of the role of strong electron-electron interactions in AlAs QWs on inter-valley scattering parameters such as inter-valley scattering time, probabilities and rates.

K1.00229 Analytical approach to neutron scattering on solitons in low dimensional systems , IRINA BARIAKHTAR, APS/Boston College, YAROSLAV NAZARENKO, Brown University — It is well known that neutron scattering, along with x-ray scattering, allows for the study of condensed matter system structures. Recently, it was revealed that in magnetic materials some nonlinear formations such as solitons of the topological type of excitation - kinks, solitons with zero topological charge - breathers, and solitons with linear excitation, analogous to spin waves, may arise. In this paper, we present the polarized neutron scattering approach for the study of such formations in magnetic materials. The formulas for the cross sections of scattering in the low-dimensional systems with solitons were obtained. We have presented the calculations for kink type solitons. Similar calculations can also be presented for breather-type solitons. We have shown that the study of neutron polarization after scattering provides for the possibility of gathering information on the static and dynamic properties of the solitons and allows for restoring of the magnetic momentum distribution in the solitons. We hope that such calculations will stimulate the formulation of a series of experiments where solitons can be experimentally observed.

K1.00230 THz imaging system with the IJJ emitter[1] , MANABU TSUJIMOTO, HIDETOSHI MINAMI, MASASHI SAWAMURA, KAVEH DELFANAZARI, TAKASHI YAMAMOTO, TAKANARI KASHIWAGI, KAZUO KADOWAKI, University of Tsukuba — The intrinsic Josephson junction (IJJ) emitter consisted of thousands of IJJs uniformly stacked in single crystalline high-T_c superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi-2212) [L. Ozyuzer *et al.*, Science **318**, (2007) 1291.] is expected to be a novel source of the continuous terahertz electromagnetic waves (THz-waves). The maximum emission power of tens of microwatts recently obtained with the mesa structure of IJJs seems to be sufficient to make use of the IJJ emitter for some practical applications such as THz imaging. According to the cavity resonance condition, we can control the radiation frequency by changing the geometrical size of the mesa. In this study, we develop the THz imaging system with IJJ emitter. In the presentation, we will show some transparent images of standard specimens obtained by the raster scanning method. Also, we will mention some problems to be solved for the future applications of the IJJ emitter.

[1]CREST-JST, WPI-MANA, Strategic Initiative A (University of Tsukuba)

K1.00231 Front instabilities, confinement effect and fracture in drying colloidal nanoparticle , DEEDER AURONGZEB, The University of Akron, Department of Polymer Science. — Drying colloidal suspension of oxide nanoparticle can fracture in fractal patterns. While similar in size TiO_2 and Al_2O_3 particles can fracture differently. We found that Alumina nanoparticle forms radially inward crack from the edge of the droplet or planer film like fluid while Titania nanoparticle form fractal cracks. Using polarized light we observe stress field formation during evaporation and crack growth. We find that crack direction is driven by surface tension rather than thermal energy of the suspended nanoparticle. Evaporation based nanoparticle assemble and effect of confinement and electric current will be also discussed.

K1.00232 High-Pressure Studies of Valence and Magnetic State in Europium Metal[1] , W. BI, G. FABBRIS, J. SCHILLING, Physics Department, Washington University in Saint Louis, N. SOUZA-NETO, D. HASKEL, J. ZHAO, E. ALP, Advanced Photon Source, Argonne National Lab, Y. MENG, HPCAT, Carnegie Institution of Washington, Argonne National Laboratory, A. ALSMADI, Hashemite University — The strong local-moment magnetism in divalent Eu metal ($4f^7$) suppresses superconductivity. At extreme pressure Eu is expected to become trivalent and nonmagnetic ($4f^6$). Recently, superconductivity in Eu was discovered by Debessai *et al.* for pressures above 80 GPa [1]. However, Eu's transition temperature lies near 2 K, nearly an order of magnitude lower than for comparable trivalent d-electron metals, possibly because Eu is not fully trivalent but rather mixed valent. Here we report recent experimental results on Eu's valence and magnetic state to Mbar pressures through synchrotron x-ray absorption near edge structure (XANES), synchrotron x-ray magnetic circular dichroism (XMCD), and synchrotron Mössbauer spectroscopy (SMS).

[1] M. Debessai, T. Matsuoka, J. J. Hamlin, J. S. Schilling, and K. Shimizu, Phys. Rev. Lett. 102, 197002 (2009).

[1]This research is supported by NSF grant DMR-0703896 and by the Carnegie/DOE Alliance Center (CDAC) through NNSA/DOE grant number DE-FC52-08NA28554.

K1.00233 Hybrid Rings for circuit Quantum Electrodynamics , E. HOFFMANN, F. DEPPE, T. NIEMCZYK, E. P. MENZEL, G. WILD, H. HUEBL, M. MARIANTONI, A. MARX, R. GROSS, Walther-Meissner-Institut and TU Muenchen, Garching, Germany, T. WIRTH, A. LUKASHENKO, A. USTINOV, Karlsruher Institut fuer Technologie (KIT), Karlsruhe, Germany, A. P. ZHURAVEL, B. I. Verkin Institute for Low Temperature Physics and Engineering, Kharkov, Ukraine — Experiments in the field of circuit QED require detection schemes for microwave signals on the single photon level. In particular, devices acting as microwave beam splitters are necessary. Using Nb thin films on silicon and sapphire substrates, we fabricated superconducting 180° microstrip hybrid rings acting as beam splitters with center frequencies of about 6 GHz. For the magnitude of the coupling and isolation we find -3.5 ± 0.5 dB and at least -15 dB, respectively, in a bandwidth of 2 GHz. We also investigate the effect of reflections at the contact between the superconducting hybrid ring and the normal conducting wiring using low temperature laser scanning microscopy. Our measurements indicate that our hybrid rings are well suited for on-chip applications in circuit QED experiments. We acknowledge financial support by the DFG via SFB 631, as well as support by and CFN, EU project SOLID and the German Excellence Initiative via NIM.

K1.00234 Magnetic behaviors in Fe(Se,Te) system , HONGLIANG SHI, Beijing Computational Science Research Center, BEIJING COMPUTATIONAL SCIENCE RESEARCH CENTER TEAM — The magnetic behaviors in Fe(Se,Te) system are investigated systematically by using the density functional theory. Our results show that for FeSe and FeTe in their respective ground state with different magnetic configurations, the easy axis of magnetization does not have any obvious preference. As for $FeSe_{0.5}Te_{0.5}$, in the collinear calculation only setting the values of magnetic moments, the ground state is in the "double stripe" magnetic phase; while the "single stripe" magnetic arrangement is found to be the ground state if the easy axis of magnetization is considered in our calculations. Our spiral calculations also successfully predict the commensurate (0.5, 0.5) ordering observed in $FeSe_{0.5}Te_{0.5}$ system experimentally. Furthermore, two incommensurate excitations near (0.5, 0.5) are also reproduced in the spin spiral states compared with the diagram of scattering plane obtained by neutron scattering.

K1.00235 Synthesis and superconductivity in Li-Fe-As-N[1] , H.H. SUNG, K.J. SYU, S.C. CHEN, W.H. LEE, National Chung Cheng University, W.H. LEE TEAM — The preparation of LiFeAs compound either in polycrystal or single crystal form is difficult to handle due to its reactivity with air and sensitivity to moisture of lithium. In this report we use Li_3N, Fe and As as starting materials. During the heating process, no high pressure, no Ta, Nb or W tube, is required to synthesize the polycrystalline sample. The crystallographic data and superconducting transition temperature (T_c) of the samples as prepared have been investigated through powder x-ray diffraction, magnetization and electrical-resistivity measurements. Discussion will be directed toward the influence of N on the superconductivity in Li-Fe-As from the viewpoint of pinning or substitute effect.

[1]Supported by the National Science Council of Republic of China under grant numbers NSC 99-2112-M-194-006-MY3 and NSC99-2811-M-194-021.

K1.00236 Evidence for intrinsic vortex pinning in 1111 Fe arsenides single-crystals , GANG LI, GAEL GRISONNANCHE, BENJAMIN CONNER, National High Magnetic Field Lab, NIKOLAI ZHIGADLO, SERGIY KATRYCH, ZBIGNIEW BUKOWSKI, JANUSZ KARPINSKI, Laboratory for Solid State Physics, ETH Zürich, CH-8093 Zürich, Switzerland, LUIS BALICAS, National High Magnetic Field Lab — We performed a study of the angular dependence of the magnetic torque $\tau(\theta)$ in $LaFeAsO_{0.9}F_{0.1}$ and in $SmFeAsO_{0.9}F_{0.1}$ single crystals. Here, θ is the angle between the magnetic field and inter-plane c-axis. As the temperature is lowered, one observes the emergence of sharp features in the magnetic torque for fields nearly aligned along the conducting planes. In particular, one observes two sharp peaks at a critical angle θ_c placed respectively slightly above and below $\theta = 90^\circ$, in the reversible component of the torque. Their position in angle, relative to $\theta = 90^\circ$, decreases as the field increases, and increases as the temperature is lowered. We conclude that θ_c corresponds to a critical pinning angle whose behavior is consistent with theoretical predictions for the intrinsic pinning of vortices by a layered crystallographic structure. However, in sharp contrast with the cuprates, in the region of temperatures where this behavior is observed the superconducting anisotropy of 1111 Fe arsenides is rather small, as measured by torque magnetometry.

K1.00237 Investigation of the role of spin-orbit coupling on transport properties of iron pnictide materials[1]

, SUDHAKAR PANDEY, HIROSHI KONTANI, DAI HIRASHIMA, Nagoya University, Japan, RYOTARO ARITA, HIDEO AOKI, University of Tokyo, Japan — A generic feature associated with the electronic structure of iron pnictides and chalcogenides, which are currently under intense investigation for their superconducting properties, is that the 3d orbitals of Fe make dominant contribution to density of states near the Fermi level. Incorporating this along with other realistic band features within a multiband tight-binding model, we investigate the role of atomic spin- orbit coupling associated with the 3d orbitals on the transport properties of these materials. Our investigation highlights the importance of some characteristic features associated with the electronic band, such as accidental degeneracy, Dirac cone, and orbital hybridization. we find significantly large spin Hall conductivity in the paramagnetic state that is comparable with Pt. We also find finite anomalous Hall conductivity in the ferromagnetic state.

[1]S P acknowledges the financial support from JSPS .

K1.00238 Anisotropic structural and magnetic properties of the field-aligned superconducting system $SmFeAsO_{1-x}F_x$ (x = 0.05, 0.1, 0.2, 0.25, and 0.3)[1]

, Y.B. YOU, J.W. WANG, M.F. TAI, H.C. KU, Dept. of Physics, National Tsing Hua University, Hsinchu, Taiwan, Y.Y. HSU, Dept. of Physics, National Taiwan Normal University, Taipei, Taiwan — Anisotropic structural and magnetic properties of the field-aligned superconducting system $SmFeAsO_{1-x}F_x$ (x = 0.05, 0.1, 0.2, 0.25, 0.3) are reported. Due to the Fe spin-orbital related anisotropic exchange coupling, all the tetragonal microcrystalline powders in epoxy were aligned at room temperature using the field-rotation method where the tetragonal ab-plane is parallel to the magnetic alignment field B_a of 0.9 T and the c-axis parallels to the rotating axis. Anisotropic magnetic properties are studied through low temperature magnetic measurements along the c-axis and paralleled to the ab-plane of aligned samples in both ZFC and FC modes. The under-doped compound (x = 0.1) is not superconducting with an antiferromagnetic Néel temperature $T_N \sim$ 40K, while the two optimum-doped compounds (x = 0.2 and 0.25) show high superconducting transition temperatures T_c of 49K and 50K, respectively. The variation of anisotropic structural and magnetic properties for this system are discussed and compared with the previously reported 52 K anisotropic superconductor $Sm_{0.95}La_{0.05}FeAsO_{0.85}F_{0.15}$.

[1]This work was supported by NSC98-2112-M-007-013-MY3.

K1.00239 COMPLEX STRUCTURED MATERIALS II —

K1.00240 The effects of asymmetric configurations on electronic properties of bilayer graphene nanoribbons[1]

, Y. -C. HUANG, Center for General Education, Kao Yuan University — Low-energy electronic properties of bilayer graphene nanoribbons subject to the effects of asymmetric configurations are studied by using the tight-binding model. They are strongly dependent on the interlayer interactions, the ribbon edges, the ribbon width (N_y), and the upper ribbon displacement (N_D). The interlayer interactions significantly modify the energy dispersions, alter the subband spacing, change the subband curvature, produce the new edge state, and induce asymmetry of energy bands. There are partial flatbands at the Fermi level and one-dimensional parabolic bands at others. These make density of states (DOS) exhibit delta- function-like structure and asymmetric prominent peaks, respectively. Energies of the extra band-edge states can be tuned by varying the upper ribbon displacement. As N_D grows from zero, the new edge states show a tendency to increase near low energy, while the curvature of the extra band-edge states display bold change about Fermi level E_F. The above-mentioned effects are completely reflected in the features of DOS, such as the generation of special structures, the shift of peak position, and the change in peak height. The predicted electronic properties could be examined by the experimental measurements on absorption spectra.

[1]This project is financially sponsored by NSC (99-2112-M-244-001-MY2)

K1.00241 Kronig-Penney Model of Graphene in a Magnetic Field of Arbitrary Strength

, NORMAN HORING, Stevens Inst. Tech., SINA BAHRAMI, Stevens Inst. Tech — We address the magneto-dynamics of a 2D graphene sheet with a one dimensional periodic array of quantum wires, using a Kronig-Penney type model. In particular we examine the role a normal magnetic field inducing Landau quantization effects in terms of a closed form integral representation involving only elementary functions which incorporates the full spectrum of magnetic-quantized graphene states and energies.

K1.00242 Effective Magnetic Fields in Graphene Superlattices[1]

, HERBERT FERTIG, JIANMIN SUN, Indiana University, LUIS BREY, Instituto de Ciencia de Materiales de Madrid — We demonstrate that the electronic spectrum of graphene in a one-dimensional periodic potential will develop a Landau level spectrum when the potential magnitude varies slowly in space [1]. The effect is related to extra Dirac points generated by the potential whose positions are sensitive to its magnitude. We develop an effective theory that exploits a chiral symmetry in the Dirac Hamiltonian description with a superlattice potential, to show that the low energy theory contains an effective magnetic field. Numerical diagonalization of the Dirac equation confirms the presence of Landau levels. Possible consequences for transport are discussed.

[1] Jianmin Sun, H.A. Fertig, and L. Brey, Phys. Rev. Lett. **105**, 156801 (2010).

[1]Support provided by the NSF through Grant No. DMR-1005035, and by MEC-Spain via Grant No. FIS2009-08744.

K1.00243 Graphene Energy Loss Spectroscopy for Perpendicular Particle Incidence

, VASSILIOS FESSATIDIS, ANTONIOS BALASSIS, Fordham University, NORMAN J.M. HORING, Stevens Institute of Technology — In this work we determine the energy loss of a fast charged particle probe moving perpendicular to a two-dimensional ($2D$) graphene sheet. The response dynamics of the $2D$ graphene sheet are modeled using the random phase approximation in the degenerate limit (zero temperature). We analyze the energy loss of the probe particle for normal incidence to the graphene sheet as a function of its velocity, examining contributions from both the particle-hole and plasmon excitations.

K1.00244 Ab initio Calculations of Geometric and Electronic Structure of Graphene-Au System

, ROBERTO NUNEZ-GONZALEZ, Dept. de Matemáticas, Universidad de Sonora, DONALD H. GALVAN, Centro de Nanociencias y Nanotecnología,Unam, ALVARO POSADA-AMARILLAS, Dept. de Inv. en Física, Unison — Structural and electronic properties of graphene with one gold atom at top were calculated using the Full-Potential Augmented Plane Waves with Local Orbitals Method and the local density approximation (LDA), within the Density Functional Theory. For the calculations, we use a 3x3x1 supercell of graphene, calculating the stability of the system with the gold atom at three different sites: Hole, Bridge and Top sites. For each site, the atoms are relaxed minimizing forces. An analysis of the structural properties is performed for each site, calculating the density of states (DOS). A comparison with pure graphene is realized.

K1.00245 Geometric and Electronic structures of deformed bilayer graphenes , JEN-HSIEN WONG, Department of Physics, National Cheng Kung University, Tainan, Taiwan, BI-RU WU, Department of nature science, Center for General Education, Chang Gung University, Taoyuan, Taiwan, MING-FA LIN, Department of Physics, National Cheng Kung University, Tainan, Taiwan — The electronic properties of bilayer AB-stacked graphene are investigated with a first-principles method when homogeneous and uniaxial strains are exerted. The two types of strains can be either tensile or compressive. The maximum deformation ratio is 36% for tensile strain, and 20% for compressive strain. The uniaxial strains along the armchair (A strain) or zigzag (Z strain) directions are considered. Bilayer AB-stacked graphene belongs to semimetal essentially. One pair of π bands owns two intersections near the Fermi level. One intersection lies at K point; the other one is near K point along the path of Γ to K. The π band overlap is approximately 2.6meV. No gap will be developed for bilayer graphene under homogenous strain or A strain. Nevertheless, tensile Z strain results in a tiny indirect band gap near R point.

K1.00246 Magneto-electronic specific heat of graphene[1] , SHIH-YANG LIN, Physics, National Cheng Kung University, Tainan, Taiwan, YEN-HUNG HO, Physics, National Sun Yat-Sen University, Taiwan, MING-FA LIN, Physics, National Cheng Kung University, Tainan, Taiwan, YUAN-CHENG HUANG, Center for education, Kao Yuan University, Kaohsiung, Taiwan — The electronic specific heat related to the Landau levels of monolayer graphene is studied by the Peierls tight-binding model. The low-temperature thermal properties are dominated by the two low-lying Landau levels with the Zeeman splitting. They give rise to rich temperature and magnetic-field dependence. The T-dependent specific heat reveals the composite form of 1/T and exponential function. Also, a prominent peak appears in the T-dependent (B-dependent) spectrum with its critical temperature T_c (critical magnetic field B_c). Moreover, there has a simple linear relationship between $T_c$and B_c. In a slightly doped graphene, there exists an extra shoulder structure in the specific heat. Such structure mainly comes from the Zeeman effect and temperature-dependent carrier distribution.

[1]NSC 99-2112-M-244-001-MY2

K1.00247 Electronic structure of a realistic model of amorphous graphene , VITALIY KAPKO, AVISHEK KUMAR, Arizona State University, DAVID DRABOLD, Ohio University, MICHAEL THORPE, Arizona State University — We calculate the electronic properties of a realistic atomistic model of amorphous graphene. The model contains odd-membered rings, particularly five and seven membered rings and no coordination defects.We show that odd-membered rings increase the electronic density of states at the Fermi level relative to crystalline graphene; a honeycomb lattice with semimetallic character. Some graphene samples contain amorphous regions, which even at small concentrations, may strongly affect many of the exotic properties of crystalline graphene, which arise because of the linear dispersion and semi-metallic character of perfectly crystalline graphene. Estimates are given for the density of states at the Fermi level using a tight-binding model for the π states. We also report preliminary density functional results for the electronic structure.

K1.00248 Vibration analysis of Graphene embedded in ordered fluids using Raman spectroscopy , MIN SANG PARK, School of Material Science and Engineering, Georgia Institute of Technology, KARTHIK NAYANI, School of Material Science and Engineering, Georgia Institute of Technolgy, JUNG OK PARK, MOHAN SRINIVASARAO, School of Material Science and Engineering, Georgia Institute of Technology — We studied the vibrational characteristics of both single- and multi-layered Graphene embedded in liquid crystal (LC), possessing various ordered phases, by polarized micro-Raman spectroscopy. The evolution of the vibrational modes (G and 2D bands) was studied in 8CB in the isotropic, nematic and smectic A phases. The shifts in the vibrational modes are discussed in the context of the phase transition in the LC system.

K1.00249 localization of plasmonic excitations in graphene induced by nanoscale potential , JUNG-JUNG SU, Theoretical Div., Los Alamos Natl. Lab., HARI DAHAL, American Physical Society, RODRIGO MUNIZ, STEPHAN HAAS, Dept. of Phys. and Astro., Univ. of Southern California, ALEXANDER V. BALATSKY, Theoretical Div., Los Alamos Natl. Lab. — The near-ballistic transport property at close to room temperature makes graphene a strong candidate for integrated nanoelectronic application. Graphene-based plasmonics is one of the devices proposed that integrate electronic and light transport. By utilizing localized plasmonic excitation, plasmonics can transport light with a sub-wavelength dimension. We report our calculation on plasmonic excitation induced by different local structures. The polarization obtained by random-phase-approximation (RPA) is diagonalized to extract plasmon modes. We have also studied the effect due to gating and due to tunning of local potential structure geometry. These prediction can be tested by scanning tunneling microscope and is important both in fundamental and in application aspects.

K1.00250 Adsorption of water on a carbon-gold surface[1] , FERNANDO MAGAÑA, GERARDO J. VAZQUEZ, Instituto de Física, Universidad Nacional Autónoma de México — Density functional theory and molecular dynamics were used at 300 K to study first the interaction of a gold atom (Au) with a graphene layer with a vacancy. The Au Atom is adsorbed on the vacancy then we studied the adsorption of H_2O on the Au anchored on the vacancy of graphene. We found that the water molecule is adsorbed on such configuration and it is not even dissociated at high temperatures like 1000 K.

[1]We acknowledge partial finantial support by DGAPA-UNAM through grant. No. IN111807 and the technical assistance Kanbalam supercomputer center, UNAM.

K1.00251 The interaction of mercury with halogenated graphene[1] , ABIGAIL KIRCHOFER, ERDEM SASMAZ, JENNIFER WILCOX, Stanford University — The interaction of mercury with halogenated graphene was studied using plane-wave density functional theory. Various configurations of H, Hg, O and Br or Cl on the zigzag edge sites of graphene were investigated. Although Hg-Br (or -Cl) complexes were found to be stable on the surface, the most stable configurations found were those with Hg adjacent to O. The surface atoms Hg, O, and Br tend to repel each other during geometric optimization, moving towards an H atom nearest-neighbor where possible. The strength of the Hg-graphene interaction is very sensitive to the local environment. The Hg-graphene binding energy is strongest when the Hg is located next to a surface O but not immediately next to a bound Br. DOS analysis revealed that Hg adsorption involves a gain in Hg 6 p-states and a loss in Hg 5 s electron density, resulting in an oxidized surface-bound Hg complex. DOS analysis suggests that Br strengthens the Hg-graphene interaction by modifying the surface carbon electron density; however, when Br is adjacent to Hg, a direct Hg-Br interaction weakens the Hg-C bond. These investigations provide insight into the mechanism associated with enhanced Hg adsorption on Br-functionalized carbon materials for Hg emissions reductions from coal-fired power plant applications.

[1]The authors acknowledge the financial support by Electric Power Research Institute (EPRI).

K1.00252 Electric-field induced modification of Landau levels in graphene nanoribbon[1] , HSIEN-CHING CHUNG, Department of Physics, National Cheng Kung University, YUAN-CHENG HUANG, Center for General Education, Kao Yuan University, MING-FA LIN, Department of Physics, National Cheng Kung University — The low energy magneto-ectronic properties of one-dimensional graphene nanoribbons are investigated by the Peierls tight-binding model with uniform magnetic and electric fields. They are mainly determined by the quantum confinement effects and the external fields. Magnetic fields result in the Landau levels (LLs), lead to the Landau wavefunctions, and enhance partial flat bands. Electric fields significantly modify the dispersionless LLs, change the band symmetry, induce more band-edge states, split the partial flat bands, and drastically alter the distribution of wavefunctions. The density of states directly reflects the main features of energy bands, such as the numbers, frequencies, heights and divergence forms of prominent peaks, which can be confirmed experimentally. The magneto-optical absorption spectra are predicted to be dramatically changed under the influence of external electric fields.

[1]NSC 99-2112-M-244-001-MY2 and NSC 95-2112-M-006-028-MY3

K1.00253 Spin-polarized energy gap opening in asymmetric bilayer graphene nanoribbons , GYUBONG KIM, Korea Institute of Science and Technology, SEUNG-HOON JHI, Pohang University of Science and Technology — Electronic and magnetic properties of bilayer zigzag graphene nanoribbon (bZGNR) are studied with the use of pseudopotential density functional method. The edge atoms in the top and bottom layers of bZGNR make a weak hybridization, which leads to band dispersion and magnetization different from monolayer ZGNR. For asymmetric bZGNR, where the top and bottom layers have different width, one edge is pinched by the interlayer bonding and the other edge sustains anti-ferromagnetic spin polarization. A small amount of charge transfer occurs from narrower to wider layer, and the band structure for each spin near the Fermi level exhibits an asymmetry. External electric field perpendicular to asymmetric bZGNR produces different energy-gap opening for each spin component, inducing half-metallicity.

K1.00254 Synthesis and Characterization of Graphene Sheets Covalently Functionalized with Polyaniline , SANJEEV MANOHAR, SRIKANTHRAO AGNIHOTRA, AKSHAY PHULGIRKAR, University of Massachusetts Lowell — Herein we report covalent functionalization of graphene oxide (GO) with conducting polymer polyaniline and aniline tetramer for the first time. The covalently functionalized rGO is electrically conducting, shows improved electrochemical properties and enhanced specific capacitance compared to rGO. We also observed enhanced thermal stability and antistatic properties can be obtained on addition of these covalently functionalized composites into the polymer matrix such as PMMA.

K1.00255 Thermoelectric Power in Dual-Gated Bilayer Graphene , CHANG-RAN WANG, VINCENT LU, WEI-LI LEE, Institute of Physics, Academia Sinica, INSTITUTE OF PHYSICS, ACADEMIA SINICA TEAM — We have performed thermoelectric transport measurements of dual-gated bilayer graphene device. The thermopower reached a maximum value of |Sm| when tuning its carrier density by gates. The |Sm| was found to monotonically increase with displacement field D introduced through the top and bottom gates. At 100K, |Sm| attains a value of $\sim$ 110 uV/K at D $\sim$ 1V/nm, which is nearly two-fold larger than that at D = 0. The detailed temperature-dependence of Sm and comparison to the resistivity data will be presented.

K1.00256 Trigonal Distortion of Valley Current in Bilayer Graphene[1] , PATRICIO VARGAS, Departamento de Física, Universidad Tecnica Federico Santa María, ALVARO NUÑEZ, Departamento de Física, FCFM, Universidad de Chile, ERIC SUAREZ, Departamento de Física, Universidad Tecnica Federico Santa María — Bilayer Graphene (BLG) is extensively explored due to its remarkably electronic properties. Its band structure has two inequivalent but degenerate points K and K' at the corners of the Brillouin Zone, because their large separation there have been proposition to use a valley index, or pseudospin to generate valley dependent currents. In BLG these currents can be created by applying an step like bias, the topology of BLG in the two zones leads to the formation of a 1D chiral zero modes transverse to the applied bias. There are two such modes per spin per valley and the current have opposite direction in each valley. We explore how the trigonal warping of BLG affects these modes. Breaking the symmetry of the unit cell in BLG opens a gap, the shape of the Berry Curvature depends of the bias applied, for very low bias (few meV) the topological charge breaks in four well defined peaks, three having the same sign and magnitude and the fourth with opposite value, the overall charge remains unaltered, these fraction charges lead to a distortion of the chiral zero modes. We calculate the currents and show how the system evolves by tuning the effect of the trigonal warping.

[1]We acknowledge FONDECYT-1100508 and CEDENNA grants from CONICYT-CHILE.

K1.00257 A Way from GHz to THz Graphene Nanosensor , YUICHI OCHIAI, AKRAM MAHJOUB, NOBUYUKI AOKI, Chiba University, JUNG WOO SONG, SUNY Buffalo, GREGORY AIZIN, CUNY Kingsborough, JONATHAN BIRD, SUNY Buffalo, DAVID FERRY, Arizona State University, YUKIO KAWANO, KOJI ISHIBASHI, ADLab, RIKEN, G-COE COLLABORATION — The unique bandstructure, and associated carrier properties, of graphene make this material of ideal interest for application as a broadly tuneable sensor, for specific application to the microwave and terahertz (THz) regime. The gapless spectrum characteristic of single-layer graphene, as well as the small forbidden gap that appears in bilayer graphene, is ideally matched to the low (meV) energy of photons near the THz regime, in marked contrast to conventional semiconductors whose relevant bandgaps are typically several orders of magnitude larger. In this presentation, we describe the results of ongoing research that is being undertaken with the objective of developing upto THz nanosensors based on graphene. We describe the preparation of graphene devices by mechanical exfoliation, after which we discuss the characterization of their electrical properties using low-temperature magneto-transport investigations [1]. These studies demonstrate the formation of open quantum-dot structures in small graphene flakes, contacted by sub-micron scale metal electrodes. The observation of quantum fluctuations in the magneto-resistance of these structures indicates the presence of quantized dot states, whose characteristics may be of use in THz sensing. [1] Y. Ujiie et al., J. Phys.: Condens. Matt. 21 (2009) 382202.

K1.00258 Photoluminescence from hydrogenated graphene[1] , VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Physics Department and NSTC, University of Central Florida, Orlando FL 32816 — We consider the optical properties of hydrogenated graphene as a function of hydrogen concentration between the graphene and graphane limits. In particular, we show that with increasing hydrogen concentration the gap in the electron density of states grows from 0 to approximately 5eV in the case of graphane. For intermediate concentrations, additional electronic states with energies smaller than 5eV appear. These states make the system optically active in the visible range. We pay special attention to the possibility of ultrafast photoluminescence in the system for different values of hydrogen concentration and hole doping. For example, for excitations by ultrafast laser pulses, the system demonstrates significant visible range photoluminescence driven by the electron-phonon interaction. In the case of graphane, the effect can be significantly enhanced by hole doping, when the phonon spectrum demonstrates a Kohn anomaly, which results in a faster partial equilibration between the electrons and an optical phonon subsystem.

[1]Work supported in part by DOE Grant No. DOE-DE-FG02-07ER46354.

K1.00259 Controllable p-n Junction Formation in Monolayer Graphene Using Electrostatic Substrate Engineering , HSIN-YING CHIU, VASILI PEREBEINOS, YU-MING LIN, PHAEDON AVOURIS, IBM Thomas J. Watson Research Center — The p-n junction is the basic element of modern electronics, providing the non-linear response essential for rectifying and switching currents. In conventional semiconductors, p-n junctions are produced by inserting donor and acceptor atoms in the crystal lattice. This approach, however, fails to produce effective results in nanoscale or low-dimensional electronic materials, such as graphene. Graphene itself is attracting much attention due to its unique electronic properties. In addition to having outstanding carrier mobilities graphene offers opportunities extending beyond CMOS technology, such as p-n junction electron (Veselago) lenses. Thus, graphene electronics depends on the ability to fabricate high-quality p-n junctions. Doping of graphene has been previously achieved by using multiple electrostatic gates, or charge transfer from adsorbants. Here we demonstrate a novel approach to create p-n junctions by changing the local electrostatic potential in the vicinity of one of the contacts without the use of extra gates. It is based on the electronic modification of the substrate and produces a well-behaved, sharp junction whose position and height can be controlled.

K1.00260 Opto-Electronic Properties of Nano-Structured Graphitic Carbon Measured Using Micro-Raman Spectroscopy , LOGAN SCHEEL, KEVIN MEAD, JEFFERY DEMERS, JEFF SIMPSON, Towson University — Nano-structured graphitic carbon allotropes offer promise for next generation optical and electronic devices. Graphene, a single atom layer of hexagonally arranged carbon atoms, is particularly interesting as the basis for other forms of graphitic carbon, e.g., single-wall carbon nanotubes (SWCNTs). The unique linear energy versus momentum band structure of graphene leads to interesting fundamental physics and potential device applications. We report on the design and implementation of a micro-Raman spectroscopy system used to measure the opto-electronic properties of graphene and SWCNTs. Using mechanical exfoliation, single and multilayer graphene flakes are deposited on Si/SiO_2 substrates. Our Raman system consists of multiple laser sources including, HeNe, Argon, and dye lasers, which provide excitation light to samples mounted in an optical microscope. Inelastically scattered light is collected and directed to a grating spectrometer with CCD detection. Analysis of the Raman spectra reveal specific phonons known as the D, G, G'_{2D} modes common to graphitic carbon. We fit the modes with Lorentzians in order to quantify the layer number and analyze electron-phonon coupling.

K1.00261 Comparing the Inner and Outer Double-resonance Raman Scattering Processes in Bilayer Graphene , DANIELA MAFRA, Universidade Federal de Minas Gerais, ELIE MOUJAES, RICARDO NUNES, Universidade Federal de Minas Gerais, Belo Horizonte, Brazil., STEVEN DOORN, HAN HTOON, Chemistry Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA., MARCOS PIMENTA, Universidade Federal de Minas Gerais, Belo Horizonte, Brazil. — The Raman spectroscopy has been widely used to study carbon materials. In this work the dispersion of phonons and the electronic structure of graphene systems can be obtained experimentally from the double-resonance (DR) Raman features by varying the excitation laser energy. The electronic structure was analyzed in the framework of the Slonczewski-Weiss-McClure (SWM) model, considering both the outer and inner DR process and the SWM parameters was obtained for each model. We show that the parameters obtained when we consider the inner DR process are in better agreement with those obtained from other experimental techniques, despite the fact that several previous studies about the DR process in graphene usually pay atention solely to the one-dimensional outer (DR) process. This result possibly shows that there is still a fundamental open question concerning the double resonance process in graphene systems.

K1.00262 A search for the dominant heat conducting phonon modes in graphene: An atomistic simulation study , HENGJI ZHANG, Department of Physics, University of Texas at Dallas, KYEONGJAE CHO, Department of Physics and Department Materials Science and Engineering, University of Texas at Dallas — We have performed an equilibrium molecular dynamic (MD) simulation study to investigate phonon thermal transport in graphene at 300K with Green-Kubo method. Using a newly optimized reactive empirical bond order carbon potential (Lindsay, et al. Physical Review B 81, 205441, 2010), our calculated thermal conductivity (TC) of defect free graphene is about 3000 W/mK in good agreement with experiments($\sim$3000-5000 W/mK). A maximum of $\sim$1000 fold reduction in TC is possible to achieve for graphene with defects and surrounding viscous medium. As we decompose the in-plane and out-plane phonon vibration modes of graphene in MD simulations, the out of plane vibration modes (ZA phonon) contribute to about 50% of the overall TC. This large contribution from ZA modes is explained with density of states analysis. We have clarified a recent controversy on which polarization mode in graphene is the main heat carrier.

K1.00263 Polarized Nonresonant Raman Spectra of Graphene Nanoribbons , GUANGFU LUO, JING LU, LU WANG, LIN LAI, JING ZHOU, RUI QIN, HONG LI, ZHENGXIANG GAO, State Key Laboratory for Mesoscopic Physics and Department of Physics, Peking University, Beijing 100871, People's Republic of China, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, Nebraska 68182-0266 — We study the non-resonant Raman scattering of armchair- and zigzag-edged graphene nanoribbons using density functional perturbation theory. We find that in both types of nanoribbon, the Raman spectrum is extremely polarized along the ribbon length direction, over 102 times larger than those of the other orientations. Also we discover that the scattering intensity of this major polarization exhibits conspicuous quantum oscillation with the ribbon width in armchair-edged nanoribbons. While in zigzag-edged nanoribbons, the Raman spectra shows relatively weak dependence on the ribbon width. We propose employing the surface-enhanced Raman spectroscopy to detect these features, a procedure which has been applied in the studies of graphene.

K1.00264 A broadband microwave study of CVD grown graphene[1] , WEI LIU, Johns Hopkins University, CARL MAGNUSON, YUFENG HAO, RODNEY RUOFF, The University of Texas at Austin, PETER ARMITAGE, Johns Hopkins University — We apply a broadband microwave Corbino spectrometer to study the complex conductivity of CVD grown graphene deposited on a high resistivity Si substrate. Explicit frequency dependency of the complex conductivity are obtained down to 300 mK and in a frequency range from 100 MHz to 20 GHz. We compare our data to the low frequency limit of the conductance of different theoretical models and make connection to other experimental results. We will also report measurements of the conductivity using time domain terahertz spectroscopy.

[1]NSF DMR-0847652

K1.00265 Graphene grown on Ni surface: quantitative analysis , IRMA KULJANISHVILI[1], DMITRIY DIKIN, Northwestern University, ALICE RILEY, Hendrx College, PAVAN PATEL, VENKAT CHANDRASEKHAR, Northwestern University — CVD growth of graphene on various substrates, e.g. Copper or Nickel, has become an increasingly popular method for production of large films. Unlike copper mediated growth, the CVD growth process of graphene on Nickel film is not self-limiting, hence understanding the main factors and/or conditions that influence the growth of one or few layers of graphene on Nickel is important. We will present our results on CVD growth of graphene on Nickel films deposited on Si/SO2 substrates. We will discuss our results of single and few layer graphene synthesis and our attempts to explain the growth mechanism of graphene. Correlation between SEM and AFM/EFM studies and optical characterization of graphene will be presented. A.R. acknowledges the support of International Institute of Nanotechnology REU Program

[1]Department of Physics

K1.00266 Experimentally determined optical-properties of monodisperse graphene quantum dots with controlled size and geometry , VIKAS BERRY, Kansas State University, NIHAR MOHANTY, ASHVIN NAGARAJA — In this talk, we will present a novel route for high throughput production of monodisperse GQDs with controlled spatial dimensions (5 nm - 100 nm at 1 nm resolution) and geometry (squares, rectangles, and triangles). We would show the first detailed experimental demonstration of the GQD optoelectronic-property-tuning via tailoring of their spatial dimensions and geometry. Further, we would be presenting the detailed structural, optical and electronic characterization of the as-obtained GQDs via various microscopic and spectroscopic techniques. While the top down methods of fabrication including lithography-based methods or sonochemical methods are either extremely low throughput or have limited control on GQDs' dimensions and geometry; the bottom-up fabrication methods are limited by the achievable size ($<$ 3 nm).

K1.00267 Magneto-transport of graphene quantum dots , KUEI-LIN CHIU, CHARLES SMITH, MALCOLM CONNOLLY, SIMON CHORLEY, JONATHAN GRIFFITHS, University of Cambridge — Graphene nanostructures continue to attract attention due to their customizable electronic properties and compatability with existing semiconductor device processing. The promise of long spin relaxation times makes graphene quantum dots small islands of confined charge - particularly suited to quantum computing architectures that manipulate the spin degree of freedom. In order to probe the spin and charge dynamics of geometrically confined Dirac quasiparticles, we have performed magneto-transport measurements on a single dot and a series-coupled double dot at temperatures down to 100 mK and magnetic fields up to 12 T. In the single dot structure we follow the energy required to add electrons to the dot in the many-electron regime. The energy levels show a rich structure of "kinks" as a function of the magnetic field, and we analyze this result in terms of Landau level formation in the quantum dot. In the double quantum dot structure we find that the conductance of the device as a function of the energy levels in the dots exhibits the typical honeycomb pattern. From the dimensions of the honeycomb we extract the capacitive coupling strength between dots and the gates, and examine how this evolves as a function of magnetic field. We analyze this result in terms of magnetic field induced changes in the capacitive coupling between the quantum dot and the plunger-gates.

K1.00268 Impurity and phonon scattering in silicon nanowires , W. ZHANG, Beijing National Laboratory for Condensed Matter Physics, China, M.P. PERSSON, H. MERA, CEA-UJF, INAC, SP2M/L-Sim, Grenoble, France, C. DELERUE, IEMN - Dept. ISEN, Lille, France, Y.M. NIQUET, CEA-UJF, INAC, SP2M/L-Sim, Grenoble, France, G. ALLAN, IEMN - Dept. ISEN, Lille, France, E. WANG, School of Physics, Peking University, Beijing, China — We model the scattering of electrons by phonons and dopant impurities in ultimate [110]-oriented gate-all-around silicon nanowires with an atomistic valence force field and tight-binding approach. All electron-phonons interactions are included. We show that impurity scattering can reduce with decreasing nanowire diameter due to the enhanced screening by the gate. Donors and acceptors however perform very differently : acceptors behave as tunnel barriers for the electrons, while donors behave as quantum wells which introduce Fano resonances in the conductance. As a consequence the acceptors are much more limiting the mobility than the donors. The resistances of single acceptors are also very dependent on their radial position in the nanowire, which might be a significant source of variability in ultimate silicon nanowire devices. Concerning phonons, we show that, as a result of strong confinement, i) electrons couple to a wide and complex distribution of phonons modes, and ii) the mobility has a non-monotonic variation with wire diameter and is strongly reduced with respect to bulk. French National Research Agency ANR project QUANTAMONDE Contract No. ANR-07-NANO-023-02 and by the Délégation Générale pour l'Armement, French Ministry of Defense under Grant No. 2008.34.0031.

K1.00269 ARTIFICIALLY STRUCTURED MATERIALS –

K1.00270 Spin splitter in a quantum ring with Rashba coupling[1] , B. TANATAR, Bilkent University, Department of Physics, 06800, Ankara, Turkey, V. MOLDOVEANU, National Institute of Materials Physics, P.O. Box MG-7, Bucharest-Magurele, Romania — We use non-equilibrium Greens' function formalism to calculate the spin currents in a one-dimensional ring coupled to three leads in the presence of perpendicular magnetic flux F and Rashba spin-orbit coupling. A finite bias is applied between the input lead and the other two output leads. We demonstrate that the spin-orbit coupling allows one to operate this system as a spin splitter, i.e. the output leads deliver spin-polarized currents with different orientations. We find that the spin splitter operation can be tuned at integer multiples of F/F_0. Efficiency depends not only on the value of the Rashba coupling but also on the bias applied between the input and output leads. The selected spin orientation of the output leads can be reversed by a slight change of their contact position. We also discuss the connection between the spin splitter operation and the spectral properties of the ring.

[1]Supported by TUBITAK and TUBA.

K1.00271 Nanoscale engineering of photoelectron kinetics in quantum dot structures , ANDREI SERGEEV, VLADIMIR MITIN, NIZAMI VAGIDOV, SUNY at Buffalo — We investigate photoelectron kinetics in advanced quantum dot (QD) structures, which combine quantum tuning of localized and conducting states with controllable photoelectron properties. Our unique approach is based on engineering of photoelectron capture processes using various configurations of manageable potential barriers around single QDs and collective barriers around QD planes (lateral structures) and QD clusters (vertical structures). Potential barriers around QDs are formed by electrons bounded in dots and ionized impurities in the depletion region. These potential barriers separate the conducting electron states from the localized intra-dot states. Besides manageable photoelectron lifetime, the novel structures will also provide high scalability, low generation-recombination noise in sensing applications and low recombination losses in QD solar cells.

K1.00272 Long-range exciton-exciton interactions in metal-semiconductor hybrid structures , ANSHU PANDEY, HSINHAN TSAI, HSING-LIN WANG, JEFFREY M. PIETRYGA, VICTOR I. KLIMOV — Establishment of long-range communication between semiconductor nanocrystals (NCs) is an important step towards their use in real-life devices. Most research towards enhancing inter-NC coupling has followed two strategies: attempts to enhance charge transfer rates in NC assemblies, and enhancement and control of energy transport via exciton transfer. We have explored the second strategy for obtaining strong coupling between distant NCs. For this purpose, we have studied the optical properties of colloidal NCs tethered to spherical gold particles coated with a silica shell. These structures exhibited clear signatures of long range coupling between the NCs which manifested in the form of cooperative decay of excitons separated by large distances (up to 40 nm apart). We further show that this coupling does not alter the overall emission efficiency of the excitons, though it significantly modifies emission rates. The observation of this regime of exciton interaction has potential applications in existing NC based devices such as lasers, and may also lead to novel applications that involve defect-tolerant energy transfer between distant chromophores

K1.00273 How to select quantum dots with smallest fine structure splitting under uniaxial stress for entangled photon sources , MING GONG, WEIWEI ZHANG, GUANGCAN GUO, LIXIN HE, Key Laboratory of Quantum Information, University of Science and Technology of China, Hefei, 230026g, HE TEAM — We propose a microscopic theory to build an exact relationship between the fine structure splitting (FSS) of exciton, the polarization of the emission lines and the amount of asymmetry in self-assembled quantum dots (QDs). Based on our model, strategy to select QDs with smallest FSS from large amount of QDs is proposed. The predilection in this work is supported by million atom empirical pseudo-potential calculation. Our theory can greatly simply the method to generate entangled photon sources using single QD.

K1.00274 Tunable Optical Switching/Routing by Negative Refraction in Liquid Crystal filled Opal and Inverted Opal Photonic Crystals , RABIA MOUSSA, Nanotech Institute, University of Texas at Dallas, RYOTARO OZAKI, Department of Electrical and Electronic Engineering, National Defense Academy of Japan, A. EFROS, ANVAR ZAKHIDOV, Nanotech Institute, University of Texas at Dallas, DEPARTMENT OF ELECTRICAL AND ELECTRONIC ENGINEERING, NATIONAL DEFENSE ACADEMY OF JAPAN TEAM, NANOTECH INSTITUTE, UNIVERSITY OF TEXAS AT DALLAS TEAM, NANOTECH INSTITUTE, UNIVERSITY OF TEXAS AT DALLAS TEAM — In this study, we investigate the optical characteristics and negative index of liquid crystal (LC) infiltrated inverse opal as a 3D photonic crystal (PC). We demonstrate that it is possible to achieve a tunable negative, by infiltrating LC into porous synthetic opal and inverted opal type PC. Using the optical anisotropy of LC and field sensitivity, the optical properties of porous PC infiltrated with LC can be easily controlled. The design of a simple and efficient wide angle optical switch/router is considered. Changing the electric field across the LC-PC, with the use of transparent electrodes, the refractive index of Opal-PC can be modulated within several percent, shifting the light beam between photonic bands with negative and positive dispersion. The calculations reveal that LC molecular orientation in the inverse opal strongly influences light propagation in 3D PC.

K1.00275 Analysis of Self-Assembled Monolayers in Nanoscale Switching Elements , MATTHEW ROBERSON, LAM YU, University of Memphis — Molecular junctions consisting of gold and silver electrodes and a self-assembled monolayer (SAM) have been shown to act as voltage-controlled electrical two-state switches due to the electrochemical migration of silver ions. In these junctions the SAM is sandwiched between the two metal electrodes. When a certain bias voltage is applied across the metal electrodes, atoms on the silver electrode surface are electrochemically oxidized, and the resulting silver ions are drawn by the local electric field toward the gold electrode. Upon deposition onto the gold electrode the silver ions are reduced to silver atoms. As more silver atoms are deposited onto the gold electrode, a metallic connection is formed between the electrodes resulting in a closed-circuit state between the two electrodes. The silver metallic bridges are metastable in these junctions, and they are dissolved when the voltage between the electrodes is swept back toward zero volts. When the silver filaments retract, the switch returns to an open-circuit state. Varying the functional group of the SAMs induces different switching characteristics in the junctions. We are analyzing the transition voltages at which this switching occurs for different SAMs under different temperature and humidity, and plotting the data to observe trends in order to isolate the key factors involved in this switching.

K1.00276 ABSTRACT WITHDRAWN —

K1.00278 Angle- and position-resolved plasmon coupling in gold nanocrystal dimers , LEI SHAO, JIANFANG WANG, The Chinese University of Hong Kong — Interactions between the localized plasmons of metal nanocrystals have attracted much attention, because of their applications ranging from photonic devices to biomolecular detection. Gold nanorods (NRs) exhibit both the transverse and longitudinal plasmon modes, with the latter being strongly polarization-dependent. We have studied the coupling in Au NR homodimers and Au NR-Au nanosphere (NS) heterodimers. Experimental observations, as well as simulations, have revealed a number of interesting phenomena in the plasmon coupling. First, both the antibonding and bonding modes are existent in the NR dimer system and their intensity ratio decreases exponentially as the NR angle increases. Second, the NR-NS heterodimers exhibit Fano resonance properties and a NS-site-dependent coupling behavior. We believe that our results will be useful for developing complex plasmon-based photonic devices and ultrasensitive plasmonic sensors. The NR-based dimers can also potentially function as building blocks for the construction of metamaterials.

K1.00279 Strain Effects in Thermoelectric $Ca_3Co_4O_9$ Thin Films[1] , ROBERT KLIE, QIAO QIAO, AHMET GULEC, TADAS PAULAUSKAS, University of Illinois - Chicago, STANISLAW KOLESNIK, BOGDAN DABROWSKI, Northern Illinois University, CIHAT BOYRAZ, MEHMET OZDEMIR, DIPANJAN MAZUMDAR, ARUN GUPTA, University of Alabama — Thermoelectric oxides have attracted increasing attention due to their high thermal power and temperature stability. In particular, $Ca_3Co_4O_9$(CCO), a misfit layered structure consisting of single layer hole-doped CoO_2 sandwiched between insulating Ca_2CoO_3 rocksalt layers, exhibits a high Seebeck coefficient at 1000 K.It was suggested that the Seebeck-coefficient can be further increased by growing doped thin films with controlled defects structures. This study combines pulsed layer deposition thin film synthesis of pristine CCO on several oxide substrates, as well as CCO thin films doped with Ti, Bi or La, with aberration-corrected scanning transmission electron microscopy and electron energy loss spectroscopy (EELS) to examine the effects of interfacial strain and doping on the atomic and electronic structures of CCO. The thermoelectric properties will be measured and correlated to the local changes in the atomic and electronic structures. We will further evaluate the role of CoO_2 stacking faults, as well as film thickness on the thermoelectric properties of CCO.

[1]This work is supported by the US Army Research Office (W911NF-10-1-0147) and the National Science Foundation (DMR-0846748).

K1.00280 First principle investigation of ZrO_2-CeO_2 heterojunction properties , MARCO FRONZI, Materials Nanoarchitectonics Department, National Institute for Material Science, ALESSANDRO DE VITA, Physics Department, King's College London, Strand,London, YOSHITAKA TATEYAMA, ENRICO TRAVERSA, Materials Nanoarchitectonics Department, National Institute for Material Science — Here we present a computational Density Functional Theory approach to analyze the structural and electronic properties of the (100) and (111) ZrO_2-CeO_2 interface. Optimization of the lattice geometry for the separate ZrO_2 and CeO_2 bulks as well as the interface is carried out and the structural morphology is analyzed. The energy formation of the oxygen vacancies are analyzed at different values of lattice parameter, in order to verify its dependency on the strain. Activation energy of the oxygen migration are also calculated in the bulk as well as at the interfaces level. The effect of the doping on the lattice geometry is analyzed for the (111) and (100) interfaces in order to verify its influence on the morphologic disorder.

K1.00281 Structure, Vibrational Dynamics and Thermodynamics of silver thin-films on Cu(100) , SAMUEL ROBERTS, JAMES WESTOVER, ABDELKADER KARA, University of Central Florida — We use a Real Space Green's function and the embedded atom method for interaction potentials, to examine the structural and vibrational properties of a silver thin-film (from one to four monolayers) on Cu(100). Due to the lattice mismatch, the first several layers of the substrate had major structural modification, in the form of buckling about 0.6A for the top two layers and 0.05A in the 6^{th} layer. For the case of a mono-layer, the vibrational densities of state of the silver atoms extend substantially beyond the maximum of the bulk density. The atoms in the first copper layer's density of state also show substantial enhancement of the high frequency end. These reflect the strong bonding between the monolayer and the substrate. The vibrational thermodynamic functions for these interface atoms will be presented

K1.00282 Improvements in 3-omega measurement of thermal conductivity for nanostructured materials , CHUANLE ZHOU, M. GRAYSON, Electrical Eng. Comp. Sci., Northwestern University, Evanston IL, USA, G. KOBLMUELLER, Walter Schottky Institut, Tech. Univ. Munich, Germany — Nanostructured materials have reduced thermal conductivity in order to enhance the thermoelectric figure of merit (ZT). The 3ω method is widely used for vertical thermal conductivity measurements in the nanostructure materials, especially layered materials. The challenge for this method is to measure the small 3ω voltage at the third harmonic, above the comparably large ω voltage from the sample at the fundamental frequency, complicated by the nonlinear signal from other components in the measurement circuit. We carefully study the 3ω method [Cahill, Rev. Sci. Instrum. 61 (2), 802 (1990)] and develop a strategy to increase the signal to noise ratio of the data, for more accurate results. We also investigate an alternate sample preparation geometry for the 3ω measurement, so that the heat flow is vertical and linear through the thin film instead of cylindrical as is standard for this method. This results in a direct measurement of the vertical thermal conductivity in such an anisotropic material. New geometries for measuring lateral thermal conductivity will also be proposed and explored.

K1.00283 PHASE TRANSITIONS AND STRONGLY CORRELATED SYSTEMS –

K1.00284 Magnetic Superstructure and Metal-Insulator Transition in Mn-Substituted $Sr_3Ru_2O_7$

M.A. HOSSAIN, UBC and SIMES, Stanford, Z.H. ZHU, UBC, B. BOHNENBUCK, MPI, Stuttgart, Y.-D. CHUANG, Berkeley Lab, Y. YOSHIDA, AIST, Z. HUSSAIN, Berkeley Lab, B. KEIMER, MPI, Stuttgart, I.S. ELFIMOV, G.A. SAWATZKY, A. DAMASCELLI, UBC — We present a temperature-dependent resonant elastic soft x-ray scattering (REXS) study of the metal-insulator transition in $Sr_3(Ru_{1-x}Mn_x)_2O_7$, performed at both Ru and Mn L-edges. Resonant magnetic superstructure reflections together with ab-initio density functional theory calculations identify the ground state as a spin checkerboard with blocks of 4 spins up and 4 spins down. Based on modelling of the REXS intensity from randomly distributed Mn impurities, we establish the inhomogeneous nature of the metal-insulator transition, with an effective percolation threshold corresponding to an anomalously low $x \sim 0.05$ Mn substitution. Perhaps more important, our results suggest that the same checkerboard instability might be present already in the parent compound $Sr_3Ru_2O_7$. In collaboration with: A.G. Cruz Gonzalez, J.D. Denlinger (Berkeley) I. Zegkinoglou, M.W. Haverkort (MPI) J. Geck, D.G. Hawthorn (UBC) R. Mathieu, Y. Tokura, S. Satow, H. Takagi (Tokyo) H.-H. Wu and C. Schussler-Langeheine (Cologne).

K1.00285 Ultrafast quasiparticle dynamics in the hidden order state of URu_2Si_2

MENGKUN LIU, Boston University, DZMITRY YAROTSKI, TOMASZ DURAKIEWICZ, STUART TRUGMAN, Los Alamos National Laboratory, RICHARD AVERITT, Boston University, ANTOINETTE TAYLOR, Los Alamos National Laboratory — The heavy-fermion compound URu_2Si_2 has attracted much interest in the past two decades due to appearance of the 'hidden order' (HO) state in this material below 17.5 K. Despite an extensive effort, the development of the theoretical description of the origin of HO has been hindered by the lack of adequate experimental evidence regarding low-energy electronic structure of this compound. We report on application of ultrafast optical spectroscopy to probe quasiparticle dynamics in the vicinity of E_F in a single crystal URu_2Si_2 undergoing the HO phase transition. The relaxation dynamics of the photoexcited carriers exhibits a strong dependence on temperature and excitation intensity. Data analysis using the Rothwarf-Talyor model demonstrates an opening of a 5 meV energy gap as the temperature decreases below 20 K. This behavior is consistent with recent results obtained from angle-resolved photoemission spectroscopy, scanning tunneling microscopy and neutron scattering experiments.

K1.00286 High Field (H,T) Phase Diagram and Anisotropy of $CeRhIn_5$ single crystals

YOSHIMITSU KOHAMA, MPA-CMMS, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, HUIQIU YUAN, LIN JIAO, Department of Physics, Zhejiang University, Hangzhou 310027, China, MARCELO JAIME, FEDOR BALAKIREV, ERIC BAUER, MPA-CMMS, Los Alamos National Laboratory, Los Alamos, NM 87545, USA — The specific heat (C_p) of a single crystal sample of composition $CeRhIn_5$ was measured as a function of temperature and magnetic field applied perpendicular and parallel to the crystallographic $c-$axis. Our experiments, carried out at temperatures below the AFM ordering temperature $T_N =$ 3.7 K, show a clear anomaly in $C_p(H)$ when the applied field is strong enough to suppress the magnetic order. This anomaly, which reduces the magnitude as the temperature is lowered, was used to map the (H,T) phase diagram for the first time to a magnetic field of 55 T and temperatures as low as 700mK.[1] Extrapolation of the low temperature phase boundary indicates the presence of a magnetic field-induced quantum critical point at $H_c \approx$ 50 T that is weakly dependent of the sample orientation, although intermediate magnetic fields reveal clear anisotropy. Our results will be discussed in the context of field-induced quantum phase transitions in strongly anisotropic correlated matter.

[1]Y. Kohama, C. Marcenat, T. Klein, and M. Jaime, *Rev. Sci. Instrum.*, **81**, 104902 (2010).

K1.00287 Transport properties in magnetic Griffiths phases

DAVID NOZADZE, THOMAS VOJTA, Department of Physics, Missouri University of Science and Technology, Rolla, MO 65409 — We study the temperature dependence of the electrical resistivity in the quantum Griffiths phases associated with the ferromagnetic and antiferromagnetic quantum phase transitions in itinerate systems. The resistivity is calculated by means of the semi-classical Boltzmann equation. We show that the contribution to the resistivity due to the scattering by spin-fluctuations in rare regions varies as T^λ with the logarithmic correction for both ferromagnetic and antiferromagnetic systems. Here λ is the usual Griffiths exponent which takes the value 0 at the critical point and increases with the distance from the criticality. We also consider other transport properties such as thermal resistivity, thermopower and Peltier coefficient.

K1.00288 Evolution of Power-Law Behavior of Temperature Dependence of Electrical Resistivity in $Pr_{1-x}Nd_xOs_4Sb_{12}$[1]

P.-C. HO, Physics/California State University, Fresno, R.E. BAUMBACH, A.A. DOORAGHI, M.B. MAPLE, Physics/University of California, San Diego, T. YANAGISAWA, Hokkaido University, Japan — The study of the $Pr_{1-x}Nd_xOs_4Sb_{12}$ series has been carried out in order to investigate the effect of ferromagnetism (FM) on the unconventional superconductivity (SC), the high field ordered phase (HFOP), and quantum critical behavior in $PrOs_4Sb_{12}$ [1, 2, 3]. Two critical concentrations $x_{cr,1} \sim 0.58$ and $x_{cr,2} \sim 0.33$ were previously identified in this system [2]: SC disappears near $x_{cr,1}$ and weak FM extends into the SC region for $x_{cr,2} < x < x_{cr,1}$ [3]. In order to further examine the possible quantum critical behavior, a power-law analysis of the temperature dependence of the electrical resistivity data is performed. Upon suppression of SC, for samples of $x_{cr,2} < x < x_{cr,1}$, the power-law exponent decreases from $\sim$ 1.8 toward 1 in the temperature region below 2.5 K, resembling non-Fermi liquid behavior.

[1] Ho, et. al., Physica B 403, 1038 (2008).
[2] Ho, et. al., arXiv:1008.5198v1 (2010).
[3] Ho, et. al., 2010 APS March Meeting, A38.00005 (2010).

[1]Research at CSU-Fresno is supported by RC CCSA #7669 and the start-up fund; at UCSD by NSF#0802478 and US DOE DE FG02-04ER46105; at Hokkaido U by MEXT, Japan.

K1.00289 Temperature Dependent Investigations on Single Crystal Gallium Ferrite Using X-ray Diffraction and Raman Spectroscopy

S. MUKHERJEE, Dept. of Physics, IIT Kanpur, India, RAJEEV GUPTA, Dept. of Physics and Materials Science Programme, IIT Kanpur, India, ASHISH GARG, Materials Science and Engineering, IIT Kanpur, India — $Ga_{2-x}Fe_xO_3$ ($0.8 \leq x \leq 1.2$) or GFO is a room temperature paramagnetic piezoelectric material with its ferrimagnetic to paramagnetic transition temperature (T_c), varying from 200 K to 300 K. We synthesized GFO ($x \sim$ 1.08-1.10) single crystals using flux growth method. Partial occupancies of the cationic sites obtained using Reitveld refinement of XRD data were used to calculate the lattice magnetic moment. We have also carried out Raman scattering as a function of temperature from 18 K to 450 K. Temperature evolution of the peak positions of most of the modes can be adequately described using an anharmonic model suggesting absence of any lattice anomaly across the phase transitions. This observation is consistent with the XRD data. However, the temperature dependence of the line width of a number of modes exhibits a change in slope across the phase transition boundary. In order to understand and quantify this change in the line width as a function of temperature we calculate the product of electron-phonon coupling strength and the density of states at the Fermi level. The deviation from anharmonicity is qualitatively explained as a consequence of a weak magneto-elastic effect in the low temperature phase.

K1.00290 Power-law Griffiths singularities in a randomly layered Heisenberg magnet , FAWAZ HRAHSHEH, THOMAS VOJTA, Department of Physics, Missouri University of Science and Technology, Rolla MO 65409, USA — We study the ferromagnetic phase transition in a randomly layered Heisenberg model using Monte-Carlo simulations. A recent strong-disorder renormalization group approach [Phys. Rev. B 81, 144407 (2010)] predicted that the critical point in this system is of exotic infinite-randomness type and is accompanied by strong power-law Griffiths singularities. Here, we show the results of simulations that provide numerical evidence in support of these predictions. Specifically, we investigate the finite-size scaling behavior of the magnetic susceptibility which is characterized by a non-universal power-law divergence in the Griffiths phase. In addition, we calculate the spin-wave stiffnesses both parallel and perpendicular to the layers. We find that the perpendicular stiffness decays to zero at lower temperatures than the parallel stiffness which vanishes at the critical point.

K1.00291 Density matrix Loschmidt echo and quantum discord in quantum phase transitions , YANCHAO LI, Beijing Computational Science Research Center (CSRC), STATE KEY LABORATORY FOR SUPERLATTICES AND MICROSTRUCTURES, INSTITUTE OF SEMICONDUCTORS, CAS COLLABORATION, BEIJING COMPUTATIONAL SCIENCE RESEARCH CENTER (CSRC) TEAM — We introduce the concept of the Loschmidt echo (LE) to the space of the reduced density matrix of spin and fermionic systems to study the relationship between the density matrix Loschmidt echos (DMLEs) and quantum phase transitions (QPTs). Our results show that the DMLEs are remarkably influenced by the criticality of the system, and the method is a convenient way to study QPT. Meanwhile, we compare quantum discord and DMLE calculations, aiming to explore the difference and connection between them in identifying QPTs.

K1.00292 Time Reversal Symmetry Breaking in 2D Lattice Model , WEI LIU, ALEXANDER PUNNOOSE, City College of New York — We use magnetic group as a tool to classify the possible spontaneous time-reversal symmetry breaking states in 2D electronic systems. We study the leading order fluctuations of the order parameter with discrete symmetry. The method is applied to the study of Topological Mott insulator phase in Graphene and orbital loop currents in CuO planes.

K1.00293 The Verwey transition in Fe_3O_4: lattice distortions on a fs time-scale , R. KUKREJA, S. DE JONG, M. HOSSAIN, C. BACK, A. SCHERZ, D. ZHU, W. SCHLOTTER, J. TURNER, W. LEE, Y. CHUANG, R. MOORE, O. KRUPIN, M. TRIGO, H. DÜRR, SLAC/ RSXS collaboration, L. PATTHEY, SLAC/ RSXS collaboration and PSI, N. PONTIUS, T. KACHEL, A. FÖHLISCH, M. BEYE, Helmholtz Zentrum Berlin, F. SORGENFREI, Uni. Hamburg and CFEL, W. WURTH, Uni. Hamburg and CFEL, C. CHANG, M. DÖHLER, C. TRABANT, Uni. Cologne, C. SCHÜSSLER-LANGEHEINE, Uni. Cologne and HZB — Magnetite, Fe_3O_4, displays a strong decrease in resistivity upon heating above $T_C = 123$ K: the Verwey transition. This transition is accompanied by a structural change from monoclinic to cubic symmetry. Despite decades of research and indications that charge and orbital ordering play an important role, the mechanism behind the Verwey transition is yet unclear. Using pump-probe soft X-ray scattering at the new LCLS SXR beamline, we have studied the role of the structural transition for the Verwey transition on ultra-fast time-scales. Focusing off-resonance on the high T forbidden (001) lattice reflection, we find a lattice response on time-scales $t < 250$ fs. The response displays a pump fluence threshold indicative of a phase transition. This strongly suggests that the lattice, via coupling to certain low energy phonon modes, plays a crucial role for the Verwey transition in Fe_3O_4.

K1.00294 Metal-insulator transition characteristics of epitaxial and polycrystalline $SmNiO_3$ thin films , SIEU HA, GULGUN AYDOGDU, SHRIRAM RAMANATHAN, Harvard University — $SmNiO_3$ (SNO) is known to exhibit a sharp insulator to metal transition at 130 °C in bulk form and is a candidate material for utilization in advanced electronic devices such as memory and neuromorphic circuits. We present growth and characterization of SNO thin films deposited on $LaAlO_3$ and Si single crystals. Structural properties such as crystallinity, strain, and stoichiometry are examined with x-ray diffraction and x-ray photoelectron spectroscopy. Temperature-dependent resistance measurements are performed, and a metal-insulator transition is observed for films on both substrates. We investigate how resistance changes are affected by thermal cycling and the role of surface oxygen loss on electrical characteristics.

K1.00295 Quantum phase diagram of the half filled Hubbard model with bond-charge interaction , ARIEL DOBRY, Instituto de Física Rosario (Argentine), ARMANDO ALIGIA, Centro Atómico Bariloche and Instituto Balseiro (Argentine) — Using field theoretical bosonization, we determine the quantum phase diagram of the one-dimensional Hubbard model with bond-charge interaction X in addition to the usual Coulomb repulsion U at half-filling, for small values of the interactions. We show that it is essential to take into account formally irrelevant terms of order X. They generate relevant terms proportional to X^2 in the flow of the renormalization group (RG). The model shows three phases separated by a charge transition at $U = U_c$ and a spin transition at $U = U_s > U_c$. For $U < U_c$ singlet superconducting correlations dominate, while for $U > U_s$, the system is in the spin-density wave phase as in the usual Hubbard model. For intermediate values $U_c < U < U_s$, the system is in a spontaneously dimerized bond-ordered wave phase, which is absent in the ordinary Hubbard model with $X = 0$. We provide an analytical expression for $U_s(X)$. The results, with only one adjustable parameter, are in excellent agreement with numerical ones for $X < t/2$ where t is the hopping.

K1.00296 Neutron diffraction study of quasi-one-dimensional lithium purple bronze: possible mechanism for dimensional crossover[1] , JOHN J. NEUMEIER, M.S. DA LUZ, Montana State University, C.A.M. DOS SANTOS, Escola de Engenharia de Lorena - USP, B.D. WHITE, Montana State University, H.J.I. FILHO, Escola de Engenharia de Lorena - USP, J.B. LEÃO, Q. HUANG, NIST Center for Neutron Research — The crystallographic structure of quasi-1D lithium purple bronze was investigated using neutron powder diffraction at temperatures T in the range 5 K $< T <$ 295 K. Lattice parameters, atomic positions, and occupation numbers are reported. At room temperature, it has a monoclinic symmetry with space group $P2_1/m$, lattice parameters $a = 12.750(1)$ Å, $b = 5.524(1)$ Å, $c = 9.491(2)$ Å, and $\beta = 90.593(1)°$. The stoichiometry was determined through chemical analysis *and* refinement of the NPD data to be $Li_{0.924}Mo_6O_{17.6}$. The bond-valence-sum method was applied to calculate the valence of each Mo ion as a function of T, which allows discussion of the mechanism by which charge is transferred between the double 1D conducting chains.

[1]Supported by the DOE-BES (DE-FG-06ER46269), the NSF (DMR-0907036), FAPESP (2009/14524-6), and CNPq (301334/2007-2 and 490182/2009-7).

K1.00297 Study of phase transitions in ternary lead indium niobate-lead magnesium niobate-lead titanate relaxor ferroelectric morphotropic single crystals[1] , PETER FINKEL, HAROLD ROBINSON, AHMED AMIN, NUWC — In this work we report on the elastic hysteretic behavior observed in ferroelectric lead indium niobate-lead magnesium niobate-lead titanate (PIN-PMN-PT) relaxor single crystals under conditions of cooperative stress, temperature, and electric field. Room temperature elastic response displays strong and sharp discontinuity associated with stress induced phase transition. Quasistatic elastic response and ultrasonic wave propagation measurements demonstrated that this strain discontinuity in PIN-PMN-PT single crystal is associated with a ferroelectric rhombohedral (FR)—ferroelectric orthorhombic (FO) phase transition. The temperature dependent elastic response and transition strain were modeled by Devonshire theory. The crystal instability under compression is significantly improved by application of a dc bias electric field.

[1]Authors acknowldge support from the ONR.

K1.00298 ^{1}H NMR Study of Proton Dynamics in the Ferroelastic Transition of $K_4LiH_3(SO_4)_4$ Cystals , MOOHEE LEE, HO HYOUN KIM, B.J. MEAN, KI HYEOK KANG, B. NDIAYE, Konkuk University, Seoul, South Korea, AE RAN LIM, Jeonju University, Jeonju, South Korea — $K_4LiH_3(SO_4)_4$ is known to show a ferroelastic transition at $T_c = 114$ K. We have performed ^{1}H nuclear magnetic resonance(NMR) measurements to investigate proton dynamics in the phase transition of $K_4LiH_3(SO_4)_4$ crystals in the temperature range of 70-300 K at 2.67 T. The ^{1}H NMR spectrum shows a composite structure with dominating broad and weak narrow components. The broad component has an extremely long T_1 whereas the narrow component exhibits a short T_1 at room temperature. The intensity of the narrow peak decreases at low temperature vanishing below 200 K. From this behavior, we find that the narrow component comes from rapidly moving protons whereas the broad component originates from rigid protons. From the temperature dependence of the short T_1 for the narrow component, the activation energy for the proton's rapid motion is deduced to be ∼1900 K. On the other hand, the long T_1 for the broad component decreases at low temperature suggesting that the proton dynamics associated with the ferroelastic transition change abruptly across T_c.

K1.00299 Ion conductivity relaxation and specific heat close to the first-order phase transition of $\gamma-RbAg_4I_5$, RUBEN A. VARGAS, Universidad del Valle, HERNANDO CORREA, Universidad del Quindo, DIEGO PEÑA-LARA, Universidad del Valle — We report on simultaneous measurements of specific heat at normal pressure and ac conductivity in single-crystalline γ-$RbAg_4I_5$ close to and below its γ-to-β first order phase transition at 121 K. We found an accurate proportionality between the specific heat, $\mathbf{c}_P$, and the temperature derivative of the product $\mathbf{nE}_\sigma$, where β **=1- n**, is the Kohlrausch stretching exponent for the conductivity relaxation and $\mathbf{E}_\sigma = \mathbf{d(ln}\sigma\mathbf{)/d(T^{-1})}$ is the dc conductivity activation energy, which is non-Arrhenius. Thus, our results show that the dc conductivity activation energy $\mathbf{E}_\sigma\mathbf{(T)}$ includes, besides the true microscopic energy "barrier" for independent ionic motion, **(1-n)** $\mathbf{E}_\sigma$ (according the coupling model), an additional contribution from the enthalpy of the mobile Ag-ions defects, **h**.

K1.00300 Critical dynamics of randomly layered magnets , HATEM BARGHATHI, THOMAS VOJTA, Missouri University of Science and Technology — We report the results of large-scale Monte-Carlo simulations of the critical dynamics in the randomly layered Heisenberg model. This system has recently been reported to display an exotic phase transition controlled by an infinite-randomness critical point [Phys. Rev. B 81, 144407 (2010)]. In agreement with this, we found the critical dynamics to be ultraslow. At criticality, the time autocorrelation function decays only logarithmically with time while it follows a nonuniversal power-law in the Griffiths phase. We also study the case of XY spin symmetry where the interplay between the randomness and the Kosterlitz-Thouless physics leads to even stronger disorder effects.

K1.00301 A second metastable spin-ordered state on ferrimagnetic single crystal Cu_2OSeO_3 , CHIH CHIEH CHOU, C.L. HUANG, K.F. TSENG, S. MUKHERJEE, J.L. HER, Y.H. MATSUDA, K. KINDO, H. BERGER, H.D. YANG — DC and AC susceptibilities were executed on ferrimagnetic single crystal Cu_2OSeO_3 under magnetic field (H) and hydrostatic pressure (P) circumstance. With increasing H, the ferrimagnetic transition at T_C ∼ 60 K tends to a higher temperature. Furthermore, the T_C rises with a linear slope and magnetization is enhanced with increasing P. Features of the ladder shown in the M vs. H curve or the peak observed in the dM/dH vs. H curve are noted at H_{SF} ∼ 0.5 kOe, exhibiting a competing ordered state in magnetic fields below T_C. Remarkably, another shoulder is observed at ∼ 1 kOe in the dM/dH vs. H curve, revealing a metastable spin ordered state in Cu_2OSeO_3. In addition, the novel state is retained and enhanced by applied pressure. However, at H up to 55 T, there is no more observable slop change in magnetization. These magnetic properties suggest a complex spin orientation in the spin-frustrated system Cu_2OSeO_3.

K1.00302 Current Bearing Electron Shock Wave[1] , MOSTAFA HEMMATI, Arkansas Tech University — For analytical solution of breakdown waves, we use a one-dimensional, steady-state, three-component (electrons, ions, and neutral particles) fluid model. The wave front is considered to be a shock front and the electron gas partial pressure is considered to provide the driving force for the propagation of the wave. The basic set of equations consists of the equation of conservation of mass flux, equation of conservation of momentum, equation of conservation of energy, plus Poison's equation. In this study, the emphasis will be on the waves propagating into a neutral medium and we will investigate breakdown waves for which a large current exist behind the wave front. We apply shock conditions to obtain breakdown wave profile for electric field, electron velocity, electron temperature, electron number density, and ionization rate behind the shock front for breakdown waves propagating in the opposite direction of the electric filed force on electrons.

[1]We would like to express our gratitude for Arkansas Space Grant Consortium's financial support of this project.

Tuesday, March 22, 2011 2:30PM - 4:54PM –
Session L1 DCMP DCP: Recent Advances in Ultrafast Studies of Condensed Matter Ballroom A1

2:30PM L1.00001 Ultrafast and Nonlinear Optical Spectroscopy of Carbon Nanotubes[1] , JUNICHIRO KONO, Department of Electrical and Computer Engineering, Rice University — Single-walled carbon nanotubes (SWNTs) provide a variety of unique opportunities for studying the dynamics and interactions of one-dimensional (1-D) electrons and phonons. We have carried out a series of ultrafast and nonlinear optical experiments on SWNTs, revealing novel properties of high- density 1-D excitons as well as coherent lattice vibrations.[2] We have shown that there exists an upper limit on the density of 1-D excitons in SWNTs, which results in photoluminescence saturation. Using a model based on diffusion-limited exciton-exciton annihilation, we provided realistic estimates for the exciton densities in the saturation regime. We also predicted and demonstrated that there is an optimum temperature at which the exciton density can be maximized, due to the existence of a dark exciton state. Using ultrashort pulses, we have also investigated the dynamics of coherent phonons (CPs) in SWNTs, including both the low frequency radial breathing mode and high frequency G-mode phonons. Pulse shaping techniques allowed us to generate and detect CPs in SWNTs in a chirality-selective manner, which provided insight into the chirality dependence of light absorption, phonon generation, and phonon-induced band- structure modulations. Finally, we observed novel large- amplitude CPs through near-band-edge excitations as well as strongly polarization-dependent CP signals in highly-aligned SWNTs.

[1]This work was performed in collaboration with Y. Murakami, A. Srivastava, T. A. Searles, L. G. Booshehri, E. H. Hároz, D. T. Morris, J.-H. Kim, K.-J. Yee, Y.-S. Lim, G. D. Sanders, C. J. Stanton, and R. Saito.

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3:06PM L1.00002 Femtosecond magnetism and spin manipulation on a time-scale of the exchange interaction , ALEXEY KIMEL, Radboud University Nijmegen — The dynamics of phase transformations on the time-scale pertinent to atomic, orbital and spin motion is a rather unexplored field in physics. This is also a particularly interesting problem of modern magnetism, a study of which may have tremendous consequences for future development of magnetic recording technology. However, generation of magnetic field pulses much shorter than 100 ps and strong enough to reverse magnetization (more than 1T) is an extremely challenging technical problem.As a result the dynamics of the magnetic phase transitions at the sub-100 ps time-scale remains to be one of the most intriguing areas of modern magnetism [1,2]. Recently it has been observed that a 40 fs laser pulse influences spins in a magnet as an equally short pulse of effective magnetic field with a strength up to 20 T [3,4]. In my talk I will discuss how these opto-magnetic pulses can be used to excite a magnet on a time-scale of the exchange interaction between the spins [5-7]. Novel insights into the physics of non-equilibrium magnetism will be provided, showing that two exchange-coupled magnetic sublattices of a ferrimagnet may have totally different spin dynamics [8]. As a result, ultrafast spin reversal of two antiferromagnetically coupled magnetic sub-lattices appears to proceed via a novel ferromagnet-like transient state.

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3:42PM L1.00003 Theory of ultrafast pump-probe phenomena in high-temperature superconductors[1] , JIAN-XIN ZHU, Los Alamos National Laboratory, Los Alamos, NM 87545 — The physics underlying the pairing mechanism for high-temperature superconductors remains a topic of current interest. The complexity lies with the existence of competing interactions in these strongly correlated electronic materials. The ultra-fast pump-probe technique can make a stride to untangle the competing degrees of freedom (DOF). In this talk, the theoretical underpinning for this technique will be reviewed. In particular, we have developed a three-temperature model [1] to simulate the real time dependence of the electron and phonon temperatures in high-temperature superconductors. The model considers anisotropic electron-phonon coupling [2]. Based on this model, we have calculated the time-resolved spectral function, which exhibits interesting features with time delay. It has been found that the excitation of phononic DOF can provide a defining signature for the evidence of electron-vibration mode coupling [1]. In addition, the time-resolved optical conductivity and Raman spectra will also be discussed within the same model [3]

[1] Jianmin Tao and Jian-Xin Zhu, Phys. Rev. B **81**, 224506 (2010);
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[3] Jianmin Tao and Jian-Xin Zhu *et al.*, unpublished (2010).

[1]This work was supported by the National Nuclear Security Administration of the U.S. DOE at LANL under Contract No. DE-AC52-06NA25396.

4:18PM L1.00004 Ultrafast Optical Excitation in $YBa_2Cu_3O_{7-\delta}$: Tracing the Optical Phonons , ALEXEJ PASHKIN, University of Konstanz — The time-resolved spectroscopy of nonequilibrium states proved to be a powerful tool for observation of the electron-phonon scattering dynamics and the recombination of photoexcited quasiparticles (QP), particularly in high-temperature cuprate superconductors. However, most of the reported experiments monitor only the electronic subsystem [1-5]. Thus, a detailed dynamics of the various phonon modes during an initial non-thermal regime has been beyond reach. Here we utilize the field-resolved ultrabroadband THz spectroscopy to resonantly trace ultrafast phonon and QP dynamics of optimally doped single crystals of $YBa_2Cu_3O_{7-\delta}$ [6]. The superconducting state is perturbed by 12-fs optical pump pulses, and the induced changes in the mid-infrared optical conductivity are probed by THz transients. Thus, we simultaneously observe the dynamics of nonequilibrium QPs and two specific phonon modes with a time resolution of 40 fs. A quantitative line shape analysis of the apex oxygen vibration allows us to separately follow its transient occupation and coupling to the Josephson plasma resonance. A strong phonon population and the maximum QP density are reached within the same time scale of 150 fs demonstrating that the lattice absorbs a major portion of the pump energy before the QPs are thermalized. Our results indicate substantial electron-phonon scattering in $YBa_2Cu_3O_{7-\delta}$ and introduce a powerful approach for characterizing transient phonon dynamics in a broad variety of solids.

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Tuesday, March 22, 2011 2:30PM - 5:30PM –

Session L2 DCMP: Single Molecule Transistors and Graphene Quantum Dots Ballroom A2

2:30PM L2.00001 Spectroscopy and read-out of STM-patterned donor based qubits[1] , MICHELLE SIMMONS, University of New South Wales — We report low temperature transport measurements of few-to single P donor based quantum dots in silicon. Dots with a high donor number (approx. 7) show a surprisingly dense spectrum of excited states with an average energy spacing of 100 micro eV. The energy spacing of these features is much too low to be accounted for by the nm-scale lateral confinement of either the dot or the leads and can be explained by lifting of valley degeneracy of the dot orbital states [1]. The use of all epitaxial in plane P:Si gates allow us to tune both the electron number in the dot and modulate the transparency of the tunnel barriers [2]. We also present transport through a deterministic single donor device, where we observe both the signature of a single donor directly through STM imaging and demonstrate that the charging energy and excited state spectrum is consistent with the orbital states of a single P-donor. Finally we present our latest results of spin read-out in STM-patterned donor based devices.

[1] M. Fuchsle et al, Spectroscopy of few electron single crystal silicon quantum dots, Nature Nanotechnology 5, 502 (2010).
[2] A. Fuhrer et al, Atomic-Scale, All Epitaxial In-Plane Gated Donor Quantum Dot in Silicon, Nano Letters 9, 707 (2009).

[1]We acknowledge the ARC and US ARO under W911NF-08-1-0527.

3:06PM L2.00002 Single-donor transport in silicon: Atomic physics in restricted momentum space[1] , SVEN ROGGE, University of New South Wales — Technology reached a level of miniaturization where we can realize transport through a single dopant atom in a transistor. Such transport spectroscopy can probe the atomic orbitals and the interaction of the atom with the environment. This interaction with the environment in a nano-device leads alters the dopants properties, such as the level spectrum and the charging energy, from those of the bulk. The system discussed here is a gated arsenic donor in a silicon field effect transistor. Electronic control over the wavefunction of dopants is one of the key elements of quantum electronics. This talk focuses on the role of the restricted momentum space which has a severe impact on the charge and spin configuration of a donor atom in a nano-device. The combined experimental and theoretical study of the gated two-electron state of the donor led to the realization of the pseudo spin nature of the valleys. We observe a blocked electronic relaxation due to combined spin and valley selection rules. Time averaged transport measurements put a lower bound of 50 ns on the rate of the blocked transition, 1000 times slower than a bulk transition. For the low lying excited states Hund's rule is violated due to vanishing exchange in orthogonal valleys. Furthermore, we observe reduced charging energies and bound singlet and triplet excited states for this negatively charged donor that can be explained in the self consistent tight binding model. Finally, experiments demonstrating coherent coupling between two donors and between a donor and the leads will be discussed.

[1]In collaboration with G.P. Lansbergen, R. Rahman, J. Verduijn, G. C. Tettamanzi, N. Collaert, S. Biesemans , G. Klimeck, and L.C.L. Hollenberg.

3:42PM L2.00003 Orbital Gating of Single Molecule Transistors , MARK REED, Yale University — Electron devices containing molecules as the active region have been an active area of research over the last few years. In molecular-scale devices, a longstanding challenge has been to create a true three-terminal device; e.g., one that operates by modifying the internal energy structure of the molecule, analogous to conventional FETs. Here we report the observation of such a solid-state molecular device, in which transport current is directly modulated by an external gate voltage. We have realized a molecular transistor made from the prototype molecular junction, benzene dithiol, and have used a combination of spectroscopies to determine the internal energetic structure of the molecular junction. Resonance-enhanced coupling to the nearest molecular orbital is revealed by electron tunneling spectroscopy, demonstrating for the first time direct molecular orbital gating in a molecular electronic device.

4:18PM L2.00004 A single-molecule optical transistor , VAHID SANDOGHDAR, ETH Zurich — This abstract not available.

4:54PM L2.00005 Optical, magnetic and electronic properties of graphene quantum dots[1] , A. DEVRIM GUCLU, National Research Council of Canada — We present a theory of optical, magnetic and electronic properties of graphene quantum dots. We demonstrate that there exists a class of triangular graphene quantum dots with zigzag edges [1-8] which combines magnetic, optical and transport properties in a single-material structure. These dots exhibit robust magnetic moment and optical transitions simultaneously in the THz, visible and UV spectral ranges due to the existence of a band of degenerate states lying at the Fermi level in the middle of the energy gap [1-6]. The magnetic and optical properties[5,7] are determined by strong electron-electron and excitonic interactions in the degenerate band, treated exactly using numerical techniques combining tight-binding, DFT, Hartree-Fock and configuration interactions methods. We show that the spin polarized degenerate band leads to quenching of the absorption spectrum at half-filling, while addition of a single electron fully depolarizes all electron spins and turns the absorption on. It is thus possible to design gate and size tunable graphene quantum dots with desired optical and magnetic properties for optoelectronic and photo-voltaic applications. Collaborators: P. Potasz, O. Voznyy, M. Korkusinski, and P. Hawrylak.

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[1]The author thanks NRC-CNRS CRP, Canadian Institute for Advanced Research, Institute for Microstructural Sciences, and QuantumWorks for support.

Tuesday, March 22, 2011 2:30PM - 5:30PM –
Session L3 DCMP: Gap Structure of the Ba-122 Iron Based Superconductors Ballroom A3

2:30PM L3.00001 Electronic structure studies of $Ba/EuFe_2As_2$ based superconductors by angle and time-resolved photoemission spectroscopy , JOERG FINK, Helmholtz-Zentrum Berlin/ IFW Dresden — We report high-resolution ARPES studies on the evolution of the electronic structure of $Ba/EuFe_2As_2$ compounds upon n-type doping by replacing Fe by Co and applying chemical pressure by substituting As by P. In particular, we have investigated the nesting conditions between the hole pockets in the centre and the electron pocket at the corner of the Brillouin zone (BZ) for various wave vectors perpendicular to the FeAs layers. In the case of chemically doped systems we observe a shift of the Fermi level in an almost rigid band system. These changes of the electronic structure upon doping cause a reduction of the nesting conditions, possibly yielding a microscopic explanation of the phase diagrams in which antiferromagnetic (AF) order is destroyed, followed by the appearance and disappearance of superconductivity at higher doping concentration. On the basis of the almost equivalent phase diagram obtained upon chemically pressurizing the compound, one expects a similar change of the electronic structure. However, in this case, with increasing P concentration, we observe a non-rigid-band-like change of the electronic structure in the centre of the BZ. In spite of this difference, also here the nesting conditions decrease with increasing P substitution, possibly providing a microscopic explanation for the phase diagram. Finally, we have performed femtosecond time-resolved ARPES studies on undoped and doped $Ba/EuFe_2As_2$ after optical pumping. Regarding the relaxation processes we obtain information on the complex dynamics of the excited electronic state in these semi metallic systems. Furthermore, we derive a small electron-phonon coupling constant making electron-phonon coupling an unlikely candidate for the mechanism of high-T_c superconductivity in these compounds. This work is performed in collaboration with S. Thirupathaiah, E. Rienks, H. A. Dürr, S. de Jong, E. van Heumen, E. Slooten, Y. Huang, R. Huisman, M. S. Golden, L. Rettig, R. Cortes, U. Bovensiepen, M. Wolf, A. Erb, T. Wolf, H.S. Jeevan, P. Gegenwart.

3:06PM L3.00002 Symmetry of spin excitation spectra in 122-ferropnictides[1] , DMYTRO INOSOV, MPI-FKF Stuttgart — We have studied the symmetry of spin excitation spectra in 122-ferropnictide superconductors by comparing the results of first-principles calculations with inelastic neutron scattering (INS) measurements on Ni- and Co-doped $BaFe_2As_2$ samples close to the optimal doping level, which exhibit neither static magnetic phases nor structural phase transitions. In both the normal and superconducting (SC) states, the spectrum does not follow the $I4/mmm$ space group of the crystal, but instead inherits its symmetry from the unfolded Brillouin zone of the Fe- sublattice. This is manifest both in the in-plane anisotropy of the normal- and SC-state spin dynamics and in the out-of-plane dispersion of the spin-resonance mode and the SC spin gap. The in-plane anisotropy is temperature-independent and can be qualitatively reproduced in normal-state density-functional theory calculations without invoking a symmetry-broken ("nematic") ground state that was previously proposed as an explanation for this effect. Below the SC transition, the energy of the magnetic resonant mode, as well as its intensity and the SC spin gap, inherit the normal-state intensity modulation along the out-of-plane direction. Apparently, it can be traced back to the three-dimensional band structure and the superconducting gap, both of which were reported to disperse along the out-of- plane direction.

[1]This work has been supported, in part, by the DFG within the Schwerpunktprogramm 1458, under Grant No. BO3537/1-1.

3:42PM L3.00003 London penetration depth as a sensitive tool for determining the superconducting gap structure in iron-pnictide superconductors , RYAN GORDON, Department of Physics and Astronomy, Iowa State University and Ames Laboratory, Ames, IA — In the high$-T_c$ cuprates, experiments and theories have relied on a single-band picture that is essentially two- dimensional with a single superconducting gap, which provided a simple way to understand the angular dependence of the superconducting order parameter. In iron-based superconductors, the experimental mapping of the superconducting gap structure is complicated by the doping- dependent, multi-band electronic structure with three- dimensional character and the existence of at least two distinct superconducting gaps. Focusing on precision measurements of the London penetration depth, $\lambda(T)$, in "122" $Ba(Fe_{1-x}T_x)_2As_2$ (T=Co,Ni,Ru,Pt,Pd,Co+Cu) single crystals, I will discuss the systematics of the ubiquitous power law temperature variation of the in-plane penetration depth, $\lambda_{ab}(T) = \lambda_{ab}(0) + \beta T^n$, and of the absolute value, $\lambda_{ab}(0)$, with the doping level, x. To understand the role of disorder and pairbreaking scattering, the effect of heavy ion irradiation has been systematically studied and the results are compared with other systems, most notably stoichiometric LiFeAs. Together with the doping dependence of the out-of- plane London penetration depth, $\lambda_c(T)$, and comparisons to thermal conductivity and specific heat data, these results strongly suggest the development of a significant in-plane anisotropy of the superconducting gap(s) and are also consistent with the appearance of accidental c-axis nodes (not imposed by symmetry) for concentrations moving away from optimal doping. By taking pairbreaking scattering into account, the data for the optimally doped compounds are well described by weak-coupling superconductivity with two nodeless superconducting gaps having amplitudes that differ by about a factor of two. I conclude by emphasizing the significant role of three-dimensionality and scattering in determining the electrodynamics of iron-based superconductors.

4:18PM L3.00004 Phase diagram and superconducting gap structure of the iron-pnictide superconductor $(Ba,K)Fe_2As_2$[1] , XIGANG LUO, Department de Physique, Universite de Sherbrooke, Sherbrook, Quebec J1K2R1, Canada — Measurements of the Nernst and Seebeck coefficients were used to delineate the T-x phase diagram of the iron-pnictide superconductor $Ba_{1-x}K_xFe_2As_2$. The sensitivity of these two coefficients to the reconstruction of the Fermi surface caused by the onset of antiferromagnetic order below a temperature T_N allowed us to track T_N precisely as a function of concentration x, even when the electrical resistivity, for example, shows no anomaly at the magnetic transition. In the region of concentrations where superconductivity appears out of an antiferromagnetic normal state ($T_c < T_N$), we investigate the evolution of the superconducting gap structure of $Ba_{1-x}K_xFe_2As_2$ by measuring the thermal conductivity in the T=0 limit. This is a sensitive and directional probe of nodal quasiparticles. As the concentration x is reduced, we find a sudden change in the gap structure from a full gap without nodes to a gap with nodes. We ascribe this change to the onset of antiferromagnetism below a critical doping x_N inside the superconducting phase, whose effect is most likely to alter both the Fermi surface and the angular dependence of the gap. We compare these results with our earlier study on $Ba(Fe_{1-x}Co_x)_2As_2$ [1,2].

[1] M. Tanatar *et al.*, Physical Review Letters **104**, 067002 (2010).
[2] J.-Ph. Reid *et al.*, Physical Review B **82**, 064501 (2010).

[1]This work was performed in collaboration with H. Shakeripour, J. Chang, F. Laliberte, J.-Ph. Reid, N. Doiron-Leyraud, L. Taillefer, M.A. Tanatar, R. Prozorov, H. Q. Luo, Z. S. Wang, H.-H. Wen

4:54PM L3.00005 Superconductivity in a 3D tight-binding model for Ba-122[1] , SIEGFRIED GRASER, University of Augsburg — Theoretical investigations of the superconducting state in the iron pnictides have shown that weak-coupling approaches based on a tight-binding parametrization of the LDA band structure can be successfully applied to describe both magnetism and superconductivity in these materials. FLEX, RPA, and fRG studies find in most cases a superconducting state with s-wave symmetry that exhibits a π-phase shift between the gap on the electron and the hole Fermi surfaces, often called a sign-changing s-wave state. Besides this general agreement about the symmetry of the superconducting state these studies have also revealed that the momentum dependence of the gap, including the possibility of gap nodes, is highly sensitive to details of the electronic structure, in particular to the orbital composition of the Fermi surface. Since superconductivity in these materials is restricted to the FeAs layers that, at least for the 1111 compounds, are well separated and only weakly coupled most tight-binding models used to study the superconducting state have been limited to two dimensions. On the other hand the 122 compounds as well as the binary compounds show a very pronounced 3D electronic structure with changing orbital weights on the Fermi surfaces along the k_z direction. An RPA based calculation of the spin susceptibility for the Ba-122 material demonstrates that the necessary averaging over the full three dimensional Brillouin zone leads to a broader and more commensurate spin response compared to a corresponding two dimensional calculation in agreement with experimental observations. In addition changes of the orbital character of the Fermi surface lead to a complicated three dimensional gap structure exhibiting V-shaped or near horizontal nodes on the hole sheets near the zone boundary that can in part explain the puzzling transport measurements.

[1]This work was supported by the German Research Foundation through TRR80.

Tuesday, March 22, 2011 2:30PM - 5:30PM –

Session L4 GQI: Quantum Information: Featured Experiments Ballroom A4

2:30PM L4.00001 Entanglement of spin waves among four quantum memories[1] , H. JEFF KIMBLE, California Institute of Technology — Quantum networks are composed of quantum nodes that interact coherently by way of quantum channels and open a broad frontier of scientific opportunities [1]. For example, a quantum network can serve as a 'web' for connecting quantum processors for computation and communication as well as a "simulator" for enabling investigations of quantum critical phenomena arising from interactions among the nodes mediated by the channels. The physical realization of quantum networks generically requires dynamical systems capable of generating and storing entangled states among multiple quantum memories, and of efficiently transferring stored entanglement into quantum channels for distribution across the network. While such capabilities have been demonstrated for diverse bipartite systems, entangled states have so far not been achieved for interconnects capable of "mapping" multipartite entanglement stored in quantum memories to quantum channels. In my presentation, I will describe an experiment [2] that demonstrates measurement-induced entanglement stored in four atomic memories; user-controlled, coherent transfer of the atomic entanglement to four photonic channels; and characterization of the full quadripartite entanglement by way of quantum uncertainty relations [3]. Our work thereby provides an important advance for the distribution of multipartite entanglement across quantum networks. Moreover, our entanglement verification method can be applied for the study of entanglement order for condensed matter systems in thermal equilibrium. With regard to quantum measurement, our multipartite entangled state can be applied for sensing an atomic phase shift beyond the limit for any unentangled state.

[1] "The Quantum Internet," H. J. Kimble, Nature **453**, 1023 (2008).
[2] K. S. Choi, A. Goban, S. Papp, S. J. van Enk and H. J. Kimble, Nature **468**, 412 (2010).
[3] S. B. Papp *et al.*, Science **324**, 764 (2009).

[1]Work supported by NSF PHY-0652914 and by NSSEFF.

3:06PM L4.00002 Quantum Networks with Atoms and Photons , CHRISTOPHER MONROE, JQI and University of Maryland — Trapped atomic ions are among the most promising candidates for quantum information processing. All of the fundamental quantum operations have been demonstrated in this system, and the central challenge now is how to scale the system to larger numbers of qubits. By entangling atomic qubits through both deterministic phonon and probabilistic photon interfaces, the trapped ion system can be scaled in various ways for applications in quantum communication, quantum computing, and quantum simulations. I will discuss several options and issues for such atomic quantum networks, along with state-of-the-art experimental progress.

3:42PM L4.00003 Quantum-logic clocks for fundamental physics and geodesy[1] , TILL ROSENBAND, NIST — We have compared the rates of two quantum-logic clocks based on the optical $^1S_0$-$^3P_0$ transition in Al^+. The performance of the newer clock is unmatched, and despite many differences, their rates agree to $1.8 \pm 0.7 \times 10^{-17}$, within the accuracy limit of the older clock. The newer clock has an accuracy of 8.6×10^{-18} and stability near $10^{-15}(\tau/s)^{-1/2}$. Quantum-correlation spectroscopy yields an improved measurement stability of $3.7 \times 10^{-16}(\tau/s)^{-1/2}$. This technique also allows Q-factors beyond 6×10^{15} to be seen. This is the highest observed Q-factor in physics. The talk will discuss the basic operation of quantum-logic clocks based on Al^+, together with recent results that include a first geo-potential difference measurement, and constraints on the temporal variation of the fine-structure constant. Potential uses of entangled states in such clocks are also explored.

[1]Supported by ONR, NIST, AFOSR, and DARPA.

4:18PM L4.00004 Towards Quantum Information Processing with Superconducting Circuits[1] , ROBERT SCHOELKOPF, Yale University — In the dozen years since the initial demonstrations that superconducting circuits based on Josephson junctions could be considered as qubits, there has been remarkable progress in the field. Several different "species" of these artificial atoms have been designed and tested, and coherence times have increased by more than 1,000, or a factor of 10 every three years. While real devices are still far from satisfying all the DiVincenzo criteria with fidelities that would meet the error correction threshold, one can nonetheless perform preparation, control, quantum logic, and measurement on multiple superconducting qubits, all with surprisingly high purity and precision given that these are man-made, solid-state systems. In recent years we have seen the preparation of highly-entangled multi-qubit states that violate the Bell and Mermin inequalities, as well as the demonstration of single quantum algorithms, which all benefit from the strong coupling, addressability, and all-electronic control that is possible with these systems. Many experiments employ the concept of a "quantum bus," where qubits couple via superconducting transmission lines that form high-quality resonant cavities. A spinoff of this work is the advent of quantum optics on a chip: microwaves are photons too! The combination of qubits coupled to cavities has allowed the preparation and detection of single gigahertz photons, as well as other highly non-classical states of microwave light. Great progress has also been made in quantum measurement, and other Josephson circuits are now delivering amplifiers that operate at or beyond the Heisenberg limit. In this talk I will attempt to give an overview of some of the key concepts, some experimental highlights from recent years, and point out some possible directions for the future in this field.

[1]I would like to acknowledge all my collaborators at Yale, and funding from ARO, NSA/LPS, NSF, and IARPA.

4:54PM L4.00005 Quantum Information and the Foundations of Quantum Mechanics: a story of mutual benefit , ANTON ZEILINGER, Faculty oft Physics, University oft Vienna, and Institute oft Quantum Optics and Quantum Information — Fundamental tests, particularly of quantum nonlocality, in the 1970s were crucial for the development of the new field of quantum information science. The consequent development of new technologies has led to novel possibilities to do fundamental tests. A most simple and clear test of noncontextuality, i.e. the existence of joint probability distributions, is due to a proposal by Klyachko et al. [PRL 101, 020403 (2008)]. There, the experimental tests became possible because of technology developed for quantum communication. It turns out that a very simple and intuitive picture of the contradiction with realism can be given. In parallel, an experiment closing the freedom of choice loophole in quantum entanglement [T. Scheidl et al., Proc Natl Acad Sci USA (2010) 19709], together with earlier experiments testing the Leggett-type inequality and objectivity, i.e. the existence of observables without the context of observation, might be challenged. Current micro-optics technology and the exploitation of external states of light like Hermite-Gauss and Laguerre-Gauss allows to extend this kind of experiments into higher-dimensional Hilbert Spaces. There, interesting connections between entanglement and mutually unbiased bases have been found.

Tuesday, March 22, 2011 2:30PM - 5:30PM –

Session L5 COM: Topics in Alternative Energy Ballroom C1

2:30PM L5.00001 Efficient High Surface Area Vertically Aligned Metal Oxide Nanostructures for Dye-Sensitized Photoanodes by Pulsed Laser Deposition[1] , RENE LOPEZ, Department of Physics and Astronomy, University of North Carolina at Chapel Hill, NC, 27599 — Dye Sensitized Solar Cells (DSSCs) differ from conventional semiconductor devices in that they separate the function of light absorption from charge carrier transport. At the heart of a DSSC is a metal oxide nanoparticle film, which provides a large effective surface area for adsorption of light harvesting molecules. The films need to be thick enough to absorb a significant fraction of the incident light but increased thickness results in diminished efficiencies due to augmented recombination. Losses in efficiency are due to the slow trap-limited diffusion process responsible for electron transport. This process limits the effective electron diffusion length to about $\sim$ 10 μm and results in an efficiency-limiting trade-off between light absorption and carrier extraction. Here we introduce a new structural motif for the photoanode in which the traditional random nanoparticle oxide network is replaced by vertically aligned bundles of oxide nanocrystals. This structure improves absorbed photon to current efficiencies (APCE) to values above 90% over most of the dye absorption range. The bundled anode is fabricated by a simple laser deposition process and features a surface area $\sim$ 2 times larger than that of traditional anodes. The direct pathways provided by the vertical structures also appear to provide for an enhanced collection efficiency for carriers generated throughout the device.

[1]This material is based upon work supported as part of the UNC EFRC: Solar Fuels and Next Generation Photovoltaics, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award N

3:06PM L5.00002 Predictive Defect Science for Cost-Effective Photovoltaics , TONIO BUONASSISI, Massachusetts Institute of Technology — Low-cost photovoltaic materials are typically defect-rich, and defects impede electronic transport and photoconversion efficiency. Since efficiency and cost are inversely related, defect-rich materials have until recently resulted in poor-quality, economically uncompetitive solar cells. In this presentation, we review defect physics in low-cost photovoltaic absorbers. Accurate identification of performance-limiting defects requires multiscale characterization, evaluating cm-size devices while probing down to the nanometer scale for defect recognition. We will review recent advances in macroscopic CCD-based PV characterization tools, and elucidate how these can be coupled to synchrotron nanoprobe techniques. Once the nature and underlying physical behavior of these defects are known, we demonstrate how manipulation of defect distribution and state, aided by predictive modeling, can enhance solar cell performance.

3:42PM L5.00003 Nanoscale heat transfer and thermoelectrics for alternative energy[1] , RICHARD ROBINSON, Cornell University — In the area of alternative energy, thermoelectrics have experienced an unprecedented growth in popularity because of their ability to convert waste heat into electricity. Wired in reverse, thermoelectrics can act as refrigeration devices, where they are promising because they are small in size and lightweight, have no moving parts, and have rapid on/off cycles. However, due to their low efficiencies bulk thermoelectrics have historically been a niche market. Only in the last decade has thermoelectric efficiency exceeded $\sim$20% due to fabrication of nanostructured materials. Nanoscale materials have this advantage because electronic and acoustic confinement effects can greatly increase thermoelectric efficiency beyond bulk values. In this talk, I will introduce our work in the area of nanoscale heat transfer with the goal of more efficient thermoelectrics. I will discuss our experiments and methods to study acoustic confinement in nanostructures and present some of our new nanostructured thermoelectric materials. To study acoustic confinement we are building a nanoscale phonon spectrometer. The instrument can excite phonon modes in nanostructures in the $\sim$100s of GHz. Ballistic phonons from the generator are used to probe acoustic confinement and surface scattering effects. Transmission studies using this device will help optimize materials and morphologies for more efficient nanomaterial-based thermoelectrics. For materials, our group has synthesized nano-layer superlattices of Na_xCoO_2. Sodium cobaltate was recently discovered to have a high Seebeck coeficent and is being studied as an oxide thermoelectric material. The thickness of our nano-layers ranges from 5 nm to 300 nm while the lengths can be varied between 10 μm and 4 mm. Typical aspect ratios are 40 nm: 4 mm, or 1:100,000. Thermoelectric characterization of samples with tilted multiple-grains along the measurement axis indicate a thermoelectric efficiency on par with current polycrystalline samples. Due to phonon confinement in nano-structures, it is expected that the thermoelectric efficiency of these sheets will be much higher than that of single crystalline $Na_{0.7}CoO_2$, when the nanosheets have single grains along the heat transport path.

[1]This work is supported by KAUST (KUS-C1-018-02), NSF (DMR 0520404), and the DOE (DE-SC0001086)

4:18PM L5.00004 Alternative Energy: A New Frontier for Microfluidics , CULLEN BUIE, Massachusetts Institute of Technology — Microfuidics is classified as the physics of fluid manipulation at sub-mm length scales. Typically, microfluidic techniques benefit from small sample volumes, low power consumption, and increased surface-to-volume ratio. Because of their high surface to volume ratio, microfluidic systems often utilize surface phenomena such as wettability (i.e. droplet microfluidics) and surface charge (i.e. electrokinetics) for actuation. To date, most applications of microfluidics are in medicine or biology with the purpose of creating "lab on a chip" devices. However, the scale of microfluidics is favorable for other engineering problems as well. In this talk we will discuss how phenomena typically applied to lab on a chip devices can be used to enhance energy systems. Specifically, we explore electric field driven fluid and particle flows such as electrophoresis, electroosmosis, and dielectrophoresis. We will show how these phenomena can solve a diverse array of problems, from water management in fuel cells to the selection of microorganisms for bio-energy applications.

4:54PM L5.00005 Fusion related physics: Understanding the basic physics of High Energy Density Plasmas (HEDP) using ultra-short pulse laser-matter interactions[1] , RONNIE SHEPHERD, Lawrence LIvermore National Lab — Nuclear fusion is one nature's most fundamental methods of generating energy. In stars, the fusion reactions that occur deep within stellar interiors generate radiation and particles that fill the Universe. For many years, a goal of scientists has been to utilize these processes on earth to generate energy. However, understanding the basic physics of the interacting particles is required to exploit this energy source. We present data and analysis from one technique (ultra-short pulse laser matter interactions) currently being used to understand this physics. High power, short pulse lasers offer the ability of studying matter heated to extremely high temperatures (as high as 700 eV) and near solid density (10^{22} part/cm^3). Two aspects of the basic physics will be presented, namely radiation absorption and particle energy exchange currently under investigation using these lasers.

[1]This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Tuesday, March 22, 2011 2:30PM - 5:30PM –

Session L6 FIAP: Complexity in Invention: The Strongly Coupled Systems that Contribute to Innovation Success Ballroom C2

2:30PM L6.00001 ABSTRACT WITHDRAWN –

3:06PM L6.00002 Value analysis for advanced technology products , MARK SOULLIERE, Corning Incorporated — Technology by itself can be wondrous, but buyers of technology factor in the price they have to pay along with performance in their decisions. As a result, the "best" technology may not always win in the marketplace when "good enough" can be had at a lower price. Technology vendors often set pricing by "cost plus margin," or by competitors' offerings. What if the product is new (or has yet to be invented)? Value pricing is a methodology to price products based on the value generated (e.g. money saved) by using one product vs. the next best technical alternative. Value analysis can often clarify what product attributes generate the most value. It can also assist in identifying market forces outside of the control of the technology vendor that also influence pricing. These principles are illustrated with examples.

3:42PM L6.00003 Innovation, Novel Solutions and New Devices: The Engines that Drive the Magnetic Storage Industry; Choosing the Right Combination , ERNESTO E. MARINERO, Hitachi GST San Jose Research Center, 3404 Yerba Buena Road San Jose, CA 95135, USA — Magnetic storage technology aims to achieve recording densities $> 10^{12}$ bits/in2 in the foreseeable future. The dimensions of the magnetic domains and sensor minimum feature sizes at this density will be $\sim$ 15 – 25 nm. These nanoscale dimensions present major challenges for both the materials utilized for magnetic recording, and to the sensors employed to reliably detect the minute magnetic fluxes emanating from such nanoscale domains. These include fundamental physical limits of material properties on account of the reduced dimensionality, as well as nanofabrication challenges to attain the required nanometer feature sizes with the stringent dimensional tolerances required. Since its invention in 1954, the storage density in magnetic recording has incremented by 10^9 and the cost of storage, measured in \$/MB, has undergone a price reduction of the same order. Impressive as these accomplishments are, is the fact that the fundamental engineering principles of the technology today are essentially the same as when it was invented. This is in spite of numerous efforts to replace it with new alternative technologies or by dire predictions by its own practitioners of its impending death based on perceived limitations. In this talk the state-of-the art and challenges facing the HDD industry in its efforts to continue incrementing the storage density will be discussed. I will illustrate how advances in materials engineering, new physical phenomena and breakthroughs in nanofabrication have facilitated such an impressive technology evolution. Moreover, the key ingredients for said innovations to be implemented as technology solutions will be discussed..

4:18PM L6.00004 Manufacturing physics: using large(r) data sets and physical insight to develop great products , STEVEN ROSENBLUM, Corning Incorporated — Early stage research does a fantastic job providing knowledge and proof-of-feasibility for new product concepts. However, the handful of data points required to validate a concept is typically insufficient to provide insight on the whole range of effects relevant to manufacturing the product. Moving to manufacturing brings larger data sets and variability; opportunistic analysis of these larger sets can yield better product design rules. In the early 2000s Corning developed an optical transmission fiber optimized to suppress stimulated Brillouin scattering (SBS). Analyzing the larger data set provided by the manufacturing environment using the same theoretical framework developed by the original researchers refined our understanding of how to improve SBS in optical fibers beyond what was known from our early efforts. This greater understanding allowed us to design better performing products.

4:54PM L6.00005 Foundational Forces & Hidden Variables in Technology Commercialization , BRANDON BARNETT, Intel Corporation — The science of physics seems vastly different from the process of technology commercialization. Physics strives to understand our world through the experimental deduction of immutable laws and dependent variables and the resulting macro-scale phenomenon. In comparison, the goal of business is to make a profit by addressing the needs, preferences, and whims of individuals in a market. It may seem that this environment is too dynamic to identify all the hidden variables and deduct the foundational forces that impact a business's ability to commercialize innovative technologies. One example of a business "force" is found in the semiconductor industry. In 1965, Intel co-founder Gordon Moore predicted that the number of transistors incorporated in a chip will approximately double every 24 months. Known as Moore's Law, this prediction has become the guiding principle for the semiconductor industry for the last 40 years. Of course, Moore's Law is not really a law of nature; rather it is the result of efforts by Intel and the entire semiconductor industry. A closer examination suggests that there are foundational principles of business that underlie the macro-scale phenomenon of Moore's Law. Principles of profitability, incentive, and strategic alignment have resulted in a coordinated influx of resources that has driven technologies to market, increasing the profitability of the semiconductor industry and optimizing the fitness of its participants. New innovations in technology are subject to these same principles. So, in addition to traditional market forces, these often unrecognized forces and variables create challenges for new technology commercialization. In this talk, I will draw from ethnographic research, complex adaptive theory, and industry data to suggest a framework with which to think about new technology commercialization. Intel's bio-silicon initiative provides a case study.

Tuesday, March 22, 2011 2:30PM - 5:30PM –

Session L7 DBP: System Biology I: The Physics of Development Ballroom C3

2:30PM L7.00001 Robustness in multicellular systems , JOAO XAVIER , Memorial Sloan Kettering Cancer Center — Cells and organisms cope with the task of maintaining their phenotypes in the face of numerous challenges. Much attention has recently been paid to questions of how cells control molecular processes to ensure robustness. However, many biological functions are multicellular and depend on interactions, both physical and chemical, between cells. We use a combination of mathematical modeling and molecular biology experiments to investigate the features that convey robustness to multicellular systems. Cell populations must react to external perturbations by sensing environmental cues and acting coordinately in response. At the same time, they face a major challenge: the emergence of conflict from within. Multicellular traits are prone to cells with exploitative phenotypes that do not contribute to shared resources yet benefit from them. This is true in populations of single-cell organisms that have social lifestyles, where conflict can lead to the emergence of social "cheaters," as well as in multicellular organisms, where conflict can lead to the evolution of cancer. I will describe features that diverse multicellular systems can have to eliminate potential conflicts as well as external perturbations.

3:06PM L7.00002 Axis Specification in Hydra , ALBRECHT OTT, Universitaet des Saarlandes — Hydra is an about cm sized polyp of roughly 10^5 cells exhibiting surprising robustness: it can regenerate even from a random cell aggregate made from its own cells. During such a reorganization, hydra first forms a hollow cell sphere. We show that even a weak temperature gradient directs the axis of the regenerating animal – but only if it is applied during the symmetry-breaking moment. We observe that the spatial distribution across the cell sphere of the early expressed, head-specific gene ks1 has become scale-free and fractal at that point. We suggest that in order to break the symmetry and define an axis during the regeneration process, the cell network organizes towards a state, that is characterized by an unusually high sensitivity to external perturbation as well as spatially self-similar gene expression patterns. The observed behavior arises naturally from next-neighbor cell communication, when long-range signaling as required for axis definition is achieved through increased synchronization of expression profiles. Numerical results in progress show that our observations can be robustly reproduced with avalanches of gene expression patterns generated from gene switching above a stimulation threshold.

3:42PM L7.00003 Surface cell differentiation controls tissue surface tension and tissue positioning during zebrafish gastrulation , S.F.G. KRENS[1], Institute of Science and Technology Austria — Differences in tissue surface tension (TST) between different tissue types are thought to guide tissue organization and cell sorting in development. Measurements of TST have been useful to predict the outcome of in vitro cell sorting and envelopment experiments. However, the outcome of cell sorting experiments in vitro often substantially differs from tissue positioning in vivo, raising questions as to the actual contribution of TST to tissue positioning within the developing embryo. Here, we show that surface tension of germ layer tissues during zebrafish gastrulation critically relies on the differentiation of their surface cells. We also show that surface differentiation of the different germ layer tissues varies and is considerably different between the situation in vitro and in vivo, explaining the apparent dissimilar outcome of cell segregation between these two situations. To analyze germ layer TST as a function of surface cell differentiation, we interfere with surface cell properties of germ layer aggregates by misexpressing genes involved in surface cell differentiation specifically within surface cells using the GAL4-UAS system, and measure tissue surface tension using both parallel plate compression and micropipette aspiration techniques. Our data provides evidence in favor of a critical function of surface cell differentiation in modulating TST and subsequently tissue positioning within the developing embryo.

[1]In collaboration with C.P. Heisenberg, Max Planck Institute of Molecular Biology and Genetics.

4:18PM L7.00004 Self-organized cytoskeletal dynamics during fruit fly epithelial morphogenesis , KONSTANTIN DOUBROVINSKI, Princeton University — Epithelial morphogenesis plays a major role in embryonic development. During this process cells within epithelial sheets undergo complex spatial reorganization to form organs with specific shapes and functions. The dynamics of epithelial cell reorganization is driven by forces generated through the cytoskeleton, an active network of protein filaments and motor proteins. In this talk, I will present a novel mesoscopic-scale physical description of force generation by the cytoskeleton, and show that this minimal description can account for a wide range of phenomena associated with fruit fly epithelial morphogenesis.

4:54PM L7.00005 Collective Chemotactic Cell Movement; a Key Mechanism of Development and Morphogenesis , CORNELIS WEIJER, College of Life Sciences University of Dundee — We investigate the molecular mechanisms by which cells produce and detect chemotactic signals and translate this information in directed movement up or down chemical gradients in the social amoebae *Dictyostelium discoideum,* and during gastrulation in the chick embryo. Investigation of Dictyostelium mutants with changes in cAMP cell-cell signalling dynamics and chemotaxis, show how cellular heterogeneity in signalling dynamics and polarised activation of the actin-myosin cytoskeleton drive aggregation, cell sorting, slug formation and migration. Chemotactic cell movement also plays a critical role during gastrulation in the chick embryo a model for amniote development. We suggest that epiblast cell movement during the formation of the primitive streak as well as the movement of the mesoderm cells after their ingression through the streak is controlled by a combination of attractive and repulsive guidance cues. We use computer models explore signalling and cell movement interact to give rise to emergent phenomena at the tissue and organism level such as pattern formation and morphogenesis.

Tuesday, March 22, 2011 2:30PM - 5:30PM –
Session L8 FHP: J. H. Van Vleck: Quantum Theory and Magnetism Ballroom C4

2:30PM L8.00001 Van Vleck from Spectroscopy to Susceptibilities: Kuhn Losses Regained , MICHEL JANSSEN, University of Minnesota — As a young assistant professor in Minneapolis, John H. Van Vleck spent much of his time between 1923 and 1926 writing a book-length Bulletin for the National Research Council. As its title, Quantum Principles and Line Spectra, suggests, the book focuses almost exclusively on spectroscopy, the core pursuit of the old quantum theory. By the time it finally appeared in 1926, the old quantum theory had given way to the new quantum mechanics. Van Vleck soon realized that matrix mechanics reinstated some well-confirmed results of the classical theory of susceptibilities that had been lost in the old quantum theory. In the history and philosophy of science literature, such losses are called 'Kuhn losses'. Using mathematical techniques similar to those presented in his NRC Bulletin, Van Vleck started to work on the theory of susceptibilities. In 1929, now a full professor in Madison, he began writing another book, which appeared in 1932 and has become a classic: The Theory of Electric and Magnetic Susceptibilities. In this talk I follow Van Vleck's trajectory from spectroscopy to susceptibilities and examine how his two books reflect and helped shape research traditions.The talk is based on joint work with Charles Midwinter.

3:06PM L8.00002 J. H. Van Vleck and Magnetism at the University of Wisconsin: 1928 -1934 , DAVID HUBER, Univ. of Wisconsin-Madison — In 1928, John Van Vleck returned to his alma mater to take a position in the Physics Department. Six years later he left to join the faculty of Harvard University. While Van Vleck was at Wisconsin, he began a series of theoretical studies that helped lay the foundation for the modern theory of magnetism in solids. In 1932 Van Vleck published his celebrated monograph, *The Theory of Electric and Magnetic Susceptibilities,* in which he made use of the new theory to explain the results of experimental studies in a variety of magnetic materials. In my talk, I will review the accomplishments of Van Vleck and his students during this period and also comment briefly on his notes for a second edition of the book.

3:42PM L8.00003 My interactions with J.H. Van Vleck as a student and colleague at Harvard , NICOLAAS BLOEMBERGEN, University of Arizona — In the summer of 1947 I participated as a graduate student in discussions with professors J.H. Van Vleck, C.J. Gorter and E.M. Purcell on exchange narrowing of magnetic resonance lines. Subsequent work on exchange broadening and narrowing in nuclear spin systems will be reviewed and interspersed with personal reminiscences.

4:18PM L8.00004 Remembering Van: Three Madison families, and other tales , CHARLES P. SLICHTER, Department of Physics, University of Illinois, Champaign/Urbana, IL61801 — The talk will present some history, in part personal, in part scientific, of Van's influence on other scientists and on magnetic resonance.

4:54PM L8.00005 Van Vleck and the magnetic susceptibilities of gaseous molecules , HORST MEYER, Duke University — In his 1927 Physical Review article and in his 1932 book, *The Theory of Electric and Magnetic Susceptibilities,* Van Vleck used the new quantum theory to derive the magnetic susceptibilities of O_2 and NO in their gaseous form and compared them with experiments. He was therefore very interested in low temperature susceptibility experiments on O_2 at Oxford University in 1954 where individual O_2 molecules were trapped in small, almost spherical cages in organic clathrates. Correspondence between him and this speaker, then at Oxford, led to further measurements of O_2 and also of NO in such clathrates, to theory and to subsequent publications and correspondence. Later communication with Van Vleck on the magnetism in rare earth iron garnets, a subject of long-term interest to him, will be described in connection with experiments carried out at Duke University. Some fond personal recollections of this speaker of his interaction with Van Vleck - both while at Harvard, during visits and through correspondence which extended into the seventies - will be presented.

Tuesday, March 22, 2011 2:30PM - 5:30PM –
Session L9 DFD: Micelles and Vesicles I D220

2:30PM L9.00001 Faceting of multicomponent charged elastic shells , RASTKO SKNEPNEK, CHEUK LEUNG, LIAM C. PALMER, Northwestern University, GRAZIANO VERNIZZI, Siena College, SAMUEL I. STUPP, MICHAEL J. BEDZYK, MONICA OLVERA DE LA CRUZ, Northwestern University — Combining coarse-grained molecular dynamics simulations with continuum elastic theory, we show that electrostatic interactions between charged lipid head groups can lead to the crystallization of the bilayer. Regions with different molecular charge ratios have distinct elastic properties and naturally tend to segregate inducing an effective line tension between neighboring patches. The line tension and local patch-dependent elastic properties, i.e., bending rigidity and Young modulus, have a drastic effect on the shell shape. We explore a wide region of parameter space and find a gallery of faceted structures, closely resembling shapes of shells recently identified experimentally.

2:42PM L9.00002 Modeling co-evolution of defects and curvature in lipid vesicles: coarse-grained simulation studies[1] , ROBIN SELINGER, JUN GENG, JONATHAN SELINGER, Kent State Univ. — To explore interaction between topological defects and curvature in lipid vesicles, we present a coarse-grained simulation approach in which defects and vesicle shape both evolve in time. First we model a vesicle cooled into the tilted gel phase. To represent the tilt field at the mesoscale, we superimpose an XY model onto a coarse-grained liquid membrane [1] where each particle represents a patch of lipid bilayer. The presence of two $+1$ defects drives the vesicle to a prolate equilibrium state as previously predicted; but extra $+1/-1$ defect pairs may induce a highly disordered shape which is deeply metastable. We discuss comparison with relevant experiments. Next we consider a lipid vesicle with nematic order, e.g. composed of lipids with a rod-shaped head group. With weak coupling between defects and curvature, the vesicle is spherical with four $+1/2$ defects. With stronger coupling, the vesicle becomes prolate with two defects clustered at each end. As coupling is further increased, pores nucleate at the defects and coalesce, producing a hollow cylinder. We compare simulation results with theoretical predictions and consider further applications e.g. to study tilt and defects in gel phase lipid rafts.

[1] H. Yuan et al, *Phys Rev E* 82 (2010) 011905

[1]Supported by NSF-DMR-0605889.

2:54PM L9.00003 Coarse-grained model for lipid bilayer membranes and vesicles[1] , JUN GENG, JONATHAN SELINGER, ROBIN SELINGER, Kent State Univ. — We present a coarse-grained model for simulation studies of lipid bilayer membranes and vesicles. We separately track the behavior of the leaflets in each bilayer, allowing us to model the mechanics of vesicles and a rich array of other phases, topologies, and defect structures. Each particle in the coarse-grain model represents a patch of lipid molecules and carries a vector degree of freedom, representing the local average lipid chain orientation. Particles interact via a pair potential depending on separation distance and relative chain orientation. Solvent is treated as implicit, and membrane fluctuations are modeled via a Langevin thermostat. Resulting bilayer structures show liquid-like diffusion within each leaflet. We show that bilayer vesicles coalesce spontaneously from a random initial state, even though no spontaneous curvature is imposed by the model. We also explore the transition from vesicles to lamellar phases as a function of increasing density. We discuss potential application to the study of vesicle fission and fusion.

[1]Work supported by NSF-DMR-0605889

3:06PM L9.00004 Molecular dynamics study of shape transitions in aqueous micelle solutions[1] , A. SANGWAI, R. SURESHKUMAR, Syracuse University, Syracuse, NY 13244, USA. — It is well known that surfactant molecules self-assemble in aqueous solutions to form various micellar structures such as spheres, rods or sheets. Although this phenomenon is widely studied experimentally, the molecular mechanisms of shape transitions are not well understood. Atomistic simulations of self-assembled micellar systems are computationally prohibitive to sample several hundred nanoseconds necessary to capture shape transitions. We demonstrate that MARTINI coarse-grained (CG) force field for CTAC is capable of accurately representing micellar assemblies by comparing the CG system to fully atomistic ones. Microsecond molecular dynamic simulations using MARTINI CG models in explicit water are used to predict sphere to rod transitions in micelles. Inter-micelle association free energies are estimated to distinguish between the chemical environments in which the micelle assumes a spherical versus rod-like shape. Presence of hydrophobic salt e.g. Sodium Salicylate, is shown to greatly promote the formation of rodlike structures. CG MARTINI molecular dynamics is benchmarked as a practical approach to study nano-scale micellar structures.

[1]NSF Grant 1049454

3:18PM L9.00005 Ordered bulk aggregates of lipid vesicles , ANA HOCEVAR, Jozef Stefan Institute, PRIMOZ ZIHERL, Faculty of Mathematics and Physics, University of Ljubljana and Jozef Stefan Institute — We study the structure of bulk assemblies of identical lipid vesicles. In our model, each vesicle is represented as a convex polyhedron with flat faces, rounded edges, and rounded vertices. Each vesicle carries an elastic and an adhesion energy and it turns out that in the limit of strong adhesion, the minimal-energy shape of cells minimizes the weighted total edge length. We calculate the shape of the rounded edge exactly and show that it can be well described by a cylindrical surface. We compare several candidate space-filling polyhedra and we find that the oblate shapes are preferred over prolate shapes for all volume-to-surface ratios. We also study aggregates of vesicles whose adhesion strength on lateral faces is different from that on basal/apical faces. We determine the anisotropy needed to stabilize prolate shapes and we show that at any volume-to-surface ratio, the transition between the oblate and the prolate shapes is very sharp. We compare the geometry of the model vesicle aggregates with the shapes of cells in certain simple animal tissues. Predictions of our model are consistent with available experimental data.

3:30PM L9.00006 Understanding crumpling lipid vesicles at the gel phase transition[1] , LINDA HIRST, School of Natural Sciences, University of California, Merced, ADAM OSSOWSKI, MATTHEW FRASER, University of California, Merced — Wrinkling and crumpling transitions in different membrane types have been studied extensively in recent years both theoretically and computationally. There has also been very interesting recent work on defects in liquid crystalline shells. Lipid bilayer vesicles, widely used in biophysical research can be considered as a single layer smectic shell in the liquid crystalline phase. On cooling the lipid vesicle a transition to the gel phase may take place in which the lipid chains tilt and assume a more ordered packing arrangement. We observe large scale morphological changes in vesicles close to this transition point using fluorescence microscopy and investigate the possible mechanisms for this transition. Confocal microscopy is used to map 3D vesicle shape and crumpling length-scales. We also employ the molecular tilt sensitive dye, Laurdan to investigate the role of tilt domain formation on macroscopic structure.

[1]Funded by NSF CAREER award (DMR - BMAT #0852791).

3:42PM L9.00007 Thin shell vesicles composed of hydrophilic plate-like nanoparticles , ANAND SUBRAMANIAM, School of Engineering and Applied Sciences, Harvard University, JIANDI WAN, Department of Mechanical and Aerospace Engineering, Princeton University, ARVIND GOPINATH, Fischer School of Physics, Brandeis University, HOWARD STONE, Department of Mechanical and Aerospace Engineering, Princeton University — Nanopowders of graphene oxide, montmorillonite and laponite spontaneously delaminate into ultrathin nanoscopic plates when dispersed in water. These plates, which are typically $\sim$ 1 nm thick and microns in lateral dimension, have found many uses as precursors to graphene, ceramics, layer-by-layer structures, and as structural modifiers of nanocomposites. Here we show that mechanical forces due to shear in a narrow gap can assemble hydrophilic plate-like particles on air bubbles, forming stable nanoplated armored bubbles. Translucent inorganic vesicles (vesicles defined here as closed thin-shelled structures with the same liquid inside and outside) of these particles are produced when the nanoplated armored bubbles are exposed to common water-miscible organic liquids and surfactants. These inorganic vesicles are mechanically robust, have walls that are about six nanometres thick, and are perforated with pores of submicron dimensions. We characterize the phenomenon and find that a wetting transition at the scale of the nanoparticles is the primary mechanism of formation. The discovery of these novel inorganic structures raises a wealth of questions of fundamental interest in materials and surface science.

3:54PM L9.00008 The effect of interlayer distance of thickness fluctuations in a swollen lamellar phase: A neutron spin echo study , MICHIHIRO NAGAO, NIST Center for Neutron Research and Indiana University — Thickness fluctuations in surfactant membranes have been measured using small-angle neutron scattering (SANS) and neutron spin echo (NSE) techniques as a function of the membrane thickness in a swollen lamellar structure composed of nonionic surfactant, water and oil. An excess dynamics from the bending motion was observed around the length scales of the membrane thickness, which originates from thickness fluctuations of the membranes. The amount of oil in the bilayers controls the interlayer distance (membrane thickness) and the bending motion of the membranes. An enhancement of the thickness fluctuations suppresses the bending motion, which introduces the increase in the bending modulus at low swelling condition. The decrease in the bending modulus with further increase in the thickness indicates the decrease of the synchronization between monolayers. In the high swelling conditions, the monolayer movement dominates the dynamics of the membranes in the measured dynamic range.

4:06PM L9.00009 The effect of interlayer distance on thickness fluctuations in a swollen lamellar phase: A molecular dynamics study , SUKHUM CHAWANG, The Univesity of Oklahoma, TAKUMI HAWA, The University of Oklahoma — Molecular dynamics simulations have been conducted to characterize thickness fluctuations in a swollen lamellar structure, composed of a non-ionic surfactant, water, and oil, to verify the results of the neutron scattering experiments by Nagao. The thickness fluctuations are measured as an excess dynamics from the bending motion around the length scales of the membrane thickness and as a function of the interlayer distance (membrane thickness). The enhancement of the thickness fluctuations is observed in all ranges of thickness we simulated; however, it decays with increase of the membrane thickness. Dependence of directions of sampling wave vectors q on the thickness fluctuation is also investigated. At more normal direction (perpendicular to the membrane surfaces) the excess dynamics is clearly observed, while at more lateral direction (parallel to the membranes) the bending motion is more clearly observed. The present results show the existence of the enhancement of the thickness fluctuations and the importance of the sampling directions.

4:18PM L9.00010 Studies of lipid vesicle mechanics using an optical fiber dual-beam trap[1] , TESSA M. PINON, School of Engineering-University of California, Merced, LINDA S. HIRST, JAY E. SHARPING, School of Natural Sciences-University of California, Merced — Fiber-based optical traps can be used for manipulating micron-sized dielectric particles such as microspheres and biological cells. Here we study the mechanics of giant unilamellar vesicles (GUVs) which are held and stretched by light forces in a fiber-based dual-beam optical trap. Our GUVs are suspended in a buffer solution and encapsulate various concentrations and molecular weights of poly(ethylene glycol) (PEG) polymer yielding a range of refractive index contrasts and trapping conditions. We find that we can trap GUVs in solution with index contrasts of less than 0.01. We explore the mechanical response of the GUV membrane to a range of forces which are proportional to laser power and refractive index contrast. Our trapping system is a compact and inexpensive platform and trapping is viewed in real time under a microscope. We hypothesize that forces within the high-tension regime will induce a linear response in vesicle surface area. This project sets the stage for membrane mechanics and lipid phase change studies.

[1]Grant: NSF award #DMR 0852791, "CAREER: Self-Assembly of Polyunsaturated Lipids and Cholesterol in the Cell Membrane"

4:30PM L9.00011 Thermal Stress of Supported Lipid Bilayer Induces Formation and Collapse of Uniform Radius Tubules , KIMBERLY WEIRICH, DEBORAH FYGENSON, University of California, Santa Barbara — Supported lipid bilayer (SLB) provides a model system in which to quantitatively investigate fluid bilayer transitions from planar to tubular and tubular to spherical morphologies. Following a small increase in temperature, flexible filaments extrude from a fluid SLB. Individual filaments can reach hundreds of microns in length before spontaneously collapsing into discs. We demonstrate that the filaments are tubular and report the effects of lipid composition and flow-induced tension on their properties. At high ionic strength, the sub-resolution tubules are adsorbed to the SLB, enabling the measurement of their radius to within $\pm$5 nm using fluorescence microscopy.

4:42PM L9.00012 A Time-Resolved Study on Nanodisc-to-Vesicle Transformation , MU-PING NIEH, IMS/CMBE, Uinversity of Connecticut, SUANNE MAHABIR, WAN KEI WAN, University of Western Ontario, JOHN KASTARAS, Oak Ridge National Lab/CNBC — Structural phase diagram of a phospholipid mixture composed of dimyristoyl phosphatidylcholine (DMPC), dihexanoyl phosphatidylcholine (DHPC) and dimyristoyl phosphatidylglycerol (DMPG) contains many rich morphologies, e.g., nanodiscs also known as "bicelles", bilayered ribbons, unilamellar vesicles (ULVs), multi-lamellar vesicles (MLVs) and perforated lamellae. In this report, we will present time-resolved small angle neutron scattering and dynamic light scattering measurements of the structural transformation from nanodiscs to ULVs as a function of temperature, lipid concentration and charge density. The result will reveal the growth rate of nanodiscs and all the intermediate structures along the transformation process. Through the understanding of the kinetic pathway, the size and polydispersity of the self-assembled nano-size ULVs can be well-controlled. These ULVs can be used as a carrier for therapeutics or imaging probes.

4:54PM L9.00013 Crystallization Induced by Electrostatic Correlations in Vesicles of Mixed-Valence Ionic Amphiphiles[1] , CHEUK YUI LEUNG, RASTKO SKNEPNEK, LIAM PALMER, GRAZIANO VERNIZZI, MEGAN GREENFIELD, SAMUEL STUPP, MICHAEL BEDZYK, MONICA OLVERA DE LA CRUZ, Northwestern University — Charged amphiphilic molecules, including molecules with biological motifs, have been predicted to organize into elastic membrane or crystalline shells with non-spherical shapes. We demonstrate that pure electrostatic interaction allow (-1) anionic water insoluble amphiphiles and (+3) cationic amphiphiles, which form only micelles in water, to co-assemble into buckled vesicles. The strong interaction between the +3 and -1 head groups increases the cohesive energy of the amphiphiles and favors the formation of crystallized membranes or shells that facet spontaneously into buckled shapes predicted by simulations of vesicles with heterogeneous elastic properties. In situ small-angle and wide-angle X-ray scattering (SAXS-WAXS) experiments conducted at the Advanced Photon Source DND-CAT confirm the presence of crystalline bilayers. Our simulations verify that ionic lateral correlations among the oppositely charged head groups of the co-assembled amphiphiles are responsible for the observed tail crystallization.

[1]This work was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering (DOE Contract No. DE-FG02-08ER46539)

5:06PM L9.00014 Endocytic internalization of nanoparticles into polymeric vesicles. , ANJA KROEGER, KARMENA JASKIEWICZ, Max Planck Institute for Polymer Research, ANTJE LARSEN, Department of Materials Science and Technology, University of Crete and F.O.R.T.H., GEORGE FYTAS, Department of Materials Science and Technology, University of Crete and F.O.R.T.H. and Max Planck Institute for Polymer Research — The monitoring of transport through cell membranes is essential for proper functioning of all living organisms. Poorly understood mechanisms of endocytosis have become the focus of intense investigations. Here we present a photon correlation spectroscopy study of the uptake of polystyrene nanoparticles (hydrodynamic radius, R_h=16nm) by poly(dimethylsiloxane)-b-poly(2-methyloxazoline) polymersomes (R_h=150nm) in aqueous solution. The relaxation function C(q,t) for a particle/polymersome mixture with a molar ratio 100:1 at different scattering wave vectors (q) reveal the presence of free and bound particles. Both the experimental form factor P(q) and the effective diffusion coefficient D(q) of the polymersome in the q-range of 0.005-0.033nm^{-1}are consistently described by modeling these q-patterns by a filled polymersome with about 30 particles under the examined conditions. The emerged picture is supported by cryo-TEM imaging.

5:18PM L9.00015 AC-Electrokinetic Characterization and Induced Encapsulation Release of Micelles in Aqueous Suspensions , VICTORIA FROUDE, YINGXI ELAINE ZHU, University of Notre Dame — Micelles and polymers vesicles have been of increasing interest as drug delivery systems for controlled release, specific cell targeting, and medical diagnostics. In addition, AC-electrokinetic techniques have emerged as a viable option for colloidal and biocolloidal manipulation. In this work, we examine the dielectrophoresis (DEP) characteristics of complex micellar nanoparticles under non-uniform AC-electric field of varied ac-field frequencies (5 kHz-20 MHz) and amplitudes (0.1-10 Vpp) by fluorescence correlation spectroscopy (FCS) at a single-molecule resolution. We focus on the AC-field induced transport of sodium tetradecyl sulfate (STS) and sodium dodecyl sulfate (SDS) micelles tagged with various fluorescent and drug encapsulates in aqueous media. We observe a strong AC-frequency dependence of micelle concentration between two microelectrodes, from which the DEP crossover frequency is determined. Surprisingly, we also observe an AC-field induced dissociation of the micelle structure and a resulting release of fluorescent encapsulates at a characteristic low AC-field frequency of approximately 1-10 kHz, where the dissociation has been found to be dependent on the surface charge of the interior encapsulate.

Tuesday, March 22, 2011 2:30PM - 5:30PM –
Session L10 DCMP: Nanoclusters and Nanowires on Surfaces D221

2:30PM L10.00001 Structure and dynamics of PtSn/γAl_2O_3[1] , F.D. VILA, J.J. REHR, U. of Washington, S.D. KELLY, EXAFS Analysis, S.R. BARE, UOP LLC — Supported metal clusters have many industrial applications, especially in heterogeneous catalysis. Their activity and durability is determined by their internal atomic and electronic structure, as well as by their interaction with the support. We have previously shown[2] that unusual phenomena such as large structural disorder and negative thermal expansion in supported Pt clusters can be understood by using a combination of MD and x-ray absorption spectroscopy simulations. Here we present results for prototypical $Pt_{10}Sn_{10}$ alloy clusters on γAl_2O_3. Our simulations show that the internal structure and surface location of the clusters varies dynamically on a time scale of a few ps. While the Sn atoms are especially mobile, the clusters have well defined Pt-Pt and Pt-Sn coordination shells at $\sim$2.75Å. Moreover, at any instant there are between 2 and 5 bonds between the Pt/Sn and the O atoms in the surface. Finally, we present simulations of the XANES spectra and their relation to charge transfers between atoms in the cluster and between the cluster and the surface.

[1]Supported by NSF Grant PHY-0835543, UOP LLC, a Honeywell Company with computer support from NERSC.
[2]F. Vila *et al.*, Phys. Rev. B **78**, 121404(R) (2008).

2:42PM L10.00002 Polarization dependent Pd deposition structure on $LiNbO_3$ {0001} surface[1] , SEUNGCHUL KIM, ANDREW M. RAPPE, Department of Chemistry, University of Pennsylvania — We investigate effects of polarization orientation on atomic structure of palladium deposited on lithium niobate ($LiNbO_3$) {0001} surface, using density functional theory (DFT) and kinetic Monte Carlo (kMC) simulations. Adsorption, diffusion, aggregation and clustering process – include geometries, paths and energies – of Pd clusters were calculated from DFT simulations. It has been observed that energy barriers of Pd motions on the negatively poled (c^-) surface are much larger than those on the positively poled surface (c^+), which indicates the Pd motions on the c^- surface are much slower than that of c^+ surface. We demonstrate, using kMC with kinetic parameters from DFT, very slow motion of Pd on c^- surface leads dispersed small clusters or atoms while fast motion on c^+ surface leads large clusters, indicating larger Pd-covered area on c^- surface than c^+ after Pd deposition.

[1]This work has been supported by US-DOE (grant DE-FG02-07ER15920), and by AROSR (FA9550-07-1-0397). Computational support was provided by HPCMO of the US-DoD.

2:54PM L10.00003 Cu/CuOx Nanoclusters on ZnO(1010): Electronic, Catalytic, Morphological Structure[1] , ZIYU ZHANG, FEI WANG, Dept. of Physics, Louisiana State University, MAOMIN REN, Dept. of Chemical Engineering, Louisiana State University, FRANK WOMACK, Dept. of Physics, Louisiana State University, MINH LE, Dept. of Chemical Engineering, Louisiana State University, YAROSLAV LOSOVYI, CAMD, Louisiana State University, RICHARD KURTZ, PHIL SPRUNGER, Dept. of Physics, Louisiana State University, JOHN FLAKE, Dept. of Chemical Engineering, Louisiana State University — To develop a high performance catalyst for CO2 reduction, we tried bi-layers based on CuOx (x=0, 1, 2) and ZnO. The highest yield rate is found for Cu(I) on ZnO. The repeatability of the experiment illustrates that the Cu(I) catalytic clusters are stable in the air, due to the interface of the bilayer.STM and ARPUS results reveal that the preparation process are highly dependent on the annealing temperature and cluster size. EELS and UPS data show that CO adsorption is distinctly different between Cu and CuOx clusters on ZnO, which explains the different yield rate. Based on TDS and EELS of adsorption such as CO2, H2O, combined with DFT calculation, the mechanism of methanol synthesis is given by introducing intermediate products.

[1]Center for Atomic-lever Catalyst Design, DOE

3:06PM L10.00004 Role of nitrogen dopants in the stabilization of nancrystalline cubic zirconia , RENAT SABIRIANOV, Univesity of Nebraska at Omaha, G. WANG, Y.L. SOO, G. LUO, H.J. LIN, W.N. MEI, F. NAMAVAR, C.L. CHEUNG — The role of the nitrogen doping in the stabilizing the nanocrystalline cubic phase of zirconia films fabricated by nitrogen beam assisted deposition (IBAD) is investigated. The IBAD zirconia films have diameters three times larger than those previously reported in a sol-gel method. Confocal Raman spectroscopy study indicates that the atomic structure of these IBAD zirconia films evolve from cubic to tetragonal and then to monoclinic phase upon annealing at elevated temperatures. The presence of nitrogen in the films is confirmed by secondary ion mass spectroscopy. X-ray absorption near edge structure study of these films infers that the nitrogen atoms are incorporated at the substitutional sites of these films. Ab-initio density functional calculations suggests that the substitutional nitrogen atoms could effectively immobilize native defect including oxygen vacancies and interstitial ions in nanocrystalline cubic zirconia.

3:18PM L10.00005 Preparation dependent neutralization efficiency of Pt/TiO2 nanoparticles

, ALEX ARJAD, YARMOFF JORY, University of California, Riverside — Metal nanoclusters resident on an oxide surface can be produced by sputtering thin films as well as by direct deposition. We previously used the neutralization of scattered low energy alkali ions to demonstrate that Au nanoclusters formed by sputtering a thin gold film on TiO_2 have similar electronic properties as those formed by deposition [1]. In this work, we compare Pt nanoclusters grown on TiO_2 by both sputtering and deposition. It is shown that Pt nanoclusters formed by deposition are more efficient at neutralizing scattered low energy Na+ ions than those formed by sputtering a thin platinum film. We attribute this difference to the strong-metal-support-interaction (SMSI) present in the Pt/TiO_2 system, but not with Au/TiO_2.

[1] P. Karmakar, G.F. Liu, Z. Sroubek and J.A. Yarmoff, Phys. Rev. Lett. 98, 215502 (2007).

3:30PM L10.00006 Nanoparticle shape instability by Coulomb interactions[1]

, NATALYA ZIMBOVSKAYA, University of Puerto Rico-Humacao — Metal atoms adsorbed on few-layer graphenes condense to form nanometer-size droplets whose growth in size is limited by a competition between the surface tension and repulsive electrostatic interactions from charge transfer between the metal droplet and the graphene. Under certain conditions a growing droplet can be unstable to a family of shape instabilities. This phenomenon was observed for Yb deposited and annealed on few-layer graphenes. A theoretical model to describe it is developed. The model describes the onset of shape instabilities for nanoparticles where their growth is limited by a generic repulsive potential and provides a good account of the experimentally observed structures for Yb on graphene [1].

[1] L. A. Somers, N. A. Zimbovskaya, A. T. Johnson, and E. J. Mele, PhPhys. Rev B 82, 115430 (2010).

[1]NSF-DMR-0934195

3:42PM L10.00007 Structure and Energy Stability of Metal Nanoparticles[1]

, HECTOR BARRON, University of Texas at San Antonio, JUAN PEDRO PALOMARES-BAEZ, Instituto Potosino de Investigacion Cientifica y Tecnologica, JESUS VELAZQUEZ-SALAZAR, University of Texas at San Antonio, JOSE LUIS RODRIGUEZ-LOPEZ, Instituto Potosino de Investigacion Cientifica y Tecnologica, MIGUEL JOSE-YACAMAN, University of Texas at San Antonio, UNIVERSITY OF TEXAS AT SAN ANTONIO COLLABORATION, INSTITUTO POTOSINO DE INVESTIGACION CIENTUFICA Y TECNOLOGICA COLLABORATION — In this work we present a theoretical model for the structural evolution and energy stability for metal nanoparticles from the small (1-2 nm) to the big ($\sim$50 nm) size ranges. We have found that the appearances of structural lattice defects as well as surface reconstructions are important factors that highly influence the growth process. A simple assembly model for a path transformation for metal nanoparticles is presented and compare with experimental evidence.

[1]Acknowledgements: Financial support from National Science Foundation Grant DMR-0934218 is acknowledged, as well as grants for the use of High Performance Computational Resources from the supercomputer center TACC-University of Texas at Austin.

3:54PM L10.00008 ABSTRACT WITHDRAWN –

4:06PM L10.00009 Attachment of Quantum Dots on Zinc Oxide Nanorods

, JARED SEAY, HUAN LIANG, PARAMESWAR HARIKUMAR, University of Tulsa — ZnO nanorods grown by hydrothermal technique are of great interest for potential applications in photovoltaic and optoelectronic devices. In this study we investigate the optimization of the optical absorption properties by a low temperature, chemical bath deposition technique. Our group fabricated nanorods on indium tin oxide (ITO) substrate with precursor solution of zinc nitrate hexahydrate and hexamethylenetramine (1:1 molar ratio) at 95C for 9 hours. In order to optimize the light absorption characteristics of ZnO nanorods, CdSe/ZnS core-shell quantum dots (QDs) of various diameters were attached to the surface of ZnO nanostructures grown on ITO and gold-coated silicon substrates. Density of quantum dots was varied by controlling the number drops on the surface of the ZnO nanorods. For a 0.1 M concentration of QDs of 10 nm diameter, the PL intensity at 385 nm increased as the density of the quantum dots on ZnO nanostructures was increased. For quantum dots at 1 M concentration, the PL intensity at 385 nm increased at the beginning and then decreased at higher density. We will discuss the observed changes in PL intensity with QD concentration with ZnO-QD band structure and recombination-diffusion processes taking place at the interface.

4:18PM L10.00010 Controlled Deposition of Nanocrystal Quantum Dots on Silicon Surfaces

, OLIVER SEITZ[1], HUE M. NGUYEN[2], DAMIEN AUREAU[3], AMANDEEP SRA[4], ANTON V. MALKO[5], YVES J. CHABAL[6], University of Texas at Dallas — Studying Forster resonant energy transfer (FRET) has constantly been a challenge because of the poor control in transferring nanocrystal quantum dots (NQDs) onto various substrates. This lack of control often resulted in formation of aggregates (3D growth), inhomogeneity, and poor adhesion. In this study, using self assembled monolayers (SAMs), dense monolayer of NQDs have been attached onto silicon substrate, with and without the presence of oxide interlayer, allowing investigating FRET effects via photoluminescence measurements. Such SAMs, directly attached to the silicon, via Si-C bonds, display an interface quality with low interface states. Moreover, the ability to be prepared with tunable thicknesses renders them ideal for FRET investigation. Such hybrid colloidal NQD/Silicon optoelectronic structures could potentially be attractive for both photovoltaic as well as light emitting applications.

[1]Department of Materials Science and Engineering
[2]Department of Physics
[3]Department of Materials Science and Engineering
[4]Department of Materials Science and Engineering
[5]Department of Physics
[6]Department of Materials Science and Engineering

4:30PM L10.00011 Synthesis of a long gold atomic strand incorporated with carbon atoms

, YOSHIFUMI OSHIMA, TOMOYA ONO, Osaka University, KUNIO TAKAYANAGI, Tokyo Institute of Technology, NGUYEN DUY HUY, Osaka University — Single metal or carbon atomic strands have attracted much interest because of their unique properties. They have been usually fabricated by stretching or thinning the junction between both electrodes, but limited to be several atoms in length at maximum. We show that a long atomic strand can be synthesized by pulling one-dimensional reconstructed structure formed on the electrode surface. In the transmission electron microscope combined with a scanning tunneling microscope, gold atoms were observed to be pulled out one-by-one from carbon contaminated gold (111) surface layer each 0.5 nm elongation till diminishing the layer. This observation was explained by the first-principle calculation, showing that two carbon atoms are incorporated at each interval (0.5 nm) between two neighboring gold atoms aligned along the [112] direction to form the one-dimensional reconstructed structure, when the gold (111) surface is contaminated with carbon atoms.

4:42PM L10.00012 Scanning Tunneling Microscopy Study of Quantum Cobalt Chains[1] , NADER ZAKI, Columbia University, DANDA ACHARYA, Pacific Northwest National Laboratory, DENIS POTAPENKO, Columbia University, PETER JOHNSON, PERCY ZAHL, PETER SUTTER, Brookhaven National Laboratory, RICHARD OSGOOD, Columbia University — We recently reported [1] on a new surface phase of the Co-vicinal-Cu(111) system, which exhibits self-assembled uniform Co quantum wires that are stable at 300K. STM images show that the wires form along the leading edge of the step rise, differentiating it from previously theoretically predicted atomic-wire phases as well as experimentally observed step-island formation. Our observations allow us to comment on the formation kinetics of the atomic-wire phase and on the fit of our data to a recently developed lattice-gas model. LT-STM measurements, taken on self-assembled Co chains, reveal a charge-density modulation that is dependent on tip bias. These charge-modulations are observed for tip-bias relatively far away from the Fermi level, both at negative and positive bias. We present arguments for the identification of these modulations as due to either charge-density-like waves (CDW) or excited states of this 1-D system.

[1] N. Zaki et al, Phys. Rev. B 80, 155419 (2009)

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

4:54PM L10.00013 ABSTRACT WITHDRAWN –

5:06PM L10.00014 Characterization of the surface environment of PbSe nanoparticles by correlating calculated and measured x-ray spectra , KEITH GILMORE, AARON HAMMACK, APRIL SAWVEL, EVELYN ROSEN, D. FRANK OGLETREE, JEFFREY URBAN, DELIA MILLIRON, BRETT HELMS, BRUCE COHEN, DAVID PRENDERGAST, Lawrence Berkeley National Lab, NANO-SURFACES TEAM — Given that defining characteristics of nanoparticles are often dictated by their surfaces, it is desirable to be able to control the surface environments. We seek this control through ligand exchange chemistry and investigate PbSe as a model system. We correlate calculated and measured x-ray spectra to quantify the extent of ligand exchange, validate our structural models, and characterize the optical and electronic properties induced by the new surface environment. Chemical shifts in x-ray photoelectron spectra indicate changes in atomic bonding at the surface, whereas x-ray absorption spectra reveal ligand conformation and binding coordination at the surface. The colloidal synthesis of PbSe particles is highly reliable and the resulting particles are technologically useful size-tunable IR absorbers. Such particles have Pb rich surfaces and native oleic acid coats. We replace the oleic acid with alternate ligands of choice, which may change the Pb:Se ratio at the particle surface.

5:18PM L10.00015 Anchoring platinum on graphene using metallic adatoms , F.G. SEN, Department of Mechanical, Automotive and Materials Engineering, University of Windsor, Windsor, ON, Canada, Y. QI, Chemical Sciences and Materials Systems Laboratory, General Motors R&D Center, Warren, MI U.S.A., A.T. ALPAS, Department of Mechanical, Automotive and Materials Engineering, University of Windsor, Windsor, ON, Canada — To anchor Pt on the graphene surface 25 different metallic adatoms were individually inserted into Pt(111)/graphene interface and the work of separation required to break the interface between Pt-adatom and C-adatom bonds were computed using first principles calculations. With the exception of Al, Zn and Au, all metals increased the strength of the Pt/graphene interface, while many transition metals with unfilled d orbitals, such as Sc, Ti, V, Cr, Co, Ni, Zr, Nb, Mo, Ru, Rh, Ta, W, Re, Os, Ir, could increase the Pt/graphene interface strength from 0.009 J/m^2 to above 0.5 J/m^2. The Pt-adatom bond had metallic character and its strength was proportional to the amount of charge transferred from the adatom to the Pt. The strength of carbon-adatom bond was proportional to the ratio of charge transferred to the carbon over charge transferred to the platinum from the adatom. As this ratio was $>$1.0 for Ir, Os, Ru, Rh and Re and these emerged as the most promising adatoms for anchoring Pt on graphene.

Tuesday, March 22, 2011 3:00PM - 4:00PM –

Session L12 APS: APS Editorial QA: APS and Open Access D223/224

3:00PM L12.00001 APS and Open Access —The movement toward Open Access continues to gain momentum. A brief review of APS efforts in this area will be presented by APS Editor in Chief, Gene Sprouse. Editors from Physical Review A, B, E, Focus, Letters, and X, Reviews of Modern Physics, and Physics will address your questions about publishing in this evolving environment.

Tuesday, March 22, 2011 2:30PM - 5:30PM –

Session L13 GSNP: Focus Session: Jamming Theory and Experiment III D225/226

2:30PM L13.00001 Relaxation of stresses and dynamical heterogeneities close to jamming in a granular experiment , CORENTIN COULAIS, OLIVIER DAUCHOT, CEA-SPEC-GIT, ROBERT BEHRINGER, Duke U — Dynamical Heterogeneities have been found to exhibit maximal size and scale invariance at Jamming. We address here the question of the link with stresses in the materials. To that end, we use a confined, vibrated layer of 8000 bidisperse grains under uniaxial compression. The vibration is horizontal, transverse to the direction of compaction. First, an intruder is pulled at constant velocity through the assembly and force measurements reveals maximal time correlations at Jamming. Then, the experimental setup is slightly modified to accept photoelastic grains, made of soft or hard materials. By measuring positions and stresses, decorrelation of forces as well as dynamics in structure, spontaneous fluctuations are probed. Both quenches and intruder pulling protocols are performed, and novel behavior at Jamming is seen.

2:42PM L13.00002 Nonlinear elasticity near jamming probed in bidisperse foams , ALEXANDER SIEMENS, MARTIN VAN HECKE — An unusual characteristic of the jamming transition is the difference in scaling of the bulk and shear modulus of frictionless soft particles near jamming. We probe this scaling by compressing a bidisperse foam monolayer sandwiched between a glass plate and a fluid surface. We also determine the weakly nonlinear effective bubble-bubble interactions in a 1D chain of bubbles under compression.

2:54PM L13.00003 Reversible plasticity near Jamming in foams , GIJS KATGERT, WILSON C.K. POON, University of Edinburgh — We study the response of a disordered foam monolayer, confined between a soapy solution and a glass plate to an oscillatory compressive strain brought about by inflating a central bubble. We show that, when driven quasistatically slowly, the foam as a whole can exhibit kinematically reversible plasticity or *anelasticity*: the bubble packing alternates between two reproducible configurations, which are separated by multiple plastic events and global displacements. After establishing that the timescale beyond which the foam behaves quasistatically is set by the scaling of the foam compressive modulus with packing fraction ϕ, we map out the boundary between reversible and irreversible plasticity in the space spanned by ϕ and the compressive strain ε and tentatively find the strain to scale as $\varepsilon \sim (\phi - \phi_c)^{1/4}$, with ϕ_c the jamming point. We finally extract a plasticity lengthscale from our experiment and show it to grow on approach to ϕ_c.

3:06PM L13.00004 Local origins of volume fluctuations in granular materials[1]

, JAMES PUCKETT, North Carolina State University, FREDERIC LECHENAULT, Universite Montpellier II, KAREN DANIELS, North Carolina State University — Recent experiments and simulations have observed that the fluctuations in the local volume fraction, ϕ, decrease as the granular material approaches jamming. We investigate the role of boundary condition and inter-particle friction, μ, on these fluctuations for a dense bidisperse granular monolayer driven at the perimeter. Using a radical Voronoi tessellation, we find a universal linear relationship between the mean variance of ϕ independent of boundary condition and μ. We examine the universality and origins of this trend using the recent granocentric model modified to draw neighbors from an arbitrary distribution $P(s)$, the edge-to-edge distance between neighbors. The mean and variance of the observed particle separation s are described by a single length scale controlled by mean ϕ. We tested diverse functional forms of $P(s)$ and found that each produces the trend of decreasing fluctuations, but only the experimentally-observed $P(s)$ provides quantitative agreement with the measured ϕ fluctuations. In conclusion, we find $P(\phi)$ and $P(s)$ encode similar information about the distribution of free volume in a driven granular system under different boundary conditions and inter-particle friction.

[1]NSF DMR-0644743

3:18PM L13.00005 Intermittent Jamming in Quasi-2D Microfunnels

, CARLOS ORTIZ, KAREN DANIELS, North Carolina State University, ROBERT RIEHN[1] — Both athermal granular jamming and thermal glass transitions have recently received extensive attention. We experimentally investigate the jamming transition in a quasi-2D system of nearly hard-sphere, micron-sized PMMA-PHSA particle suspension in a density and index-matched medium flowing through a microfunnel. We observe a packing fraction driven transition from a gas-like to a liquid-like to a solid-like phase. At sufficiently high packing fractions we observe intermittent jamming under constant pressure. Further increase in the packing fraction forms a stable solid-like jammed phase which is disordered on long-ranges, and susceptible to re-melting by reverse flow, agitation, and diffusion. By displaying properties of both athermal granular jamming and thermal glass transitions, our experiment provides a useful testing ground for understanding the jamming transition as a unifying framework.

[1]North Carolina State University

3:30PM L13.00006 Controllable jamming of amorphous granular materials applied to robotics[1]

, ERIC BROWN, RODENBERG RODENBERG, The University of Chicago, JOHN AMEND, HOD LIPSON, Cornell University, ANNAN MOZEIKA, ERIK STELTZ, iRobot G&I Research, MITCHELL ZAKIN, DARPA, HEINRICH JAEGER, The University of Chicago — We demonstrate the practicality of using a controlled jamming transition in an amorphous mass of granular material for applications to robotic gripping, and how the gripping capabilities depend on the properties of the jammed state. A mass of granular material contained in a flexible membrane in an unjammed state flows and conforms to almost any object it is pressed against. Upon application of a vacuum, the external pressure on the membrane jams the granular mass with a volumetric contraction $< 1\%$, allowing it to pinch the object. By measuring the holding force on a test sphere at different levels of envelopment, we show that three mechanisms contribute to the holding force: friction, suction, and interlocking. We use a solid mechanics model to relate the holding force from each mechanism to the measured stress response of jammed granular materials to compressional, extensional, and bending strains. This opens up new possibilities for the design of simple systems that excel at gripping objects of arbitrary shape.

[1]E. Brown et al., PNAS 107(43) (2010). Videos: http://ccsl.mae.cornell.edu/jamming_gripper

3:42PM L13.00007 Jamming in Vertical Channels[1]

, G. WILLIAM BAXTER, FIONA STEEL, Penn State Erie, The Behrend College — We study jamming of low aspect-ratio cylindrical Delrin grains in a vertical channel. Grain heights are less than their diameter so the grains resemble antacid tablets, coins, or poker chips. These grains are allowed to fall through a vertical channel with a square cross section where the channel width is greater than the diameter of a grain and constant throughout the length of the channel with no obstructions or constrictions. Grains are sometimes observed to form jams, stable structures supported by the channel walls with no support beneath them. The probability of jam occurrence and the strength or robustness of a jam is effected by grain and channel sizes. We will present experimental measurements of the jamming probability and jam strength in this system and discuss the relationship of these results to other experiments and theories.

[1]Supported by an Undergraduate Research Grant from Penn State Erie, The Behrend College.

3:54PM L13.00008 Geometry Dependence of the Clogging Transition in a Tilted Hopper

, CHARLES THOMAS, DOUGLAS DURIAN, University of Pennsylvania — We report the effect of system geometry on the clogging of granular material flowing out of a flat-bottomed hopper. We vary the hopper tilt angle, aperture shape, and granular media shape, investigating smooth spheres (glass beads), compact angular grains (beach sand), and rod-like grains (rice). We measure the average number of grains discharged before a clog halts the flow. This value grows with hole size as a power law, diverging above a critical hole size. We determine the critical value by performing a least-squares fit to the data. Beyond that critical hole size, the flow does not clog for any given tilt angle. This critical hole size grows with increasing tilt, diverging at $\pi - \theta_r$, where θ_r is the angle of repose. The value of the critical hole size as a function of tilt angle describes a well-defined transition on a clogging phase diagram. For circular apertures, the shape of this transition is similar for all grain types. However, this is not the case for the narrow slit apertures, where the rate of growth of the critical hole size with tilt angle depends on the material. The growth rate is the fastest for angular grains, then smooth spheres, with rod-like grains showing the slowest growth. This suggests a profound link between the aperture geometry and the particle shape.

4:06PM L13.00009 Jamming of Granular Flow in a Two-Dimensional Hopper[1]

, JUNYAO TANG, SEPEHR SADIGHPOUR, ROBERT BEHRINGER — We seek an understanding of the physics of jamming for hopper flow using high speed spatio-temporal video data for photoelastic disks flowing through a two-dimensional hopper. We have found experimental support for the hypothesis that jamming events of granular flow in a hopper is approximately a Poisson process. The mean flow time between two consecutive jams increases rapidly with the hopper opening size, but it is insensitive to changes of the hopper wall angle.Through particle tracking and photoleastic measurements, we measure stress fields, velocity fields and density fields, as well as their fluctuations during the flow. Current work is focusing on understanding how to combine these results to give us further insights of the relation between mean flow properties and jamming and their dependence on hopper configuration.These data are part of an IFPRI-NSF Collaboratory for comparing physical data and simulations.

[1]This work is funded by IFPRI. (International Fine Particle Research Institute)

4:18PM L13.00010 Structural Stability and Jamming of Self-Organized Cluster Conformations in Granular Materials[1] , A. TORDESILLAS, U. of Melbourne, B. BEHRINGER, Duke U, Q. LIN, J. SHI, U. of Melbourne, J. ZHANG, Indiana U-Purdue University-Fort Wayne — We probe emergent self-organized particle cluster conformations in slowly deforming dense granular materials. We invoke structural mechanics to devise a new stability measure for clusters, and use this measure to explore stability of jammed states of cluster conformations consisting of particles in force chains and minimal contact cycles. Knowledge of the spatio-temporal evolution of the (relative) stability of jammed conformations offers valuable clues to granular rheology and self-assembly. We use data from assemblies of bi-/poly-disperse disks subject to 2D deformation in two biaxial strain tests: one computational and one experimental. Self-assembly occurs on multiple length scales with jammed force chains and minimal cycles forming the basic building blocks. Three-cycles are stabilizing agents acting as granular trusses to load-bearing force chain columns. The co-evolution of minimal cycles and force chains form a generic feature of these materials and loading paths.

[1]Work supported by US ARO grants W911NF-07-1-0370/1031, ARC Discovery Grant DP0772409, and NSF-DMR0906908.

4:30PM L13.00011 Decoupling of Rotational and Translational Diffusion in Supercooled Colloidal Fluids[1] , KAZEM V. EDMOND, GARY L. HUNTER, Emory University, MARK T. ELSESSER, HYUNJOO PARK, DAVID J. PINE, New York University, ERIC R. WEEKS, Emory University — Using high-speed confocal microscopy, we directly observe the three-dimensional rotational dynamics of rigid clusters of microspheres suspended in dense colloidal suspensions. The clusters are highly ordered packings of fluorescently-labeled PMMA particles, fabricated using a recently developed emulsification technique. Our colloidal suspensions serve as good approximations to hard-sphere fluids, while the clusters probe the system's local rotational and translational dynamics. Far from the colloidal liquid's glass transition, both rotational and translational motion of the clusters are purely Brownian. However, in the liquid's supercooled regime, we observe a decoupling between the two types of motion: as the glass transition is approached, rotational diffusion slows down even more than translational diffusion. Our observation supports the notion that supercooled liquids are not merely liquids with large viscosities but that diffusion takes place by fundamentally changed mechanisms.

[1]Supported by NSF Grant No. CHE-0910707

4:42PM L13.00012 Confinement of Colloidal Suspensions in a Cylindrical Geometry , NABIHA SAKLAYEN, GARY L. HUNTER, KAZEM V. EDMOND, ERIC R. WEEKS, Emory University — We study binary colloidal suspensions confined within a glass microcapillary to model the glass transition in confined cylindrical geometries. We use high speed three-dimensional confocal microscopy to observe particle dynamics. The use of a slightly tapered microcapillary enables us to probe a range of local volumes for a single colloidal sample. We observe that confinement of the sample slows down particles. In addition, the particles form layers against the capillary walls; these layers also influence particle mobility. We see that even though confinement is primarily responsible for slowing down particles, particles within a layer are seen to move even slower. Within each region of the microcapillary, the mobility perpendicular to the confining boundaries is influenced by distance from the confinement boundary, while the parallel component of mobility is not.

4:54PM L13.00013 Shear-induced dynamics of polydisperse jammed emulsions , ERIC R. WEEKS, JOAQUIM CLARA RAHOLA, Physics Dept., Emory University — We study dense and highly polydisperse emulsions at droplet volume fractions ranging from phi = 0.65 to 0.85. We apply oscillatory shear and observe the subsequent droplet motions using confocal microscopy. Both affine and nonaffine droplet motions are observed, with the large droplets typically moving affinely and pushing the smaller droplets around in non-affine ways. Despite the polydispersity of the sample and the complex droplet trajectories, we observe dynamic correlation length scales. These length scales grow from one to four times the mean droplet diameter, with larger length scales corresponding to higher strain amplitudes (up to strains of about 6%).

5:06PM L13.00014 A Jamming Phase Diagram for Pressing Polymers , CHAO TENG, Nanjing University, ZEXIN ZHANG, Soochow University, XIAOLIANG WANG, GI XUE, Nanjing University, NANJING UNIVERSITY TEAM, SOOCHOW UNIVERSITY COLLABORATION — Molecular glasses begin to flow when they are heated. Other glassy systems, such as dense foams, emulsions, colloidal suspensions and granular materials, begin to flow when subjected to sufficiently large stresses. The equivalence of these two routes to flow is a basic tenet of jamming, a conceptual means of unifying glassy behavior in a swath of disordered, dynamical arrested systems. However, a full understanding of jamming transition for polymers remains elusive. By controlling the packing densities of polymer glasses, we found that polymer glasses could once flow under cold-pressing at temperatures well below its calorimetric glass transition temperature (Tg). The thermomechanical analysis (TMA) results confirmed that Tg changed with density as well as the applied stress, which is exactly what to be expected within the jamming picture. We propose a jamming phase diagram for polymers based on our laboratory experiments.

5:18PM L13.00015 Visualization of force networks in a three-dimensional granular system , CHANTAL CARPENTIER, KINGA LORINCZ, PETER SCHALL, DANIEL BONN, FRED BROUWER, University of Amsterdam — Force networks form the skeleton of granular matter. The understanding of the rigidity to flow transition of granular materials requires the study of the three-dimensional distribution of forces between the particles. Here we propose a new method to visualize and measure contact forces in three-dimensional suspensions. We use a rigidochromic dye which we attach chemically to the surfaces of the particles to measure local forces at the contact point. This dye exhibits non-fluorescent transitions, when it is free to relax mechanically, but shows strong fluorescence when confinement blocks mechanical relaxation. Preliminary experiments suggest that the fluorescent intensity is a direct measure of the local contact force. We use confocal microscopy to create spatial intensity maps to reconstruct the entire contact force distribution.

Tuesday, March 22, 2011 2:30PM - 5:18PM –

Session L14 FEd: Physics Education Research D227

2:30PM L14.00001 A Proactive Approach for Improving the Mathematical Foundation of Students Taking College Physics , LEIGH SMITH, JAMES SULLIVAN, HOWARD JACKSON, Department of Physics, University of Cincinnati, Cincinnati, OH 45221 — We report on preliminary results using the mathematics teaching program ALEKS (see aleks.com) along with the use of Just-in- Time-Teaching (JiTT) and Peer Instruction (PI) to improve the performance of students in College Physics, an algebra-based course. ALEKS, an adaptive program based on artificial intelligence and long-used in the mathematics community, was made available to students 5 weeks ahead of the first class session with participation encouraged by the award of a small class credit. Student participation and engagement was remarkable with many students making significant gains in their mathematics performance. Preliminary data suggests that performance on the first midterm was strongly correlated with performance within ALEKS. The use of JiTT and PI in two out of the four classes suggested overall a modest increase over standard lecture sections, but with women performing significantly better in these classes. We acknowledge the financial support of McGraw-Hill and ALEKS and the National Science Foundation through CCLI grant DUE-1022563.

2:42PM L14.00002 Improving Students' Interest and Motivation in Introductory Physics Laboratory: A Comparative Study , YEVGENIYA V. ZASTAVKER, JENNIFER A. SIMONOVICH, EMILY TOWERS, F. W. Olin College of Engineering — Project-based learning (PjBL) has shown to be an effective method to enhance student learning in many disciplines, including science and engineering fields. Due to the complex nature of PjBL, however, the effectiveness of this learning environment has been linked, to a large degree, to the specifics of its implementation. This talk will present a comparative study of two technical PjBL courses required for engineering majors at a small technical school, *Introductory Mechanics Laboratory* and *Introductory Engineering Design*. Twelve semi-structured in-depth interviews are analyzed using grounded theory approach. The results indicate that despite similarity in the course goals of these PjBL environments, students' interest and motivation varies dramatically based on the relative levels of student autonomy and scaffolding provided in each course. We propose a framework for creating appropriate PjBL environments in *Introductory Physics Laboratories* with an emphasis on improving engineering and physics students' interest and motivation in the relevant coursework and improving student retention.

2:54PM L14.00003 Integrating pre-, in- and post-lecture activities to improve students' learning in a large introductory physics course[1] , KWAN CHENG, MEHMET CAGLAR, AMY PIETAN, HANI DULLI, Texas Tech University — Monitoring and assessing the students' learning activities before, during and after lecture teaching in a large (more than 150 students) introductory physics class setting are important to evaluate the efficacies of various teaching pedagogies and methods. At Texas Tech, an online and integrative computer-based approach of using an interactive pre-lecture tutorial, an in-class concept test using a wireless student response system and a homework/tutorial system has been implemented in Fall 2010. The strategy of implementation of this integrative approach and the assessment results from various in-house and standard Mechanics tests will be presented. In addition, how this approach may create synergism of lab and lecture teaching efforts will also be addressed.

[1]This project is supported by the NIH grant 5RC1GM090897-02.

3:06PM L14.00004 Design and development of physics simulations in the field of oscillations and waves suitable for k-12 and undergraduate instruction using video game technology , TREVOR TOMESH, University of Wisconsin - River Falls, COLIN PRICE, University of Worcester, England — Using the scripting language for the Unreal Tournament 2004 Engine, Unreal Script, demonstrations in the field of oscillations and waves were designed and developed. Variations on Euler's method and the Runge-Kutta method were used to numerically solve the equations of motion for seven different physical systems which were visually represented in the immersive environment of Unreal Tournament 2004. Data from each system was written to an output file, plotted and analyzed. The over-arching goal of this research is to successfully design and develop useful teaching tools for the k-12 and undergraduate classroom which, presented in the form of a video game, is immersive, engaging and educational.

3:18PM L14.00005 A Physics of Semiconductors Concept Inventory , EMANUELA ENE, Oklahoma State University, BRUCE J. ACKERSON COLLABORATION[1], ALAN CHEVILLE COLLABORATION[2] — Following the trend in science and engineering education generated by the visible impact that the Force Concept Inventory (FCI) has created, a Physics of Semiconductors Concept Inventory (PSCI) has been developed. Whereas most classroom tests measure *how many* facts students can remember, or if they *can manipulate* equations, PSCI measures *how well* students interpret concepts and *how well* they can infer new knowledge from already learned knowledge. Operationalized in accordance with the revised Bloom's taxonomy, the multiple–choice items of the PSCI address the "understand", "apply", "analyze" and "evaluate" levels of cognition. Once standardized, PSCI may be used as a predictor for students' academic performance in the field of semiconductors and as an assessment instrument for instructional strategies.

[1]Department of Physics; Oklahoma State University; bruce.ackerson@okstate.edu
[2]NSF and Oklahoma State University; rchevill@nsf.gov

3:30PM L14.00006 A semantic space mapping of introductory physics concepts , NIC RADY — We know that physics students and their professors organize knowledge differently, but exactly how do they organize knowledge. The Physics Perception Assessment (PPA) has been designed to create a map of the semantic space of 15 commonly encountered concepts in a first-semester physics course. Preliminary data taken with the PPA will be presented and from this data, an "expert" semantic space configuration will be presented.

3:42PM L14.00007 A student's guide to searching the literature using online databases[1] , CASEY W. MILLER, DUSTIN BELYEA, MICHELLE CHABOT, University of South Florida, Department of Physics, TROY MESSINA, Centenary College of Louisiana, Department of Physics — A method is described to empower students to efficiently perform general and specific literature searches using online resources [Miller et al., Am. J. Phys. **77**, 1112 (2009)]. The method was tested on undergraduate and graduate students with varying backgrounds in scientific literature. Students involved in this study showed marked improvement in their awareness of how and where to find scientific information. Repeated exposure to literature searching methods appears worthwhile, starting early in the undergraduate career, and even in graduate school orientation.

[1]Supported by NSF-CAREER, and the Mattie Allen Broyles and Gus S. Wortham Endowments.

3:54PM L14.00008 Mutual Mentoring Makes Better Mentors , CINDY BLAHA, Carleton College, AMY BUG, Swarthmore College, ANNE COX, Eckerd College, LINDA FRITZ, Franklin & Marshall College, BARBARA WHITTEN, Colorado College — In this talk we discuss one of the impacts of an NSF ADVANCE sponsored horizontal, mutual mentoring alliance. Our cohort of five women physicists at liberal arts colleges has found that mutual mentoring has had a profound impact on many aspects of our professional lives. In this talk we will describe how our peer-to-peer mentoring has enabled us to become better mentors for our undergraduate students, for recent graduates beginning their careers and for colleagues at local and neighboring institutions.

4:06PM L14.00009 Impact of Mutual Mentoring on Research , BARBARA WHITTEN, Colorado College, CYNTHIA BLAHA, Carleton College, AMY BUG, Swarthmore College, ANNE COX, Eckerd College, LINDA FRITZ, Franklin and Marshall College — In this talk we discuss one of the impacts of an NSF ADVANCE sponsored horizontal, mutual mentoring alliance. Our cohort of five women physicists at liberal arts colleges has found that mutual mentoring has had a profound impact on many aspects of our professional lives. In this talk we will give some specific ways that we have supported and helped to expand each other's research. For some new areas of research were opened, for others new focus was brought to existing areas, and still others found acceptance for where they were.

4:18PM L14.00010 Developing Effective Undergraduate Research Experience , MICHAEL EVANS, CAROLINA C. ILIE, Dept. of Physics, SUNY Oswego — Undergraduate research is a valuable educational tool for students pursuing a degree in physics, but these experiences can become problematic and ineffective if not handled properly. Undergraduate research should be planned as an immersive learning experience in which the student has the opportunity to develop his/her skills in accordance with their interests. Effective undergraduate research experiences are marked by clear, measurable objectives and frequent student-professor collaboration. These objectives should reflect the long and short-term goals of the individual undergraduates, with a heightened focus on developing research skills for future use. 1. Seymour, E., Hunter, A.-B., Laursen, S. L. and DeAntoni, T. (2004), "Establishing the benefits of research experiences for undergraduates in the sciences: First findings from a three-year study". *Science Education*, 88: 493–534. 2. Behar-Horenstein, Linda S., Johnson, Melissa L. "Enticing Students to Enter Into Undergraduate Research: The Instrumentality of an Undergraduate Course." *Journal of College Science Teaching* 39.3 (2010): 62-70.

4:30PM L14.00011 Seriously? Freshmen In A Physics Research Lab?[1] , ROSA ELIA CÁRDENAS, ISAAC MANZANERA ESTEVE, JOHN T. MARKERT, The University of Texas at Austin, Department of Physics, SARAH SIMMONS, The University of Texas at Austin, Office of Honors, Research, and International Studies — We report on the University of Texas College of Natural Sciences Freshman Research Initiative (FRI) program as a whole and more specifically, its physics stream. The FRI program was developed in an effort to improve retention in the College of Natural Sciences (CNS). The general goal of the program is to bring students at the freshman level into a research laboratory. The reasoning is that as students become part of a research laboratory he or she will feel more involved with science, both academically and socially, and will be more likely to continue on a research science route. We will present the college wide statistical tracking data which shows that the FRI program has indeed improved retention in the CNS, has improved GPA and has improved graduate school matriculation. We will also discuss the tracking of three generations of physics stream participants. We describe the curriculum, training, precautions and techniques used as we bring freshmen into a physics research laboratory.

[1]We acknowledge support from NSF-DMR 0605828, Welch F-1191, HHMI-52005907, and NSF-0629136.

4:42PM L14.00012 Mentoring undergraduates for experimental research in physics[1] , JEREMY LEVY, U. Pittsburgh — Undergraduate research experiences are pivotal in shaping careers in physics. I will support this thesis—the implicit focus of this session—with anecdotes highlighting research performed by undergraduates in my group at the University of Pittsburgh, as well as my own recollections as an undergraduate researcher.

[1]This work was supported by NSF DMR-0704022.

4:54PM L14.00013 Modular Curriculum Approach (MCA) for teaching of introductory physics: Tablet PCs and flexible instructional space to stimulate active learning , TIKHON BYKOV, McMurry University, Department of Physics, YELENA KOSHELEVA, McMurry University, Departments of Psychology, Curriculum and Instruction — Modular Curriculum Approach is an innovative model designed at McMurry University and adopted for teaching of introductory physics courses. In MCA, traditional lab/lecture structure is converted into a system of flexible instructional modules, with lecture, lab, and discussion being merged into one technologically and collaboratively rich experience. Different elements are integrated with Tablet PCs as a single unifying platform to improve continuity among module components. A technology suite incorporated with tablets includes: Physlets, tablet-adapted personal response systems, data acquisition systems, and tablet-based note-taking tools. The MCA has been further reinforced by creating a new instructional space with movable partitions, allowing for easy transformation between lecture and lab modes. The space is supportive of small peer- group activities with easy-to-reconfigure table clusters, multiple white and black board surfaces, multiple TVs and projection screens.

5:06PM L14.00014 Impact E-Learning Platform Moodle on the Physic's Learning Process in the High School's Students , JONAS TORRES-MONTEALBAN, GREGORIO RUIZ-CHAVARRIA, ENRIQUE ARMANDO GOMEZ-LOZOYA, Universidad Autonoma Chapingo — As a didactic proposal, moodle e-learning platform was implemented in one of two Physics High School's group at UACH, in order to show how the use of new technologies can improve the learning progress linked to physics concepts. As a result, the first group worked at the same time with inside class activities as well as outside resources from the moodle e-platform. The second group only worked with inside class activities. This teaching application was developed in six sections. Section I defines the educational framework. Section II identifies the key physic's concepts to be studied in each proposed activity. Section III describes the didactic model. Section IV displays the compared results between similarities and differences in both groups. Section VI shows the gathered information in order to be discussed as a topic related on how new technologies improve the Physic's learning process in the high school' students.

Tuesday, March 22, 2011 2:30PM - 5:30PM –

Session L15 DMP GMAG FIAP: Focus Session: Spins in Semiconductors - Spin Torque and Spin Injection D171

2:30PM L15.00001 Spin Torque Switching in GaMnAs Magnetic Tunnel Junctions[1] , LIN XUE, R. A. BUHRMAN, D.C. RALPH, Cornell University, D.W. RENCH, M.J. WILSON, P. SCHIFFER, N. SAMARTH, Physics Dept., Penn State University — We have fabricated and measured submicron magnetic tunnel junctions made from GaMnAs multilayers: GaMnAs/GaAs/GaMnAs/MnAs, where GaMnAs is a ferromagnetic semiconductor, GaAs serves as the tunneling barrier, and MnAs is a ferromagnet that provides an exchange bias to the upper GaMnAs (reference) layer. The devices have magnetoresistances of order 50% at 4.2 K and exhibit clear spin-torque switching of the lower GaMnAs layer between parallel and antiparallel orientations relative to the reference layer. We report the switching phase diagram as a function of current and magnetic field. We also describe efforts to probe the high-speed magnetic dynamics in GaMnAs driven by spin torque from ns-scale current pulses and microwave-frequency currents that can drive ferromagnetic resonance.

[1]This work is supported by ONR MURI.

2:42PM L15.00002 Theory of current-induced torque in uniform ferromagnets , KAREL VYBORNY, LIVIU ZARBO, Institute of Physics, Academy of Sciences of the Czech Rep, T. JUNGWIRTH, Institute of Physics, Academy of Sciences of the Czech Rep; School of Physics and Astronomy, University of Nottingham — In a model ferromagnetic semiconductor (Ga,Mn)As with strong spin-orbit interaction, it has been experimentally shown that magnetization can be manipulated by injection of unpolarized currents [Chernyshov et al., Nat. Phys. 5, 656 (2009)]. We critically review the existing theoretical approaches to this phenomenon and present a model whose results are compared to more recent measurements of the current-induced torque driven by ferromagnetic resonance in (Ga,Mn)As. The results entail the dependence of the effect on carrier concentration, various types of strain, and temperature.

2:54PM L15.00003 Intrinsic spin-orbit coupling effects on spin and charge pumping in magnetic tunnel junctions with microwave-driven precessing magnetization , FARZAD MAHFOUZI, BRANISLAV NIKOLIC, Department of Physics and Astronomy, University of Delaware, Newark, DE 19711, USA, NAOTO NAGAOSA, Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan — We develop a microscopic quantum transport approach to the problem of spin pumping by precessing magnetization in one of the ferromagnetic layers within FIF or FIN (F-ferromagnet; N-normal metal; I-insulating barrier) magnetic tunnel junctions (MTJs) in the presence of intrinsic spin-orbit couplings (SOC) at the FI interface. Our approach evaluates the nonequilibrium Green functions (NEGFs) by starting from the time-dependent Hamiltonian of these junctions. To express the time-averaged charge current, or the corresponding dc pumping voltage in open circuits that was measured in recent experiments on MTJs [T. Moriyama *et al.*, Phys. Rev. Lett. **100**, 067602 (2008)], we construct a novel solution for the double-time-Fourier-transformed NEGFs where their two energy arguments are connected by the Floquet theorem describing emission and absorption of finite number of photons. Within this fully quantum-mechanical treatment of the conduction electrons, we find that only in the presence of the interfacial Rashba SOC non-zero dc pumping voltage in F|I|N junctions emerges at the adiabatic level (i.e., proportional to microwave frequency).

3:06PM L15.00004 Manipulation of ferromagnetic state by means of spin-orbit interactions , LEONID ROKHINSON, Purdue University — The current state of information technology accentuates the dichotomy between processing and storage of information, with logical operations performed by charge-based devices and non-volatile memory based on magnetic materials. The major obstacle for a wider use of magnetic materials for information processing is the lack of efficient control of magnetization. Reorientation of magnetic domains is conventionally performed by non-local external magnetic fields or by externally polarized currents. Efficiency of the latter approach is greatly enhanced in materials where ferromagnetism is carrier-mediated. In such materials control of carriers' polarization provides an alternative mean to manipulate orientation of magnetic domains. In some crystalline conductors the charge current couples to spin via intrinsic spin-orbit (SO) interactions and generates electron spin polarization. Unlike the Oersted field, the SO-induced polarization is spatially localized and can be controlled by local electric fields. This non-equilibrium electron spin polarization couples to magnetic moments of magnetic ions and is capable of controlling magnetization of the ferromagnet. We show that magnetization can be reversibly manipulated by SO-induced polarization of carrier spins generated by the injection of unpolarized currents. We demonstrate domain rotation and hysteretic switching of magnetization between two orthogonal easy axes in a model ferromagnetic semiconductor GaMnAs.

3:42PM L15.00005 Ferromagnetic resonance driven by current-induced torque in uniform ferromagnetic micro-structures , H. KUREBAYASHI, D. FANG, University of Cambridge, J. WUNDERLICH, Hitachi Cambridge Laboratory, K. VYBORNY, L.P. ZARBO, Institute of Physics, ASCR, R.P. CAMPION, A. CASIRAGHI, B.L. GALLAGHER, University of Nottingham, T. JUNGWIRTH, Institute of Physics, ASCR, A.J. FERGUSON, University of Cambridge, EU GRANTS FP7-214499 NAMASTE COLLABORATION — We show that the recently demonstrated current induced torque (CIT) [A. Chernyshov, et al. Nat. Phys. 5, 656 (2009)] can excite magnetisation dynamics in micro-bars of uniform ferromagnetic semiconductors. Due to the combined effects of the spin-orbit and exchange interactions, a microwave current injected into (Ga,Mn)As (or (Ga,Mn)(As,P)) micro-bars generates an oscillating effective magnetic field. By using a sensitive electrical detection technique, we accurately measure the magnitude and direction of driving fields for samples under different strain. We confirm the observation of a field with the symmetry of the Dresselhaus spin-orbit interaction and observe an additional field with the symmetry of the Rashba spin-orbit interaction. Our work demonstrates a new scalable FMR technique which provides a sensitive method to study the nature of current-induced torques and to perform magnetic characterisation of uniform ferromagnetic micro-structures.

3:54PM L15.00006 Non-local spin transport devices with a tunable channel[1] , J. MISURACA, J.-I. KIM, P. XIONG, S. VON MOLNAR, Department of Physics, Florida State University, K.K. MENG, J. LU, J.H. ZHAO, Institute of Semiconductors, Chinese Academy of Sciences — The spin lifetime in GaAs is known to vary strongly with carrier density near the metal to insulator transition [1]. However, a detailed study to optimize this lifetime is complicated because many replica samples need to be made and measured. This difficulty can be circumvented by employing Si:$Al_{0.3}Ga_{0.7}As$, a persistent photoconductor, as the spin transport medium. This material, which is structurally similar to GaAs, has been characterized and shown to have an effective carrier density which can be tuned *in situ* via photo-excitation from 10^{14} to 10^{18} cm^{-3}[2]. Heterostructures (2-μm Si:$Al_{0.3}Ga_{0.7}As$, a thin epitxial Fe layer, and a GaAs graded junction to create linear contacts between them) have been grown by MBE and non-local spin devices have been patterned by photolithography and wet etching. Magnetic measurements on Fe micro-patterns demonstrated the possibility of controlling the coercivity of the Fe electrodes [3]. Electrical characterization of the devices will be presented. [1] J. Kikkawa et al., Phys. Rev. Lett. 80, 4313 (1998) [2] J. Misuraca et al., Phys. Rev. B. 82, 125202 (2010) [3] K. K. Meng et al., Appl. Phys. Lett. 97, 072503 (2010).

[1]This work is supported by NSF DMR-0908625 and NSFC 10920101071.

4:06PM L15.00007 Electron Charge and Spin Transport in Ferromagnet/Semiconductor Schottky Barrier Heterostructures , QI HU, CHRIS PALMSTROM, University of California at Santa Barbara, ERIC GARLID, CHAD GEPPERT, PAUL CROWELL, University of Minnesota — Previous studies of Fe/n^+-GaAs/n-GaAs heterostructures in the lateral non-local geometry have shown that spin accumulation is observed only when tunneling current across ferromagnet/semiconductor Schottky barrier is sufficiently large. The tunneling mechanism is modeled by band diagram simulations and transport calculation using the WKB approximation for the barrier. These suggest that tunneling from localized states in the quantum well (QW) which forms just inside the Schottky interface dominates over tunneling directly from the semiconductor bulk. Electron tunneling spectroscopy is utilized to probe the predicted localized states in the QW. Valleys in the derivative of tunneling conductance spectra were observed at discrete forward bias voltages which are attributed to localized 2-dimensional energy states. The spin escape time of the 2D energy states in the QW is calculated using a spin-dependent WKB approximation. The results are compared with the spin lifetime and escape time extracted from three-terminal spin Hanle measurements. This work was supported by the NSF MRSEC and ONR MURI programs, and NSF DMR-0804244.

4:18PM L15.00008 Dependence of spin-injection spectra of CoFe/GaAs contacts on temperature and annealing conditions , GIAN SALIS, IBM Research - Zurich, ANDREAS FUHRER, SANTOS F. ALVARADO — Spin injection from CoFe contacts into bulk GaAs epilayers is studied experimentally. Close to the metal/semiconductor interface the GaAs epilayer is highly n-doped, allowing efficient spin injection through the Schottky tunnel barrier. Spin polarization in the GaAs channel is measured as a non-local voltage at CoFe detection contacts. Similar to spin injection from Fe contacts, an inversion of the sign of injected spin polarization is found at a finite forward bias U_c applied to the injection contact. We investigate the dependence of the nonlocal signal on U_c. From the data, the spin polarization of the differential interface conductance is obtained, providing spectral information on the spin-polarized density of states. The dependence of these spectra on measurement temperature as well as on annealing and growth conditions is discussed and compared to samples with Fe injection contacts.

4:30PM L15.00009 Electrical Measurements of the Extrinsic Spin Hall Effect in $Fe/In_xGa_{1-x}As$ Heterostructures[1] , CHAD GEPPERT, ERIC GARLID, MUN CHAN, PAUL CROWELL, University of Minnesota, QI HU, CHRIS PALMSTRØM, University of California at Santa Barbara — We report on all-electrical measurements of the extrinsic spin Hall effect in $Fe/In_xGa_{1-x}As$ heterostructures with n-type channel doping (Si) and highly doped Schottky tunnel barriers. The spin Hall effect refers to the transverse spin current generated by application of a longitudinal unpolarized charge current. Complementary spin accumulation at opposing edges of the channel is detected via a Hanle effect in the voltage measured by pairs of ferromagnetic Hall contacts. The spin Hall conductivity is extracted by fitting the data to a drift-diffusion model incorporating spin precession and relaxation. Tuning the channel conductivity with applied bias allows the skew and side-jump contributions to be determined independently. The resulting magnitude is in agreement with models based on ionized impurity scattering. Further quantitative comparison to theoretical models is achieved by increasing the In concentration beyond previously reported values.

[1]Supported by ONR and NSF.

4:42PM L15.00010 Ab initio Investigation of the Failure of Efficient Spin-Injection in Fe/GaAs Superlattices , SINEAD GRIFFIN, NICOLA SPALDIN, ETH Zürich — Magnetic metal-semiconductor systems have been widely studied for use as spintronic devices. The injection of elemental ferromagnetic Fe into GaAs shows great device potential because of the relativity high Curie temperature of Fe compared to other possible injection materials. However, spin-injection in Fe/GaAs has not been successful with several phases such as FeAs and Fe_2As forming at the interface. We perform Density Functional Theory calculations on bulk FeAs and Fe_2As to elucidate the structural and magnetic ground states. We then incorporate these Fe-As layers into GaAs/FeAs superlattices and investigate the resulting structures. Both the effects of Fe content and the number of layers in the heterostructure on the magnetic and electronic properties are considered. Our results show that the magnetic ground state of the FeAs compounds helps to explains the failure of spin-injection in these superlattices.

4:54PM L15.00011 Lateral spin injection and detection through electrodeposited Fe/GaAs interfaces[1] , SARMITA MAJUMDER, ANTHONY ARROTT, KAREN KAVANAGH, SFU, ANTHONY SPRING THORPE, CMC, SFU TEAM, CMC COLLABORATION — We report results on spin injection and detection through epitaxial, electrodeposited Fe/GaAs tunnel barriers formed ex-situ on epitaxially grown GaAs (001). The BCC-Fe ?lms are predominantly single crystalline with large mosaic spread [1]. Tunnel junctions, fabricated with bulk GaAs wafers, and epitaxially grown MBE or MOCVD GaAs (001), showed the expected increase in tunneling current with increasing surface Si dopant concentration. Spin transport through in situ coherently strain, MBE Fe/GaAs interfaces have been reported at spin polarization levels as high as 42% at 50K.[3]. In our experiments the design of the epitaxially grown GaAs substrates followed those used successfully for in situ MBE Fe spin contacts. [2]. A spin voltage (4 mV) has been detected for $2x10^{18}$/cm3 doped tunnel junctions at liquid nitrogen temperatures (77 K) using an injection current of 20 A/cm2 while varying the applied in-plane magnetic ?eld ($\pm$ 300 Gauss) along a <100> easyaxis of the Fe contacts. 1. Z. L. Bao, S. Majumder, A. A. Talin, A. S. Arrott, K. L. Kavanagh, JES 155 (2008) H841. 2. X. Lou, C. Adelmann, A. S. Crooker, E. S. Garlidi, J. Zhang, K. S. Reddy, S. D. Flexner, C. J. Palmstrøm, and P.A. Crowell, Nature Phys. 3 (2007) 197.

[1]Acknowledgments: NSERC

5:06PM L15.00012 All-electrical spin injection and detection in an AlGaN/GaN two-dimensional electron gas[1] , D.R. HOY, Department of Physics, The Ohio State University, Columbus, OH, Y. PU, Department of Physics and Center for Emergent Materials, The Ohio State University, Columbus, OH, S.D. CARNEVALE, Department of Materials Science and Engineering, The Ohio State University, Columbus, OH, E. JOHNSTON-HALPERIN, Department of Physics and Center for Emergent Materials, The Ohio State University, Columbus, OH, R.C. MYERS, Department of Physics and Department of Materials Science and Engineering, The Ohio State University, Columbus, OH — Materials with low spin-orbit coupling, including wide band gap semiconductors, may allow practical semiconductor spintronics. Here we investigate all-electronic spin injection and detection using ferromagnetic Fe electrodes on a polarization doped AlGaN/GaN two-dimensional electron gas (2DEG) grown by molecular beam epitaxy. The ultrathin AlGaN cap provides polarization doped electrons and serves as a thin tunnel barrier for spins. The surface morphology is characterized by atomic force microscopy and the electron density, resistivity, and mobility are characterized by Hall measurements. Through the Hanle effect, we investigate the dependence of the spin injection efficiency and spin lifetime with temperature and bias.

[1]This work was supported by the Center for Emergent Materials at the Ohio State University, an NSF MRSEC.

5:18PM L15.00013 Studies of spin injection into thin film InSb from CoFe , YONG-JAE KIM, R.L. KALLAHER, J.J. HEREMANS, Virginia Tech — Spin-based electronics requires manipulation of spin-polarized carriers in materials. The narrow gap semiconductor InSb is a promising material for spin-based devices due to its strong spin-orbit interaction, allowing spin manipulation using electric fields. Yet, spin injection from spin-polarized electrodes into InSb has not yet been demonstrated. In order to electrically characterize spin injection and detection in InSb, we use InSb/CoFe lateral spin valve geometries studied at low temperatures and in tilted magnetic fields. The geometries are fabricated by depositing two non-epitaxial CoFe electrodes at mesoscopic separations on high-mobility InSb thin films through an insulator window. The anisotropy of the ferromagnetic electrodes provides parallel and anti-parallel configurations. We have observed two-state non-local output voltages, which are consistent with a spin injection signal. Interestingly, the switching signal is very sensitive to temperature in the range studied. The switching signal appears at low external fields due to CoFe magnetic anisotropy effects. The results are discussed in the light of the CoFe anisotropy and expected spin-coherence properties of InSb (partial support from DOE DE-FG02-08ER46532).

Tuesday, March 22, 2011 2:30PM - 5:30PM –

Session L16 DMP GMAG: Focus Session: Magnetic Nanostructures: Probing Using Advanced Methods D173

2:30PM L16.00001 Soft X-ray Spectroscopy of Magnetic Nanostructures: New Phenomena and Applications[1]

, ELKE ARENHOLZ, Advanced Light Source, Lawrence Berkeley National Laboratory, 1 Cyclotron Rd, Berkeley, CA 94720 — The delicate balance between charge, spin, orbital, and lattice degrees of freedom in transition metal oxides leads to unique phenomena such as colossal magnetoresistance, high temperature superconductivity, as well as a remarkable diversity of charge, spin, and orbital ordered phases. The rich phase diagrams are determined by the strong local interaction of electrons in transition metal d orbitals. Subtle changes in d occupancy and overlap—and thereby phase transitions—can be induced by variations in temperature, by external fields, through doping and lattice distortions. In particular, interfaces can hold surprising electronic and magnetic properties that differ remarkably from the adjacent layers. Soft x-ray based techniques are ideal tools to study these systems as they are inherently element-specific, allow characterizing the valence state and the symmetry of lattice sites and provide detailed information about the electronic and magnetic structure with nanometer spatial resolution and on ultrafast time scales. Here we show that the to-date little explored angular dependence of the x-ray magnetic dichroism provides unique insights in the correlation between atomic, magnetic and electronic structure in these systems [1-4]. Taking advantage of this approach will prove invaluable for the engineering of novel nanoarchitectures to be used in low cost and energy efficient devices with improved performance and multiple functionalities.

[1] G. van der Laan *et al.*, Phys. Rev. Lett. **105**, 067405 (2010).
[2] E. Arenholz *et al.*, Phys. Rev. B **82**, 140103(R) (2010).
[3] G. van der Laan *et al.*, Phys. Rev. Lett. **100**, 067403 (2008).
[4] E. Arenholz *et al.*, Phys. Rev. Lett. **98**, 197201 (2007).

[1]Supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

3:06PM L16.00002 Investigation of ferromagnetic/antiferromagnetic nanostructures using X-ray magnetic dichroism

, J. WU, National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32310, USA, J.S. PARK, Department of Physics, University of California at Berkeley, Berkeley, California 94720, USA, W. KIM, Korea Research Institute of Standards and Science, Yuseong, Daejeon 305-340, Koera, E. ARENHOLZ, M. LIBERATI, A. SCHOLL, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA, CHANYONG HWANG, Korea Research Institute of Standards and Science, Yuseong, Daejeon 305-340, Koera, Z.Q. QIU, Department of Physics, University of California at Berkeley, Berkeley, California 94720, USA — The spin structure of epitaxially grown antiferromagnetic/ferromagnetic bilayer was investigated using X-ray Magnetic Circular Dichroism (XMCD) and X-ray Magnetic Linear Dichroism (XMLD) techniques. The XMLD measurement on the antiferomagnetic film (NiO or CoO) gives a direct probe of the spin orientation of the compensated antiferromagnetic spins. This capability enables us to give a clear clue to the mechanism of the exchange bias in the bilayer and to give a direct observation of the antiferromagnetic vortex.

3:18PM L16.00003 XPCS Study of Antiferromagnetic Domain Fluctuation[1]

, KEOKI SEU, SUJOY ROY, Lawrence Berkeley National Laboratory, SAN-WEN CHEN, XIANGSHUN LU, HONGYU GUO, SUNIL SINHA, Dept. of Physics, University of California, San Diego, KARINE DUMESNIL, Univeristy of Nancy, France — We have studied magnetic domain fluctuations in Yttrium-Dysprosium-Yttrium trilayer films using X-ray Photon Correlation Spectroscopy (XPCS) in conjunction with resonant soft X-ray magnetic scattering. Dysprosium thin film possesses a helical antiferromagnetic phase below Tn = 180 K and a ferromagnetic phase below Tc = 64 K. With coherent soft x-rays we observed magnetic speckle in the scattering from the antiferromagnetic domains. We determined critical points and found a shift of Curie temperature from the bulk value. Hysteresis associated with a first order phase transition was also observed. We observed magnetic speckle around the magnetic satellite peak at (0,0,q_m) due to static disorder as well as magnetic domains. At temperatures above Tn the system showed static behavior on times scales up to $\sim$ 300 sec which is indicative of non-fluctuating static disorder that persists above Tn. Close to Tc, there appears to be time-dependent fluctuations due to slow domain wall motion and these will be discussed.

[1]Work supported by U.S. Dept. of Energy Basic Energy Sciences under grant DE-FG02-03 ER46680.

3:30PM L16.00004 Deposition-order dependent magnetization reversal of graded anisotropy Co/Pd films[1]

, PETER GREENE, University of California, Davis, BRIAN J. KIRBY, JULIE A. BORCHERS, JUNE W. LAU, NIST, Gaithersburg, KAI LIU, University of California, Davis — We report deposition-order-dependent, and depth-dependent, magnetization reversal in Co/Pd with graded anisotropy, which are technologically important as they address both writability and thermal stability challenges. Multilayers of $[Co(0.4nm)/Pd(0.6nm)]_{60}$ have been deposited by sputtering, where the Ar pressure has been varied from 5 to 12 and 20 mtorr in type A samples and in the reverse order in type B samples. An extensive set of structural and magnetization reversal studies with depth-resolution has been performed using XRD, cross-sectional TEM, magnetometry, PNR and XMCD. In type A samples, due to the larger grain size, lower interfacial roughness and less disorder in the magnetically softer layer, magnetization reversal proceeds via domain nucleation, propagation, and annihilation. Type B samples show a more localized reversal. Layers grown at higher pressure contain more disorder and rougher interfaces, which is carried into the magnetically softer layers deposited on top, thus impeding domain movement.

[1]Work supported by NSF (DMR-1008791& ECCS-0925626).

3:42PM L16.00005 ABSTRACT WITHDRAWN –

3:54PM L16.00006 Magnetization reversal and magnetic imprinting in a giant exchange bias system

, M.R. FITZSIMMONS, LANL, J.A. BORCHERS, NIST, M. LAVER, PSI, K.L. KRYCKA, W.C. CHEN, S. WATSON, NIST, C. DUFOUR, K. DUMESNIL, Laboratoire de Physique des Matériaux, Université H. Poincaré Nancy — We present compelling experimental evidence, obtained with small angle neutron scattering (SANS) that magnetization reversal of an exchange biased $DyFe_2/YFe_2$ superlattice occurs via reversal of magnetic domains with at least two different length scales. Our SANS studies used both unpolarized neutron beams (with a high field magnet) and polarized neutron beams using ^{3}He filter polarization analysis. Magnetic length scales ranging from tens of nanometers to greater than several hundreds of nanometers were observed. The magnetization contained within nanometer large domains constituted a significant fraction of the total magnetization at the exchange bias field. During magnetization reversal some of the domains were arranged in a quasi-periodic manner. Because the ferromagnetic domains are so small, they exchange couple to relatively small portions of the pinned magnetic layer (i.e., $DyFe_2$), which at the nm length scale may appear relatively perfect. This reasoning may explain why the $DyFe_2/YFe_2$ system is a system that exhibits among the largest exchange bias observed to date. This work was supported by the Office of Basic Energy Science, U.S. Department of Energy and the National Science Foundation. ML acknowledges support from DanScatt.

4:06PM L16.00007 Polarized Neutron Reflectivity and Electron Microscopy Analysis of the Magnetic Microstructure in Antiparallel-Coupled Co Multilayers , JOHN UNGURIS, BENJAMIN MCMORRAN, Center for Nanoscale Science and Technology, JULIE BORCHERS, BRIAN MARANVILLE, BRIAN KIRBY, THERESA GINLEY, Center for Neutron Research, National Institute of Standards and Technology — Antiparallel exchange-coupled thin films are a convenient way to provide a ferromagnetic surface in situations where zero net magnetization is required, for example, when studying superconducting-ferromagnetic proximity effects with spin-triplet superconducting correlations.[1] We use the complementary techniques of polarized neutron reflectivity (PNR) and scanning electron microscopy with polarization analysis (SEMPA) to characterize the magnetic structure of such an antiferromagnetically coupled Co/Ru/Co multilayer. We find that, although the average macroscopic magnetization follows the simple antiparallel coupling picture, at the nanoscale the 3-dimensional magnetic structure is much more complex. The films are mostly antiparallel, but the magnetization directions fluctuate by as much as $\pm$ 40° over lengths as small as 100 nm. This structure has significant implications when trying to understand the local spin-dependent transport properties at the ferromagnetic interface. Applying magnetic fields further complicates the structures, leading to spin-flop related magnetic arrangements.

[1]T. Khaire, etal. Phys. Rev. Lett. 104, 137002 (2010)

4:18PM L16.00008 Distinguishing the ultrafast dynamics of orbital and spin magnetic moments in solids , CHRISTINE BOEGLIN, CNRS-IPCMS-UMR7504 — Ultrafast magnetization dynamics is an important issue for both fundamental science and for applications in order to optimize spin manipulation on a microscopic level. Since the first observation of laser induced spin dynamics,[1] the mechanisms of angular momentum dissipation at picosecond timescales have been widely debated. In order to progress in the understanding of such microscopic ultrafast mechanisms, it is now possible to probe absolute values of magnetization with a high temporal resolution (100 fs). In this context, we have used ultrashort optical laser pulses (60 fs duration) to induce changes of the magnetization in a ferromagnetic CoPd alloy film with perpendicular anisotropy. The dynamics was probed with ultrashort circularly polarized femtosecond X-ray pulses, measuring the X-ray magnetic circular dichroism (XMCD) at Co $L_{2,3}$ edges.[2,3] We observe that the two components of the magnetic moments (L and S) show different ultrafast dynamics and that the spin-orbit coupling related to the magneto-crystalline anisotropy in solids is strongly affected by fs laser pulses in the ultrashort time scales. These dynamics can be compared to the purely electronic effect at the CoL_3 edge. Electronic excitations and their response to the laser pump pulse will be discussed and related to the modifications in the spin-orbit coupling. We will compare our results with time resolved MOKE experiments recently performed on CoPd alloys.

[1]Beaurepaire, E., Merle, J.C., Daunois, A., and Bigot, J.-Y. *Phys. Rev. Lett.* **76**, 4250 (1996).
[2]Stamm, C. Kachel, T., Pontius, N., Mitnzer, R., Quast, T., Holldack, Khan, S., Lupulescu, C., Aziz, E. F., Wietstruk, M., Dürr, H. A., and Eberhardt, W. *Nature Mater.* **6**, 740-743 (2007).
[3]C. Boeglin, E. Beaurepaire, V. Halté, V. Lopez-Flores, C. Stamm, N. Pontius, H. Dürr, J. -Y. Bigot "Observing how fast the spin-orbit interaction branches spin and orbital moments in solids" Nature 465, 458 (2010).

4:54PM L16.00009 Neutron Reflectivity Study in Py/CoO Exchange Bias System , SAN-WEN CHEN, XIANGSHUN LU, SUNIL SINHA, Dept. of Physics, University of California, San Diego, AMI BERKOWITZ, ERIC FULLERTON, KEITH CHAN, Center of Magnetic Recording Research, University of California, San Diego, VALARIA LAUTER, HAILEMARIAM AMBAYE, Neutron Science Divn., Oak Ridge National Laboratory, ELIZABETH BLACKBURN, University of Birmingham, UK — We have studied the permalloy-cobalt monoxide exchange bias system using polarized neutron reflectivity. Both polycrystalline and epitaxial single crystalline (with the (111) and (100) CoO planes at the interface) CoO films were studied. By fitting the reflectivity for both directions of the applied field relative to the cooling field, we are able to obtain both the nuclear and spin depth profiles, as well as locating the pinned spins which are responsible for the exchange bias effect. The pinned spins at the interface can be resolved in the polycrystalline sample, which is consistent with our previous study with resonant soft x-ray reflectivity. One could reasonably have expected a stronger exchange bias effect in the (111) single crystal CoO film, because it has more uncompensated spins at the interface. The neutron reflectivity, however, shows lesser pinned spins. In the presentation, we will show the difference between the magnetic density profiles of the samples involving polycrystalline, (111) and (100) single crystalline CoO films respectively.

5:06PM L16.00010 Effects of hydrogen/deuterium absorption on the magnetic properties of Co/Pd multilayers , KINESHMA MUNBODH, FELIO PEREZ, CAMERON KEENAN, DAVID LEDERMAN, West Virginia University, MIKHAIL ZHERNENKOV, MICHAEL FITZSIMMONS, Los Alamos National Laboratory — The effects of hydrogen and deuterium absorption were studied in two Co/Pd multilayers with perpendicular magnetic anisotropy using Polarized Neutron Reflectivity (PNR). PNR measurements were performed with the field in the plane of the sample with the magnetization M saturated at H = 6.0 T and unsaturated at 0.65 T. The nominal thicknesses of the Co/Pd layers were 2.5 Å/21 Å. Therefore, the actual layer chemical composition, thickness, and interface width parameters were defined from the nuclear scattering length density (SLD) profile obtained from both x-ray reflectivity (XRR) and PNR and their derivatives. The nuclear PNR SLD profile showed that although deuterium absorption occurred throughout the sample, the multilayer stack did not expand. The magnetic SLD showed that M in both the Pd and Co layers was affected. At saturation, M decreased, while at H = 0.65 T M increased upon deuterium exposure. Magnetization measurements confirmed hydrogen absorption decreased the total M at saturation and increased the component of M parallel to the field when not at saturation. These results indicate that hydrogen or deuterium absorption decreases both the perpendicular anisotropy and total magnetization of the samples.

5:18PM L16.00011 Revisit of Magnetism of Fe overlayers on Cu(001) , CHANYONG HWANG, Korea Research Institute of Standards and Science, YONG ROK OH, Pukyung National University, Y.S. PARK, WONDONG KIM, Korea Research Institute of Standards and Science, LEELA POORNIMA, Chungnam National University, Z.Q. QIU, University of california at Berkeley — Fe films on Cu(001) have drawn a great attention due to the complicated structural and magnetic properties. It is known from the previous investigations that depending on the Fe thickness, Fe/Cu system has three distinguishable regions in terms of the structural and magnetic properties. Especially the spin structure in region II, where the film thickness ranges from 5 ML to 11 ML, has been controversial for the last two decades. We have studied the spin structure of Fe films on Cu(001) in region II via x-ray magnetic circular dichroism (XMCD) and surface magneto-optic Kerr effect (SMOKE) measurements. Wedge-shaped Fe films, which ranged from 6 ML to 10 ML, have been grown on Cu(001) at room temperature by an e-beam evaporator. Our results suggest a new model, which is totally different from the previous models, based on the incommensurate spin density wave.

Tuesday, March 22, 2011 2:30PM - 5:30PM –

Session L17 GMAG DMP: Focus Session: Magnetic Oxide Thin Films - Ferroic and Oxide Tunnel Junctions D174

2:30PM L17.00001 All-Manganite Tunnel Junctions with Interface-Induced Barrier Magnetism[1]

, ZOUHAIR SEFRIOUI, Grupo de Física de Materiales Complejos, Universidad Complutense de Madrid, 28040 Madrid (Spain) — The recent discovery of several unexpected phases at complex oxide interfaces is providing new insights into the physics of strongly correlated electron systems. The possibility of tailoring the electronic structure of such interfaces has triggered a great technological drive to functionalize them into devices. In this communication, we describe an alternative strategy to produce spin filtering by inducing a ferromagnetic insulating state in an ultrathin antiferromagnetic layer in contact with a ferromagnetic layer. This artificially induced spin filtering persists up to relatively high temperatures and operates at high applied bias voltages. The results suggest that after playing a key role in exchange-bias for spin-valves, uncompensated moments at engineered antiferromagnetic interfaces represent a novel route for generating highly spin-polarized currents with antiferromagnets.

Work done in collaboration with M. Bibes, C. Carrétéro, A. Barthélémy (Unité Mixte de Physique CNRS/Thales, Campus de Polytechnique, 1, Avenue A. Fresnel, 91767 Palaiseau (France) and Université Paris-Sud, 91045 Orsay (France)), F.A. Cuellar, C. Visani, A. Rivera-Calzada, , C. León, J. Santamaria (Grupo de Física de Materiales Complejos, Universidad Complutense de Madrid, 28040 Madrid (Spain)), M.J. Calderón, L. Brey (Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, 28049 Madrid (Spain)), K. March, M. Walls, D. Imhoff (Laboratoire de Physique des Solides, CNRS, Université Paris-Sud, 91405 Orsay (France)), R. Lopez Anton, T.R. Charlton (ISIS, Rutherford Appleton Laboratory, Chilton, Oxon OX11 0QX (United Kingdom)), E. Iborra (Universidad Politécnica de Madrid, Escuela Técnica Superior de Ingenieros de Telecomunicaciones, 28040 Madrid (Spain)), F. Ott (Léon Brillouin, CEA/CNRS, UMR 12, 91191 Gif-sur-Yvette (France)).

[1]This work was supported by the Spanish Ministry for Science and Education programs MAT2008 06517, and the Réseau Thématique de Recherche Avancée (RTRA) "Triangle de la Physique"

3:06PM L17.00002 Nanostructured $CoFe_2O_4$ Films for Magnetic Logic Applications

, RYAN COMES, MAN GU, University of Virginia, MIKHAIL KHOKHLOV, Guilford College, JIWEI LU, STUART WOLF, University of Virginia — $CoFe_2O_4$ (CFO) offers unique properties as a magnetoelectric material due to its large magnetoelastic response when strained. Previous work has shown that when CFO is co-deposited with $BiFeO_3$ (BFO) nanostructured phase segregation occurs and electrical control of the magnetic anisotropy is possible [1]. Such a system offers unique possibilities for an electrically-controlled spintronic logic scheme. To that end, CFO films were grown on MgO and $SrTiO_3$ (STO) substrates using pulsed electron deposition. Films grown on MgO substrates exhibit large perpendicular anisotropy due to epitaxial strain, while films on STO exhibit mixed anisotropy. Using electron-beam lithography, nanopillars were etched into the film in dense arrays and characterized using magnetic force microscopy. Pillar arrays were produced with diameters between 30 and 75 nm with pitch ranging from 90 to 200 nm. The dipole interactions in these pillars were examined and their potential applications for spintronic logic were evaluated. Thinner $CoFe_2O_4$ islands were also patterned on STO with EBL and then used as a template for a co-deposited BFO/CFO film. Results of this work will also be presented.

[1] Zavaliche, F., et al. *Nano Lett.*, 2007, 7 (6), pp 1586–1590

3:18PM L17.00003 Spin-polarized tunnelling across single or double ferrite-based spin-filters

, SYLVIA MATZEN, JEAN-BAPTISTE MOUSSY, CEA-Saclay, RICHARD MATTANA, KARIM BOUZEHOUANE, CYRILE DERANLOT, FREDERIC PETROFF, UMP CNRS/Thales, JAGADEESH MOODERA, GUOXING MIAO, Francis Bitter Magnet Laboratory, CEA-SACLAY, FRANCE TEAM, UMP CNRS/THALES, FRANCE TEAM, FRANCIS BITTER MAGNET LABORATORY, MIT, USA TEAM — The generation of highly spin-polarized electron currents at room temperature is the basis of most spin-based device technologies. One approach known as spin filtering, has the potential of generating 100% spin-polarized currents by the spin selective transport of electrons across a ferromagnetic tunnel barrier. In this work, we investigate the spin-polarized tunnelling characteristics of ferrites (CoFe2O4, NiFe2O4 and MnFe2O4), which are exciting candidates for spin filtering at room temperature. Tunnel junctions containing epitaxial ferrite tunnel barriers have been grown by oxygen plasma-assisted molecular beam epitaxy. Their structural, chemical and magnetic properties having previously been optimized by a number of in situ and ex situ methods, we focus on the spin-polarized tunnelling in the ferrite-based systems using different measurement techniques and we propose an unconventional device combining two ferrite magnetic tunnel barriers in order to get large tunnelling magnetoresistance without the necessity of magnetic electrodes.

3:30PM L17.00004 Effect of Strain on Electronic and Magnetic Structure of Fe-doped $CoFe_2O_4$[1]

, JARRETT MOYER, CARLOS VAZ, Dept. of Applied Physics and Center for Research on Interface Structures and Phenomena, Yale University, EZANA NEGUSSE, Dept. of Physics, Montana State University, DARIO ARENA, National Synchrotron Light Source, Brookhaven National Laboratory, VICTOR HENRICH, Dept. of Applied Physics and CRISP, Yale University — The development of new materials with large room temperature spin polarizations and small conductivity mismatches with semiconductors is key for more complex spintronics devices. $CoFe_2O_4$ has a high Curie temperature (T_C = 793 K), a large predicted spin polarization, and, when doped with iron, a conductivity similar to semiconductors; however, the magnetic properties of thin films are different from the bulk. To investigate the effect of strain, $Co_{1-x}Fe_{2+x}O_4$ thin films ($0 \leq x \leq 0.65$) are grown epitaxially on MgO (001) and $SrTiO_3$ (001) by MBE. UPS probes filled valence band states, while X-ray Linear Dichroism (XLD) determines d-orbital occupations. SQUID magnetometry and XMCD are used to determine bulk and site-specific magnetic moments, respectively. These measurements allow us to understand how strain affects the electronic and magnetic structure of $Co_{1-x}Fe_{2+x}O_4$ thin films.

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

3:42PM L17.00005 Fabrication and properties of LuFe2O4 thin film[1]

, WENBIN WANG, University of Tennessee & Oak Ridge National Lab, XIAOSHAN XU, ZHENG GAI, PAUL C. SNIJDERS, THOMAS Z. WARD, Oak Ridge National Lab, JIAN SHEN, University of Tennessee & Fudan University — We have succeed in growing the LuFe2O4 polycrystalline thin film on the MgO(111) substrate with the Pulsed laser deposition(PLD) method. The surface structures, crystallographic and magnetic properties of the sample were characterized by XRD, AFM, SEM and SQUID. XRD pattern shows the sample crystallized in both (001) and (110) directions, which is also reflected in their morphological appearance in both AFM and SEM images. SQUID measurements reveal strong ferromagnetic signal in the thin film.

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

3:54PM L17.00006 Magnetic Force Microscopy of Magnetite Thin Films with Transition Metal Buffer Layers[1]

, ALFRED KH. LEE, MARK C. MONTI, JOHN T. MARKERT, ALEX DE LOZANNE, Department of Physics, The University of Texas at Austin, PRIYANGA B. JAYATHILAKA, CHRIS A. BAUER, CASEY W. MILLER, Physics Department, University of South Florida — Magnetite (Fe_3O_4) has been the subject of interest as a material for use in spin devices. Its ideal properties for this application break down in thin film morphologies due to the occurrence of antiphase boundaries (APBs). The density of APBs can be adjusted to some degree via film strain. This is accomplished in this work by including a variety of transition metal buffer layers between Fe_3O_4 and its MgO substrate. We investigate the microscale magnetic domain structure via magnetic force microscopy of Fe_3O_4 films on MgO with no, a Mo, or an Fe buffer layer across a temperature range surrounding the Verwey temperature ($T_V \sim$ 120K) and compare to bulk measurements from a SQUID magnetometer.

[1]Supported by NSF-ECCS (USF), NSF-DMR (UT), NSF-IGERT (UT), and the Welch Foundation (UT).

4:06PM L17.00007 A structural, electronic and magnetic study of ultrathin iron oxides , M. MONTI, B. SANTOS, J. MARCO, J. DE LA FIGUERA, CSIC-Rocasolano Madrid-SPAIN, M.A. NIÑO, T.O. MENTEŞ, A. LOCATELLI, ELETTRA Trieste-ITALY, K.F. MCCARTY, Sandia Nat Labs Livermore-USA, A. MASCARAQUE, O. RODRÍGUEZ DE LA FUENTE, Complutense Univ Madrid-SPAIN — Iron oxides continue to fascinate us after nearly a century of "modern" science devoted to their growth, properties and structure. Recently, a revival of research has been spurred by the multiferroic character of magnetite, and by its predicted half-metal character, both interesting for spintronic applications. Maghemite is, on the other hand, an interesting counterpart to magnetite. They both present the same inverse spinel structure but maghemite is a ferrimagnetic insulator. In this work we individually characterize flat triangular islands, less than 10 atomic layers thick, of magnetite and maghemite on Ru(0001) by means of selected-area X-ray photoemission and absorption, X-ray circular dichroism and low-energy electron diffraction and reflectivity. We grow magnetite islands in-situ, with well-defined magnetic domains inside, surrounded by a wüstite wetting layer by depositing iron in a molecular oxygen background pressure. Further exposure to NO_2 transforms the magnetite islands into maghemite, while changing the wüstite wetting layer into hematite.

4:18PM L17.00008 Giant tunnel electroresistance and electrical control of spin polarization with ferroelectric tunnel barriers , VINCENT GARCIA, Unité Mixte de Physique CNRS/Thales, Palaiseau, France — At room temperature, we use piezoresponse force microscopy to show robust ferroelectricity in $BaTiO_3$ ultrathin films, and conductive-tip atomic force microscopy to demonstrate the resistive readout of the polarization state via its influence on the tunnel current [1]. This giant electroresistance nondestructive readout paves the way for ferroelectric memories with simplified architectures, higher densities and faster operation. Additionally, ferroelectric tunnel junctions with ferromagnetic electrodes were engineered to demonstrate local, large and non-volatile control of carrier spin polarization by switching ferroelectric polarization [2]. Our results represent a giant interfacial type of magnetoelectric coupling and suggest a new low-power approach for spin-based information control.

[1] V. Garcia *et al.*, Nature 460, 81 (2009)
[2] V. Garcia *et al.*, Science 327, 1106 (2010)

4:54PM L17.00009 Electrically Controlled Spin Valve at a Complex Oxide Interface , EVGENY TSYMBAL, J.D. BURTON, University of Nebraska - Lincoln — Since the discovery of giant magnetoresistance exploration of spin-dependent electronic transport has proved promising for applications. To avoid the costly generation of magnetic fields in these devices there have been recent efforts toward manipulating magnetization by *electric* fields. Such magnetoelectric effects can be induced at the surfaces and interfaces of many ferromagnetic metals. Ferroelectric materials are especially helpful in this because their spontaneous electrical polarization can induce a large response at the interface with a magnetic metal. One example is the ferroelectric control of magnetic order at the interface between $La_{1-x}A_xMnO_3$ (where A is a divalent cation), and the ferroelectric $BaTiO_3$ [1]. Importantly, ferroelectric films can now be made thin enough (less than a few nm) to allow measurable electron tunneling while still maintaining a stable and switchable polarization [2]. Here we show that those few atomic layers near the interface sensitive to the ferroelectric polarization can act as an atomic scale spin-valve in series with the ferroelectric tunnel barrier. Switching the ferroelectric barrier induces more than an order of magnitude change in the conductance due to the interfacial spin-valve, constituting a substantial spin-dependent transport phenomenon controlled by an electric field alone.
[1] J. D. Burton and E. Y. Tsymbal, Phys. Rev. B **80**, 174406 (2009).
[2] A. Gruverman *et al.*, Nano Lett. **9**, 3539 (2009).

5:06PM L17.00010 Magnetic state switching controlled by a voltage in $La_{0.7}Ca_{0.3}MnO_3$/(Ba, Sr)TiO_3/$La_{0.7}Ca_{0.3}MnO_3$ tunneling junctions , WEIJIN HU, Department of Physics, Pennsylvania State University, University Park, PA 16802, KE CHEN, XIAOXING XI, Department of Physics, Pennsylvania State University, University Park, PA 16802 and Department of Physics, Temple University, Philadelphia, PA 19122, QI LI, Department of Physics, Pennsylvania State University, University Park, PA 16802, ZHIDONG ZHANG, Shenyang National Laboratory for Materials Science, Institute of Metal Research, CAS, Shenyang 110016, China — We report the switching of the two magnetic states (parallel and antiparallel states) in $La_{0.7}Ca_{0.3}MnO_3$/(Ba, Sr)TiO_3/$La_{0.7}Ca_{0.3}MnO_3$ magnetic tunneling junctions by measuring the tunneling magnetoresistance after applying a voltage pulse. The junction size ranges between 5x5 to 20x20 μm^2 with the barrier thickness in the range of 1-3 nm. We have found that magnetic state of the junction can be switched both from the antiparallel to parallel state and from the parallel to antiparallel state in certain and different field ranges, respectively. The switching does not depend on the polarity of the electrical field direction and the magnetic field direction. The critical voltage for the switching depends on the magnetic field with higher voltage needed for lower magnetic field. The critical voltage depends almost linearly on the bias magnetic field when the switch occurs.

5:18PM L17.00011 Four resistance states in $La_{0.7}Sr_{0.3}MnO_3$/(Ba, Sr)TiO_3/$La_{0.7}Sr_{0.3}MnO_3$ multiferroic tunnel junction at room temperature , PENG XU, YUEWEI YIN, WEIJIN HU, MURALIKRISHNA RAJU, QI LI, Department of physics, The Pennsylvania State University, University Park, PA 16802, USA, XIAOGUANG LI, Hefei National Laboratory for Physical Sciences at Microscale, Department of Physics, University of Science and Technology of China, 230026, China — Multiferroic tunnel junction (MFTJ), composed of two ferromagnetic electrodes separated by a thin ferroelectric barrier, has been predicted to serve as a four-state device as a result of the coexistence of tunneling magnetoresistance and tunneling electroresistance effects. Our previous results have demonstrated such devices, but only at low temperatures. Here, we report a MFTJ composed of $La_{0.7}Sr_{0.3}MnO_3$/(Ba, Sr)TiO_3/$La_{0.7}Sr_{0.3}MnO_3$ fabricated by pulsed-laser deposition. A typical R-H loop with a sharp-switched resistance states (magnetic parallel and antiparallel) similar to that of magnetic tunnel junctions has been observed up to room temperature. Upon polarization reversal of the barrier, both the parallel and antiparallel resistances will switch to a different value. Clear tunneling magnetoresistance and tunneling electroresistance, hence the four-resistance states, have been observed at room temperature. The resistance states can be switched between them by electric and magnetic fields and the manipulation of the states will be discussed.

Tuesday, March 22, 2011 2:30PM - 5:30PM –
Session L18 GMAG DMP: Focus Session: Low D/Frustrated Magnetism - 2D Lattices D172

2:30PM L18.00001 Exotic quantum phases in a frustrated quantum spin model on a honeycomb lattice[1] , CHRISTOPHER VARNEY, University of Maryland / Georgetown University, KAI SUN, VICTOR GALITSKI, University of Maryland, MARCOS RIGOL, Georgetown University — A quantum spin liquid is a phase that defies the usual conventions, i.e. quantum fluctuations prevent long range order even at $T = 0$. The search for models that exhibit this type of behavior has intensified in recent years. In this work, we utilize the Lanczos algorithm to study hard-core bosons on a frustrated honeycomb lattice with nearest-neighbor (t) and next-nearest-neighbor hoppings (t'). The two limits of this model, $t'/t = 0$ and $t'/t = \infty$, favor two different superfluid phases. In between, we find that an anomalous phase is stabilized by the strong frustration in this system and compare its properties with a quantum spin liquid and a fragmented Bose-Einstein condensate.

[1]This research is supported by by US-ARO, JQI-NSF-PFC, and the Office of Naval Research.

2:42PM L18.00002 Protecting the Kitaev honeycomb model from external fields[1] , HAITAN XU, JACOB TAYLOR, Joint Quantum Institute, University of Maryland, College Park, MD 20742, and National Institute of Standards and Technology, Gaithersburg, MD 20899 — We propose an approach to generate many-body interactions from two-body interactions with stable cat states. Applied to the celebrated Kitaev honeycomb model, our approach opens a spectral gap in the gapless phase of the model without any external magnetic field. We confirm the non-Abelian topological properties of a generalized Kitaev model and demonstrate our approach's robustness to sources of error. Our work provides a complete framework for experimentally realizing and manipulating non-Abelian anyons, with direct application in topological quantum computation.

[1]Supported by NSF JQI PFC

2:54PM L18.00003 Paramagnetic ground states and field-driven Néel order in S=3/2 Heisenberg antiferromagnets on a honeycomb lattice , GANESH RAMACHANDRAN, Department of Physics, University of Toronto, D.N. SHENG, Department of Physics and Astronomy, California State Univ., Northridge, Y.J. KIM, A. PARAMEKANTI, Department of Physics, University of Toronto — We study the spin-3/2 Heisenberg antiferromagnet on a honeycomb lattice with exchange interactions which frustrate Néel order. Our motivation stems from the recent synthesis of $Bi_3Mn_4O_{12}(NO_3)$, a spin-3/2 bilayer honeycomb lattice antiferromagnet which remains paramagnetic to the lowest temperature, but shows a field-induced Néel transition. We use a combination of spin wave theory, exact diagonalization, and bond operator theory to study the effects of quantum and thermal fluctuations, second-neighbor exchange, biquadratic exchange and bilayer coupling. Biquadratic terms give rise an AKLT valence bond solid ground state, and bilayer coupling leads to an interlayer dimer solid. Upon applying a magnetic field, both these states undergo a phase transition into a Néel long range ordered state. We comment on experimental consequences and disorder effects.

3:06PM L18.00004 Gapped Z_2 spin liquid and chiral antiferromagnetic phase in Hubbard model on the honeycomb lattice , YUAN-MING LU, YING RAN, Boston College — In Schwinger-fermion representation we identify a Z_2 spin liquid called the sublattice-pairing state (SPS) as the gapped spin liquid phase discovered in recent Quantum Monte study of Hubbard model on a honeycomb lattice. We show that SPS is identical to the zero-flux Z_2 spin liquid state in Schwinger-boson representation by an explicit duality transformation. SPS is connected to an *unusual* antiferromagnetic ordered phase, which we term as chiral-antiferromagnetic (CAF) phase, through an $O(4)$ critical point. CAF phase breaks $SU(2)$ spin rotation symmetry completely and has three Goldstone modes. Our results indicate that there is likely a hidden phase transition between CAF phase and the usual antiferromagnetic (Neel) phase at large U/t. We also propose numerical measurements to reveal the CAF phase and the hidden phase transition.

3:18PM L18.00005 Exotic phases in Mott insulating Iridates with strong spin-orbit coupling: Phase diagram of the Kitaev-Heisenberg model in a magnetic field , HONG-CHEN JIANG, Microsoft Research, Station Q, UCSB, ZHENG-CHENG GU, Kavli Institute for Theoretical Physics, UCSB, XIAO-LIANG QI, SIMON TREBST, Microsoft Research, Station Q, UCSB — Motivated by the recent proposal of a Mott insulating state with strong spin-orbit coupling for the Iridate Na_2IrO_3[1], we discuss the collective ground states of the effective Iridium moments in the presence of Heisenberg-Kitaev exchange interactions and a time-reversal symmetry breaking magnetic field. For a field pointing in the (111) direction we find a rich phase diagram with both symmetry breaking magnetically ordered phases as well as an unconventional topological phase which is stable over a small range of coupling parameters. Our numerical simulations further indicate two exotic multicritical points at the boundaries between these ordered phases, which we will discuss.

[1] J. Chaloupka, G. Jackeli, and G. Khaliullin, Phys. Rev. Lett. 105, 027204 (2010).

3:30PM L18.00006 Schwinger boson spin liquid states on honeycomb lattice: projective symmetry group analysis and critical field theory , FA WANG, Department of Physics, MIT — Motivated by the numerical evidence of a gapped spin liquid in the honeycomb Hubbard model [Meng et al. Nature 464, 847 (2010)], we analyse possible Z_2 spin liquids with gapped bosonic spinons coupled to Z_2 gauge field on honeycomb lattice within the Schwinger boson formalism. By the projective symmetry group method we find that there are only two relevant Z_2 spin liquids on honeycomb lattice with different (zero or π) gauge flux in the elemental hexagon. The zero-flux state seems to be a good candidate for the numerically observed spin liquid. It can acquire collinear AFM Neel order via a continuous O(4) transition. In the critical field theory of this transition the coupling of bosonic spinons to the Higgs field contains cubic powers of spatial derivatives, therefore does not break honeycomb lattice symmetry and allows for a continuous transition to a commensurate collinear Neel order. We will also discuss several observable features of this spin liquid.

3:42PM L18.00007 Nature of the spin liquid state of the Hubbard model on the honeycomb lattice , BRYAN CLARK, DMITRY ABANIN, PCTS, Department of Physics, Princeton University, SHIVAJI SONDHI, Department of Physics, Princeton University — Recent numerical work (Nature 464, 847 (2010)) indicates the existence of a spin liquid phase (SL) that intervenes between the antiferromagnetic and semimetallic phases of the half filled Hubbard model on a honeycomb lattice. To better understand the nature of this exotic phase, we study the quantum $J_1 - J_2$ spin model on the honeycomb lattice, which provides an effective description of the Mott insulating region of the Hubbard model. Employing the variational Monte Carlo approach, we analyze the phase diagram of the model, finding a phase transition between antiferromagnet and an unusual Z_2 SL state which we identify as the SL phase of the Hubbard model. At higher $J_2/J_1 > 0.3$ we find a transition to a dimerized state with spontaneously broken rotational symmetry.

3:54PM L18.00008 Finite-temperature phase transition to $m = 1/2$ plateau phase in a S=1/2 XXZ model on Shastry-Sutherland Lattices , TAKAFUMI SUZUKI, Institute for Solid StatePhysics — We study the finite-temperature transition to the $m = 1/2$ magnetization plateau in a model of interacting $S = 1/2$ spins with longer range interactions and strong exchange anisotropy on the geometrically frustrated Shastry-Sutherland lattice. This model was shown to capture the qualitative features of the field-induced magnetization plateaus in the rare-earth tetraboride, $\mathrm{TmB_4}$. Our results show that the transition to the plateau state occurs via two successive transitions with the two-dimensional Ising universality class, when the quantum exchange interactions are finite, whereas a single phase transition takes place in the purely Ising limit. To better understand these behaviors, we perform Monte Carlo simulations of the classical generalized four-state chiral clock model and compare the phase diagrams of the two models. The magnetic properties and critical behavior of the finite-temperature transition to the $m = 1/2$ plateau state are also discussed.

4:06PM L18.00009 Study of spin-lattice coupling in the Shastry-Sutherland compound $SrCu_2(BO_3)_2$, RAMZY DAOU, MPI-CPfS, MARCELO JAIME, SCOTT CROOKER, NHMFL-Los Alamos, FRANZISKA WEICKERT, MICHAEL NICKLAS, FRANK STEGLICH, MPI-CPfS, HANNAH DABKOWSKA, BRUCE GAULIN, McMaster University — $SrCu_2(BO_3)_2$ supports a network of orthogonally coupled spin-dimers whose ground state consists of localized spin-singlets which can be described by the exactly solvable Shastry-Sutherland Hamiltonian. On applying strong magnetic fields (>20T), however, the spin gap in $SrCu_2(BO_3)_2$ is closed and triplet excitations are generated. As a consequence of the strong geometric frustration, the triplet band is nearly dispersionless and a sequence of steps and plateaux in the magnetisation at integer fractions of the saturation magnetisation are observed, corresponding to static magnetic textures that are commensurate with the lattice. Here we present high resolution measurements in pulsed magnetic fields up to 65T of the magnetostriction and magnetocaloric effect which 1) shed light on the coupling between spin and lattice degrees of freedom and 2) are aimed to address discrepancies between existing data and theoretical predictions for the sequence of field-induced plateaus. Experiments were carried out at the Dresden High Magnetic Field Laboratory and the pulsed field facility of the National High Magnetic Field Laboratory.

4:18PM L18.00010 Phase Transitions in the $J_1 - J_2$ Ising Model on the Square Lattice[1] , SONGBO JIN, ARNAB SEN, ANDERS SANDVIK, Boston University — The $J_1 - J_2$ Ising model on the square lattice is one of the simplest classical models to study the effects of competing interactions and the resulting phase transitions. In spite of previous studies, there remains a controversy regarding the nature of the transition into the "stripe" phase in this model for $J_2/J_1 > 0.5$. In this study, we use the Binder cumulant of the order parameter to address this question. We use the Wang-Landau and Metropolis algorithms to simulate the model in the relevant parameter space. From our numerics, we determine that the transition is first-order for $0.5 < J_2/J_1 < g_{tri}$ ($g_{tri} \approx 0.8$) and becomes continuous in nature for larger values of J_2/J_1. We also discuss the order parameter distribution and correlation lengths at the first-order transition.

[1]Funding/Support: NSF DMR-0803510

4:30PM L18.00011 Low Temperature ^{31}P-NMR Study of the Frustrated Square-Lattice Compound $BaCdVO(PO_4)_2$[1] , B. ROY, R. NATH, D.C. JOHNSTON, Y. FURUKAWA, Ames Laboratory, Dept. of Phys. and Astro., Iowa State Univ., C. GEIBEL, MPI CPfS, Dresden — $BaCdVO(PO_4)_2$ is known to be a S = 1/2 frustrated square-lattice (FSL) system with a ferromagnetic nearest neighbor exchange coupling $J_1 \sim$ -3.36 K and an antiferromagnetic next nearest neighbor exchange coupling $J_2 \sim$ 3.53 K. We have carried out ^{31}P-NMR measurements at low temperatures down to 0.1 K to investigate magnetic properties of this compound from a microscopic point of view. ^{31}P spin-lattice relaxation rates ($1/T_1$) measured at H = 0.8 T are almost independent of temperature above 2 K, show a peak at 1.05 K and become constant below 0.4 K. The temperature dependence of $1/T_1$ indicates the existence of antiferromagnetic ordering at $T_N \sim$ 1.05 K which is also evidenced by the broadening of the NMR spectrum below that temperature. We will compare our NMR results with those of a similar FSL system, $Pb_2VO(PO_4)_2$ and discuss the similarities and differences in the magnetic properties of these two systems.

[1]Supported by USDOE under the Contract No. DE-AC02-07CH11358.

4:42PM L18.00012 Magnetic phase diagram of spatially anisotropic, frustrated spin-1/2 Heisenberg antiferromagnet on square and stacked square lattices , KINGSHUK MAJUMDAR, Department of Physics, Grand Valley State University, Allendale, MI 49401 — Magnetic phase diagram of a spatially anisotropic, frustrated spin-1/2 Heisenberg antiferromagnet on a square and a stacked square lattice is investigated using second-order spin-wave expansion. It is shown that with increase in next nearest neighbor frustration the second-order corrections play a significant role in stabilizing the magnetization. We obtain two ordered magnetic phases (Neél and stripe) separated by a paramagnetic disordered phase. Within second-order spin-wave expansion we find that the width of the disordered phase diminishes with increase in the interlayer coupling (for the 3D case) or with decrease in spatial anisotropy but it does not disappear. Our obtained phase diagram differs significantly from the phase diagram obtained using linear spin-wave theory.

4:54PM L18.00013 Study of Orbital Degenerate System in Frustrated Checkerboard Lattice , JOJI NASU, Tohoku University, SUMIO ISHIHARA — Orbital degree of freedom is one of the recent attractive themes in transition-metal oxides. In contrast to the spin degree of freedom, the orbital interaction explicitly depends on the bond direction, and a certain kind of frustration exists. In the geometrical frustrated lattice, cooperating and competing effects between the orbital frustration and the geometrical frustration provide new features in the static and dynamical properties of orbital. The present purpose is to study the intrinsic orbital frustration effect in a geometrical frustrated lattice. We introduce the spin-less Hubbard-type model with the doubly degenerate d_{yz} and d_{zx} orbitals in the checkerboard lattice. The effective Hamiltonian for the strong correlation limit is derived. We have the $J_z S_i^z S_j^z$ type Ising interaction for the nearest-neighbor bonds and the $J_x S_i^x S_j^x$ type Ising one for the next nearest-neighbor bonds. Here **S** is the orbital pseudo-spin operator. In the mean-field approximation, there is a macroscopic number of degeneracy at the frustration point J_x/J_z=2. In the classical Monte-Carlo simulation, we have a staggered orbital order and the reentrant phase-boundary. In the analyses by the spin-wave approximation and the exact diagonalization method, a large damping of the high-energy orbital dynamics due to the frustration is observed.

5:06PM L18.00014 Thermodynamics of the AF Heisenberg Model on the Checkerboard Lattice; a Numerical Linked-Cluster Expansion Study[1] , EHSAN KHATAMI, MARCOS RIGOL, Georgetown University — Employing numerical linked-cluster expansions (NLCEs) along with exact diagonalizations of finite clusters with periodic boundary condition, we study the energy, specific heat, entropy, and various susceptibilities of the antiferromagnetic (AF) Heisenberg model on the checkerboard lattice. NLCEs, combined with extrapolation techniques, allow us to access temperatures much lower than those accessible to exact diagonalization and other series expansions. We find that the high-temperature peak in specific heat decreases as the frustration increases, consistent with the large amount of unquenched entropy in the region around maximum classical frustration, where the nearest-neighbor and next-nearest-neighbor exchange interactions (J and J', respectively) have the same strength, and with the formation of a second peak at lower temperatures. The staggered susceptibility shows a change of character when J' increases beyond $0.75J$, implying the disappearance of the long-range AF order at zero temperature. For $J' = 4J$, in the limit of weakly-coupled crossed chains, we find large susceptibilities for stripe and Néel order with $\mathbf{Q} = (\pi/2, \pi/2)$ at low temperatures with AF correlations along the chains. Other magnetic and bond orderings, such as a plaquette valence-bond solid and a crossed-dimer order suggested by previous studies, have also been investigated.

[1]Supported by NSF Grant No. OCI-0904597 and Teragrid Account No. TG-DMR100026

5:18PM L18.00015 Quantum Phases of the Cairo Pentagonal Lattice , IOANNIS ROUSOCHATZAKIS, ANDREAS M. LAEUCHLI, RODERICH MOESSNER, Max Planck Institute for the Physics of Complex Systems, NEW STATES OF QUANTUM MATTER TEAM — We present an analytical and numerical study of the spin S=1/2 antiferromagnetic Heisenberg model on the Cairo pentagonal lattice. This is the dual of the Shastry-Sutherland lattice and has been discussed as a possible new candidate for having a spin liquid ground state [1]. More recently a S=5/2 version of this model has been realized in the Bi2Fe4O9 system [2]. Here we use a model with two different types of exchange couplings and investigate the nature of the ground state as a function of their ratio. This strategy allows us to understand the nature of a number of phases and derive effective models for their description with and without a magnetic field. Of particular interest is a surprising interplay between a collinear and a four-sublattice orthogonal phase due to an underlying order-by-disorder mechanism. Furthermore we address the issue of possible nonmagnetic ground states such as singlet and spin nematic phases.

[1] K. S. Raman, R. Moessner, and S. L. Sondhi, PRB 72, 064413 (2005)
[2] E. Ressouche, V. Simonet, B. Canals, M. Gospodinov, and V. Skumryev, PRL 103, 267204 (2009)

Tuesday, March 22, 2011 2:30PM - 5:30PM –

Session L19 GMAG DMP: Focus Session: Spin Transport & Magnetization Dynamics in Metals V D170

2:30PM L19.00001 Thermal spin fluctuations in itinerant ferromagnets: Aspects of magnetic thermodynamics and transport properties , KIRILL BELASHCHENKO, University of Nebraska-Lincoln — The character of thermal spin fluctuations in itinerant ferromagnets is a long-standing problem. Our recent theoretical results offer new insights in this issue. First, I will discuss a classical effective spin model with both rotational and longitudinal spin fluctuations, which allows for a variable degree of itinerancy. Magnetic thermodynamics in this model was analyzed for fcc and bcc lattices using Monte Carlo simulations compared (favorably) with mean-field and generalized Onsager approximations. It was found that magnetic short-range order is relatively weak and almost independent on the degree of itinerancy. The ambiguity of the phase space measure will be emphasized. Next, I will discuss our first-principles calculations of spin-disorder resistivity (SDR) of Fe, Ni, and heavy rare-earth metals (Gd-Tm series), in which the Landauer conductance is explicitly averaged over spin disorder configurations. For Fe the SDR agrees very well with experiment. For Ni, comparison with experiment suggests that the average local moment in the paramagnetic state is reduced to $\sim$0.35 μ_B. The effect of magnetic short-range order on SDR is found to be weak in both Fe and Ni. Overall, the results suggest that thermal spin fluctuations in Fe and Ni have an effectively classical character. While the crystallographically averaged paramagnetic SDR for rare earth metals agrees quite well with experiments, its anisotropy systematically and significantly exceeds the available measurements. This discrepancy is critically evaluated, suggesting the need for additional experiments.

[1] A. L. Wysocki, J. K. Glasbrenner, and K. D. Belashchenko, Phys. Rev. B **78**, 184419 (2008).
[2] A. L. Wysocki, R. F. Sabirianov, M. van Schilfgaarde, and K. D. Belashchenko, Phys. Rev. B **80**, 224423 (2009).

3:06PM L19.00002 Theory of the Kondo Temperature in Multilevel Quantum Dots[1] , ION GARATE, IAN AFFLECK, University of British Columbia and Canadian Institute for Advanced Research — We develop a simple but general method to evaluate the Kondo temperature in a multilevel quantum dot that is weakly coupled to conducting leads. Our analysis reveals that the Kondo temperature is strongly enhanced when the intradot energy-level spacing is smaller than the charging energy.

[1]We acknowledge financial support from NSERC and CIFAR.

3:18PM L19.00003 Role of initial quantum correlation in transient linear response , CHIKAKO UCHIYAMA, Univ. of Yamanashi, Japan, MASAKI AIHARA, Nara Institute of Science and Technology, Japan — We study the transient linear response of a two-level system coupled with an environmental system for correlated and factorized initial conditions. We find the significant differences between the transient linear response in these cases, especially for strong system-environment interaction at intermediate temperatures. This means that we need to pay attention to the initial conditions when we analyze experiments on transient linear response. This is because the conventional factorized initial condition, in which the system-environment correlation is disregarded, results in an incorrect response.
Reference: C. Uchiyama and M. Aihara, Phys. Rev. A, **82**, 044104(2010).

3:30PM L19.00004 Even-odd parity effects of a spin-1 Heisenberg chain on long-range interaction and entanglement[1] , SANGCHUL OH, University at Buffalo, SUNY, MARK FRIESEN, University of Wisconsin-Madison, XUEDONG HU, University at Buffalo, SUNY — A strongly coupled spin chain can be used as a quantum data bus, to mediate long-range interactions and entanglement between remote qubits.By obtaining numerical solutions for finite size systems, we investigate even-odd parity effects in a spin-1 chain and their consequences for long-range interactions and entanglement. We observes some similarities with a spin-1/2 chain [1]. For example, we find that an even-size chain mediates an RKKY (Ruderman-Kittel-Kasuya-Yosida)-like interaction between weakly coupled attached spins, while an odd-size chain acts as a central spin to the attached spins. On the other hand, we find that the RKKY-like interactions have a different character. For a spin-1/2 chain, the interactions decay with qubit separation as they oscillate between ferro and antiferromagnetic couplings. For a spin-1 chain, the interactions also oscillate, but they decay very little as a function of qubit separation. We believe this behavior is a manifestation of the finite Haldane gap of an integer spin chain in the thermodynamic limit.

[1] S. Oh, M. Friesen, X. Hu, Phys. Rev. B **82**, 140403(R) (2010).

[1]This work is supported by the DARPA/MPO QuEST program through a grant from AFOSR.

3:42PM L19.00005 Theory of Magnetization of Interacting Bloch Electrons , PRASANTA MISRA, University of Houston, GOURI TRIPATHI, Berhampur University, India — We derive a theory of magnetization of interacting Bloch electrons in the paramagnetic limits. We start with a thermodynamic potential, which includes both the quasi-particle and correlation contributions. The startling result obtained by us is that the modifications brought about by the electron-electron interactions for the magnetization in the quasi-particle interaction is precisely cancelled by the contributions due to electron correlations and thus the magnetization is devoid of explicit many-body corrections. In contrast, it is well known that both the spin susceptibility and the spin Knight-shift are exchange enhanced by electron-electron interactions. This is due to second order effects in the sense that while both the spin vertices are renormalized, the renormalization of only one of the vertices is cancelled by the contribution due to electron correlations. However, there is only one spin-vertex in the expression for magnetization which is renormalized in the quasi-particle approximation. We discuss the importance of self-energy corrections on the single-particle spectrum and we have shown as how to predict that the interacting electron system is magnetic or not by considering a variant of the Hubbard Hamiltonian in the momentum space.

3:54PM L19.00006 Exact solution for permeability of a ferromagnet under parametric bichromatic irradiation , ADIL-GERAI KUSSOW, University of Massachusetts, Lowell, Department of Physics, ALKIM AKYURTLU, University of Massachusetts, Lowell, Department of Electrical and Computer Engineering — If two parametrically coupled electromagnetic fields are applied to a ferromagnet, a non-linearity of the equation of precession of magnetic moment strongly affects the permeability. If the coupling constant $|\beta| < 1$ between the probe (p) wave and the support (s) wave is small, the permeability $\hat{\mu}(\omega)$, at the frequency of the probe wave $\omega = \omega_p = 2\omega_s$, is still monochromatic-like, with the re-normalized resonance spin waves frequency $\Omega_r \to \Omega(1+\beta)$. If a coupling is strong, $\beta \leq -1$, unusual response effects are possible (the magnetic transparency and profoundly non-monochromatic permeability $\hat{\mu}(\omega)$. Possible optical applications to the homogeneous negative refractive index materials are discussed.

4:06PM L19.00007 Element specific analysis of magnetic anisotropy in practical Mn-based antiferromagnetic alloys from first principles , KHMELEVSKYI SERGII, Institute of Applied Physics, Vienna University of Technology, Austria, ALEXANDR B. SHICK[1], Institute of Physics ASCR, v.v.i., Na Slovance 2, 182 21 Praha 8, Czech Republic, PETER MOHN, Institute of Applied Physics, Vienna University of Technology, Austria — Magnetic Anisotropy Energy (MAE) and element specific contribution to MAE has been studied for practical Mn-based antiferromagnetic alloys with layered $L1_0$ structure in the framework of the Local Spin Density Approximation and fully relativistic torque method. It is found that the contribution to the total MAE from non-magnetic 3d and 4d-elements in MnNi and MnPd alloys is comparable to the contribution of the magnetic Mn atoms. In the 3d-5d MnIr alloy the Ir contribution is found to be dominating. The origin of this contribution from the elements with total zero atomic spin moment is linked to the calculated non-trivial spin density distributions on the corresponding atom, which gives a zero moment only on average. We have also found and discuss a strong dependence of the total and element specific contribution to MAE on the state of the magnetic order.

[1]shick@fzu.cz

4:18PM L19.00008 Theoretical search for new permanent magnets with no rare earth atoms , LIQIN KE, VLADIMIR ANTROPOV, Ames Laboratory — We performed the extensive computational search for better permanent magnets containing no rare earth atoms. Our initial studies are concentrated on the intrinsic properties of magnetic materials such as magnetization, the Curie temperature and magnetic anisotropy. A computational tool based on the electronic structure methods has been developed to describe these physical properties as a function of electronic concentration. The application of this technique allowed us to provide several possible directions to perform a search for new materials. We discuss some physical limitations of required properties in iron based materials using the analysis of their electronic structure and simplified magnetic models. The issues of chemical substitutions, modification of geometry and changing the dimensionality of systems will be discussed as well. The specific results will be shown for Fe and Co based systems with the additions of N, C, W, Al and other atoms.

4:30PM L19.00009 Ab initio study of $d^{\bigcirc}$ magnetism in CaC , HADI AKBARZADEH, ZAHRA NOURBAKHSH, S. JAVAD HASHEMIFAR, Isfahan University of Technology — The half-metallic ferromagnetism in d^0 ionic compounds has attracted considerable attention in the spintronics community [Phys. Rev. B 73 024404, 2006]. In this work we employ density functional theory to study electronic, magnetic, and mechanical properties of the high ionic CaC compound in the Zinc Blend (ZB), Rock Salt (RS), B_2, Wurtzite (WZ), NiAs, and tetragonal structures.The observed ferromagnetic equilibrium state in the RS, NiAs, WZ, tetragonal and ZB structures is attributed to the partially filled sharp p band of carbon around the Fermi level. Half-metallicity has been found in the equilibrium ZB and expanded WZ structures with a magnetic moment of 2 μ_B/formula units. Comparing the Gibbs free energy of various structures indicates favorability of the half metallic phases in negative pressures. Topological analysis of the electronic charge density reveals topological character of the paramagnetic-ferromagnetic phase transition of the revised NiAs and B_2 structures as well as the geometrical character of the magnetic phase transitions of the RS and ZB structures.

4:42PM L19.00010 Greigite and Spinorbitronics[1] , BAOMIN ZHANG, GILLES DE WIJS, Institute for Molecules and Materials, Radboud University Nijmegen, ROB DE GROOT, Institute for Molecules and Materials, Radboud University Nijmegen; Institute for Advanced Materials, University of Groningen, ELECTRONIC STRUCTURE OF MATERIALS TEAM, SOLID STATE MATERIALS FOR ELECTRONICS TEAM — Greigite(Fe_3S_4) and magnetite(Fe_3O_4) are isoelectronic and isostructural ferrimagnets. In biology, the motility of magnetotactic bacteria is based on any or both of them. Not much work is known on greigite. Unlike half-metallic magnetite, greigite is a normal metal. Although the constituent elements are light, the complex Fermi-surface of greigite is remarkably sensitive to relativistic effects. The existence of several Fermi-surface sheets is dependent on the direction of the magnetization. This implies spintronics based on a homogeneous material rather than a device. Since this effect is intrinsically relativistic, spin-contamination is irrelevant here.

[1]Thanks to FOM and NWO for support.

4:54PM L19.00011 Experimental and theoretical investigations into the twinning energy of an FSMA system , P.K. MUKHOPADHYAY, MADHUPARNA KARMAKAR, RAJINI KANTH B., LCMP, S.N.B.N.C.B.S., Kolkata 98, India, S.N. KAUL, SoP, Central University, Hyderabad 46, India — Ferromagnetic shape memory alloys (FSMA) are smart materials with largest magnetic field induced strain below austenite - martensite transformations. The lower temperature martensitic state is characterized by the presence of structural twins that have this exceptional magnetoelastic coupling. To understand this behavior, we carried out sound velocity and attenuation measurements on a typical FSMA material, NiFeAl system, and determined the Young's moduli under various stresses and associated strains. We found that the effect of stress is to alter the martensite temperature. We also studied a theoretical thermodynamic constitutive model and Clausius-Duhem inequality, to determine the stress resulting from an applied strain for an isothermal system. In the absence of an applied magnetic field the free energy of the system consists of only the mechanical energy contribution which in turn is dependent upon the elastic moduli pertaining to the elastic and twinning strains. The paper describes the details of measurements and the model chosen, along with the discussions on the correspondence between the experimental observations and various theoretically determined quantities.

5:06PM L19.00012 Influence of Goldstone modes on the electronic properties of helical magnets , YAN SANG, DIETRICH BELITZ, University of Oregon, KWAN-YUET HO, TED KIRKPATRICK, University of Maryland — We have investigated the influence of Goldstone modes on the electronic properties of helical magnets, such as MnSi, in which a Dzyaloshinsky-Moriya term in the action leads to helical order with a pitch wave number q [1]. In the presence of a homogeneous external magnetic field H the helix is superimposed by a homogeneous magnetization, which leads to a conical phase [2]. The Goldstone mode in this conical phase has the form $\Omega^2 \propto c_z k_z^2 + c_\perp k_\perp^4/q^2 + c_H k_\perp^2$, where k_z and $k_\perp$ denote the components of the wave vector parallel and perpendicular to H, respectively. The elastic constants c_z and $c_\perp$ are independent of H for small H, whereas $c_H \propto H^2$. This Goldstone mode couples to the conduction electrons and leads to nonanalytic temperature dependences of various observables. In the conical phase, the strongest effect is on the thermal conductivity and the single-particle relaxation rate, which both are proportional to $T^{3/2}$. We also report results for the specific heat and the electrical resisitivity, both in the conical phase and in other phases of MnSi [3]. [1] P. Bak and M.H. Jensen, J. Phys. C 13, L881 (1980). [2] Y. Ishikawa, G. Shirane, J.A. Tarvin, and M. Kohgi, Phys. Rev. B 16, 4956 (1977). [3] Kwan-yuet Ho, T.R. Kirkpatrick, Yan Sang, D. Belitz, Phys. Rev. B 82, 134427 (2010)

5:18PM L19.00013 Is CrO_2 Fully Spin Polarized? Analysis of Andreev Spectra and Excess Current , TOMAS LOFWANDER, Department of Microtechnology and Nanoscience - MC2, Chalmers University of Technology, SE-412 96 Goteborg, Sweden, ROLAND GREIN, MATTHIAS ESCHRIG[1], Institut fuer Theoretische Festkoerperphysik and DFG-Center for Functional Nanostructures, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — We report an extensive theoretical analysis of point-contact Andreev reflection data available in the literature on ferromagnetic CrO_2. We find that the spectra can be well understood within a model of fully spin-polarized bands in CrO_2 together with spin active scattering at the contact. This is in contrast to analyses of the data within extended Blonder-Tinkham-Klapwijk models, which lead to a spin polarization varying between 50% and 100% depending on the transparency of the interface. We propose to utilize both the temperature dependence of the spectra and the excess current at voltages above the gap to resolve the spin-polarization in CrO_2 in a new generation of experiments.

T. Löfwander, R. Grein, and M. Eschrig, Phys. Rev. Lett. **105**, 207001 (2010)

[1]Fachbereich Physik, Universitaet Konstanz, D-78457 Konstanz, Germany

Tuesday, March 22, 2011 2:30PM - 5:30PM –

Session L20 DMP GERA FIAP: Focus Session: Thermoelectric Materials: Skutterudites, Novel and Nanostructured Materials D168

2:30PM L20.00001 Synthesis and thermoelectric property of Ca-doped n-type $Bi_{85}Sb_{15}$ alloy , KAMAL KADEL, WENZHI LI, Florida International University, GIRI JOSHI, GMZ, ZHIFENG REN, Boston College — $Bi_{1-x}Sb_x$ (0.09<x<0.20) alloys are n-type semiconducting materials that exhibit a good thermoelectric property at low temperature, around 80 K. In the present work we investigated the thermoelectric properties of undoped $Bi_{85}Sb_{15}$ and different Ca-doped $Bi_{85}Sb_{15}Ca_x$ alloys (x=0.5, 2, and 5) synthesized via arc-melting first and followed by ball milling and hot pressing. Effect of different Ca doping levels on transport properties of $Bi_{85}Sb_{15}$ alloys has been investigated. It is found that thermal conductivity decreases with increasing Ca. Electrical transport measurements show that power factor increases with doping level of Ca up to $Bi_{85}Sb_{15}Ca_2$ and then decreases, yielding the maximum value of power factor of 3.8×10^{-3} $Wm^{-1}K^{-2}$ and ZT of 0.39 at room temperature for $Bi_{85}Sb_{15}Ca_2$. Properties at below room temperature will also be presented.

2:42PM L20.00002 Exploration of Electron Poor Materials and their thermoelectric properties , DARYN BENSON, ULRICH HAUSSERMANN, OTTO SANKEY, Arizona State University — The Electron Poor Materials (EPM); ZnSb, ZnAs which have an average 3.5 valence electrons are explored via ab initio calculations. These materials are of interest for thermoelectric research. The EPM are then compared to valence balanced zinc-blende materials; InSb, GaSb, ZnSe, and ZnTe. Analysis of binding to assess the interesting electronic properties such as the role of nonclassical four-center bonds and the thermoelectric Seebeck coefficient are discussed. Bandstructure comparisons to a simple tight-binding model (Linear Combination of Atomic Orbitals (LCAO)) are preformed in order to test the effects of the atomic orbitals on the electronic structure.

2:54PM L20.00003 Chemical Doping Effect on the Thermoelectric Properties of $T$$Ga_3$($T$ = Fe, Ru, Os) , NEEL HALDOLAARACHCHIGE, AMAR KARKI, ADAM PHELAN, YIMIN XIONG, RONGYING JIN, JULIA CHAN, SHANE STADLER, DAVID YOUNG, Louisiana State University, USA — Thermoelectric properties of chemically-doped intermetallic narrow-band semiconductors: $T$$Ga_3$($T$ = Fe, Ru, Os) are reported. The parent compounds show semiconductor-like behavior (E_g $\sim$ 0.2 eV, n_{290K} $\sim$ $10^{18}$$cm^3$) with large $n-$type Seebeck coefficients at room temperature (S_{290K} $\sim$ -300 μV/K). The semiconductor-like $FeGa_3$ becomes metallic upon chemical doping (adding electron carriers), but $RuGa_3$ and $OsGa_3$ remain semiconducting. While the electrical resistivity and the Seebeck coefficients of all the compounds decrease with electron doping, the Seebeck coefficients remain fairly large and $n-$type, which leads to larger power factors than those of the pure samples. The thermal conductivity (κ_{290K}= 1.6 W/m K) of electron-doped $FeGa_3$ decreases, which increases the room temperature power factor by a large percentage (S^2/ρ_{290K} = 60 μW/m K^2) over that of pure $FeGa_3$. This improvement in the power factor leads to a corresponding enhancement in the thermoelectric figure of merit (ZT) – a factor of 5 increases above undoped polycrystalline $FeGa_3$ and two orders of magnitude improvement over that of pure single crystalline $FeGa_3$.

3:06PM L20.00004 Doping dependence of thermoelectric performance in Mo_3Sb_7: first principles calculations[1] , DAVID PARKER, MAO-HUA DU, DAVID SINGH, Oak Ridge National Laboratory — Experimental studies have indicated the substantial thermoelectric promise of doped Mo_3Sb_7, with a figure-of-merit ZT of 0.9 (H. Xu *et al*, J. Appl. Phys. **105**, 053703 (2009)) already achieved at high temperature. However, optimal doping levels have not yet been achieved. We study doping of Mo_3Sb_7 with transition metals (Ni,Fe,Co,Ru) via first principles calculations, including electronic structure, lattice dynamics and Boltzmann transport. We discuss the selection of dopant and the potential thermoelectric performance of optimally doped Mo_3Sb_7.

[1]Research sponsored by the U.S. Department of Energy, Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Vehicle Technologies, as part of the Propulsion Materials Program, under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

3:18PM L20.00005 Giant Seebeck Coefficient in V-TCNE thin films[1] , AUDREY CHAMOIRE, CHRISTOPHER JAWORSKI, Department of Mechanical Engineering, OSU, CHI-YUEH KAO, Department of Chemistry, OSU, JOSEPH HEREMANS, Department of Mechanical Engineering and Department of Physics, OSU, ARTHUR EPSTEIN, Department of Physics and Department of Chemistry, OSU — The disordered structure of organic conductors results in a naturally low thermal conductivity (κ) but their ZT is known to be low because of their low thermopower (S) and electrical conductivity (σ). Here we report an exception, with results obtained from 220 to 320K for the thermopower of V-$TCNE_x$ (V-$(C_2(CN)_4)_x$) thin films deposited on a Si wafer (111). At room temperature S=+21.8 mV/K and increases with decreasing temperature. Those values are matched only by very pure semiconductors such as Si at low temperature, Bi nanowires, or strongly correlated electron systems like $FeSb_2$. The valence band of V-TCNE has a very high density of states over a very narrow energy range, ascribed mostly to vanadium 3d(t_{2g}) orbitals,[2] which is consistent with the exceptionally large value of S. The dependence of S and σ upon illumination will also be shown, alongside preliminary estimates for the ZT.

[1]Work supported by DOE-EFRC 61-32128 (through MSU).

[2]Y-J Yoo et al., Nat. Mat. **9** 638 2010

3:30PM L20.00006 Einstein Modes in the Phonon Density of States of the Single-Filled Skutterudite $Yb_{0.2}Co_4Sb_{12}$

, IVO K. DIMITROV, Brookhaven National Laboratory, MICHAEL E. MANLEY, Lawrence Livermore National Laboratory, STEVEN M. SHAPIRO, Brookhaven National Laboratory, JIONG YANG, WENQING ZHANG, LIDONG CHEN, Shanghai Institute of Ceramics, Chinese Academy of Sciences, QING JIE, Brookhaven National Laboratory, GEORG EHLERS, ANDREY PODLESNYAK, Spallation Neutron Source, Oak Ridge National Laboratory, JORGE CAMACHO, QIANG LI, Brookhaven National Laboratory — Measurements of the phonon density of states by inelastic neutron scattering and specific heat measurements along with first principles calculations, provide compelling evidence for the existence of an Einstein oscillator (*rattler*) at $\omega_{E1} \approx$ 5.0 meV in the filled skutterudite $Yb_{0.2}Co_4Sb_{12}$. Multiple dispersionless modes in the measured density of states of $Yb_{0.2}Co_4Sb_{12}$ at intermediate transfer energies (14 meV $\leq \omega \leq$ 20 meV) are exhibited in both the experimental and theoretical *density of states* of the Yb-filled specimen. A peak at 12.4 meV is shown to coincide with a second Einstein mode at $\omega_{E2} \approx$ 12.8 meV obtained from heat-capacity data. The emergence of local modes at intermediate transfer energies is attributed to altered properties of the host $CoSb_3$ cage as a result of Yb filling. It is suggested that these modes are owed to a complementary mechanism for the scattering of heat-carrying phonons in addition to the mode observed at $\omega_{E1} \approx$ 5.0 meV.

3:42PM L20.00007 On the role of nanostructure on the thermal conductivity of skutterudite thermoelectrics[1]

, MARCO FORNARI, Central Michigan University, DMITRI VOLJA, JIVTESH GARG, Massachusetts Institute of Technology, DAEHYUN WEE, Ewha Womans University, BORIS KOZINSKY, Robert Bosch LLC, NICOLA MARZARI, University of Oxford — One of the most effective strategies to improve the thermoelectric figure of merit in skutterudites is to reduce thermal conductivity via alloying, filling, or nanostructuring. The latter is most effective when the dimension of the domains is comparable in size to the mean free path of the dominant heat-conducting phonons. In bulk, pristine semiconductors and insulators thermal conductivity and phonons' mean-free paths can nowadays be calculated fully from first-principles from the anharmonic terms in the ionic displacements. We show here our results for the lattice thermal conductivity of several compounds with the skutterudite structure, obtained from the Boltzmann transport equation using phonon lifetimes determined from density functional calculations. We will also discuss the effect of fourth-order terms, albeit as obtained using phenomenological approaches. Last, we comment on the interplay between the different length scales for the nanostructured domains and the relevant heat-carrying phonons.

[1]Support from Robert Bosch LLC/MIT Energy Initiative.

3:54PM L20.00008 Thermoelectric Properties of p-type Yb Filled Skutterudite $Yb_yFe_xCo_{4-x}Sb_{12}$[1]

, CHEN ZHOU, DONALD MORELLI, Michigan State University, XIAOYUAN ZHOU, GUOYU WANG, University of Michigan, CTIRAD UHER, University of Michgan — Since the discovery in 1995 of high thermoelectric figure of merit in skutterudite compounds, much work has been done to optimize the thermoelectric properties of these materials. As a result of this effort, n-type skutterudites are available today with figure of merit ZT approaching 1.8. By contrast, p-type skutterudites have lagged behind, with the best materials having figure of merit less than unity. In this study, we report the thermoelectric and magnetic properties of p-type Yb-filled skutterudites of nominal composition $Yb_yFe_xCo_{4-x}Sb_{12}$ with the aims of extending our knowledge of the filled skutterudite family and enhancing the thermoelectric properties of these p-type materials.

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

4:06PM L20.00009 First principles calculations of the interactions of a filling atom with its neighboring atoms in a skutterudite (LaFe4Sb12)[1]

, JOSEPH FELDMAN, NRL, DAVID SINGH, ORNL, NOAM BERNSTEIN, NRL — The room temperature lattice thermal conductivity of filled skutterudites is about a factor of 5 smaller than that of unfilled skutterudites which has caused a great deal of attention to be focused on these materials from a scientific standpoint, as well as a technological one, i.e., thermoelectric applications. In an effort to gain a microscopic understanding of this we have previously used a central force model and Green-Kubo techniques with force parameters heavily based on first principles results [Bernstein et al., Phys Rev. B **81**, 134301 (2010)]. However, as we had no first principles information on the La-Fe cubic anharmonic parameters in LaFe4Sb12 we have performed new direct method calculations for a larger supercell than the Bravais cell used previously to compute not only the six independent La-Fe cubic anharmonic parameters but numerous other parameters. Atomic forces were computed in various structural configurations differing only by the coordinates of one of the two La positions in the simple cubic supercell. DFT results are compared for LAPW, PAW, and plane-wave pseudopotential methods.

[1]Work at ORNL was supported by DOE, EERE, Vehicle Technologies, Propulsion Materials Program. Work at NRL was supported by ONR.

4:18PM L20.00010 Thermoelectric Technology for Automotive Waste Heat Recovery[1]

, GREGORY MEISNER, GM Global Research and Development — Essential to the long term success of advanced thermoelectric (TE) technology for practical waste heat recovery is fundamental physics and materials research aimed at discovering and understanding new high performance TE materials. Applications of such new materials require their development into efficient and robust TE modules for incorporation into real devices such as a TE generator (TEG) for automotive exhaust gas waste heat recovery. Our work at GM Global R&D includes a continuing investigation of Skutterudite-based material systems and new classes of compounds that have potential for TE applications. To assess and demonstrate the viability of a TEG using state-of-the-art materials and modules, we have designed, fabricated, installed, and integrated a working prototype TEG to recover exhaust gas waste heat from a production test vehicle. Preliminary results provide important data for the operation and validation of the mechanical, thermal, and electrical systems of the TEG in combination with the various vehicle systems (e.g., exhaust bypass valve and controls, thermocouples, gas and coolant flow and pressure sensors, TE voltage and output power). Recent results from our materials research work and our functioning automotive TEG will be presented.

[1]This work is supported by US DOE Grant # DE-FC26-04NT 42278.

4:30PM L20.00011 Bottom-Up Strategy for Thermoelectric Nanocomposites[1]

, ANUJA DATTA, Department of Physics, University of South Florida — Thermoelectric (TE) materials that incorporate nano-scale domains offer potential control over electrical and thermal properties simultaneously. A bottom-up strategy may provide cost-effective, scalable, and reproducible processing of TE materials with improved TE properties above existing materials. The strategy involves composition and size controlled syntheses of TE materials as nanocrystals by employing facile solution based processes followed by densification into bulk nanocomposite pellets using Spark Plasma Sintering. In this talk an overview of the various solution phase synthesis processes for preparing nanocrystals of different TE materials will be presented. In addition the TE properties after SPS densification will be discussed in relation to composition and grain size within the nanocomposites. Experimental results will be assessed together with theoretical modeling in describing the effect of the nano-scale domains on the TE properties.

[1]This work is supported by the U.S. Army Medical Research and Material Command under Grant No. W81XWH-07-1-0708 and the National Science Foundation under Grant No. CMMI-0927637, and CBET-0932526, Professor George S. Nolas, Principal Investigator.

5:06PM L20.00012 Formation Mechanisms of Embedded Zincblende and Wurtzite Nitride Nanocrystals , ADAM WOOD, University of Michigan, X. WENG, Penn State University, Y.Q. WANG, Materials Science & Tech. Division, LANL, R.S. GOLDMAN, University of Michigan — Semiconductor nanocomposites have been proposed for high figure of merit thermoelectrics. A promising approach to nanocomposite synthesis is matrix-seeded growth, which involves ion-beam-amorphization of a semiconductor film, followed by nanoscale re-crystallization via rapid thermal annealing (RTA) [1]. In this work, we are studying the formation and evolution of N ion-implanted InAs and GaAs. Low temperature (77K) N ion implantation into InAs leads to the formation of an amorphous layer with crystalline InAs remnants. RTA at up to 550 $^\circ$C leads to the nucleation of zincblende (ZB) InN nanocrystals (NC). RTA at 600 $^\circ$C leads to nucleation of both ZB and wurtzite (WZ) InN, with an increase in average NC size. These results are consistent with the predictions of a thermodynamic model for the nanoscale-size-dependence for nucleation of ZB and WZ InN. We are also developing a novel approach to *direct* the seeding of nanostructure arrays, using a combination of focused-ion-beam (FIB) implantation and conventional ion implantation. To date, we have demonstrated the selective positioning of WZ and ZB GaN NCs using 75keV and 100keV N implantation, followed by FIB patterning and 800 $^\circ$C RTA. [1] X. Weng, et al, *J. Appl. Phys.* **97,** 64301 (2005).

5:18PM L20.00013 Thin film thermocouples for thermoelectric characterization of nanostructured materials , MATTHEW GRAYSON, CHUANLE ZHOU, ANDREW VARRENTI, SEUNG HYE CHYUNG, JIEYI LONG, SEDA MEMIK, Electrical Eng. Comp. Sci, Northwestern University — The increased use of nanostructured materials as thermoelectrics requires reliable and accurate characterization of the anisotropic thermal coefficients of small structures, such as superlattices and quantum wire networks. Thin evaporated metal films can be used to create thermocouples with a very small thermal mass and low thermal conductivity, in order to measure thermal gradients on nanostructures and thereby measure the thermal conductivity and the Seebeck coefficient of the nanostructure. In this work we confirm the known result that thin metal films have lower Seebeck coefficients than bulk metals, and we also calibrate the Seebeck coefficient of a thin-film Ni/Cr thermocouple with 50 nm thickness, showing it to have about 1/4 the bulk value. We demonstrate reproducibility of this thin-filmSeebeck coefficient on multiple substrates, and we show that this coefficient does, in fact, change as a function of film thickness. We will discuss prototype measurement designs and preliminary work as to how these thin films can be used to study both Seebeck coefficients and thermal conductivities of superlattices in various geometries. The same technology can in principle be used on integrated circuits for thermal mapping, under the name "Integrated On-Chip Thermocouple Array" (IOTA).

Tuesday, March 22, 2011 2:30PM - 5:30PM –

Session L21 DMP GIMS DCP: Focus Session: Imaging and Modifying Materials at the Limits of Space and Time Resolution II D161

2:30PM L21.00001 Nanoscale phase transitions within single ion tracks. , WILLIAM WEBER, University of Tennessee, RAM DEVANATHAN, Pacific Northwest National Laboratory, PEDRO MOREIRA, Universidade Estadual de Campinas — The dynamics of track development due to the passage of energetic ions through solids is a long-standing issue relevant to nuclear materials, age-dating of minerals, space exploration, and nanoscale fabrication of novel devices. We have integrated computer simulation and experimental approaches to investigate nanoscale phase transitions under the extreme conditions created within single tracks of energetic ions in the $Gd_2Zr_{2-x}Ti_xO_7$ system and $ZrSiO_4$. Based on the inelastic thermal spike model, we have used molecular dynamics simulations to follow the time evolution of the structure of individual tracks and to reveal the phase transition pathways to experimentally observed concentric track structures. The molecular dynamics simulations clearly demonstrate the dependence of track evolution on composition, deposited energy density, and the complex competition among melting, disordering and recrystallization processes.

2:42PM L21.00002 Exploring electron beam induced heat and mass transport at the atomic scale[1] , CHRISTIAN KISIELOWSKI, Lawrence Berkeley National Laboratory — In recent years the performance of mid-voltage electron microscopes was significantly boosted to reach deep sub-Ångstrom resolution around 0.5 Å at 300 kV in broad beam (TEM) and focused probe (STEM) modes. Atomic resolution microscopy at voltages as low as 50 kV (and possibly below) was fostered. As a result the detection of single atoms across the Periodic Table of Elements is now possible even if light atoms are considered. After decades of striving for resolution enhancement, electron microscopy has now reached a limit that is given at a fundamental level by the Coulomb scattering process itself and by beam-sample interactions, which set a maximum dose limit that can be easily reached for soft and hard materials with the developed high-brightness electron guns. Consequently, new frontiers for electron microscopy emerge and this contribution addresses dynamic processes at the single atom level that can now be captured in time series of images at frequencies below 1 Hz reaching towards kHz. In this frequency range much of the observed atom dynamics is electron beam induced and the control of beam-sample interaction imposes constraints as well as opportunities. In this contribution it is shown that it seems feasible to exploit beam sample interactions to gain better insight into heat and mass transport in soft and hard matter at atomic resolution.

[1]This work was supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

2:54PM L21.00003 Gold nanoislands for sensitivity enhancement in organic and imaging mass spectrometries (LDIMS, keV- and MeV-SIMS) , ARNAUD DELCORTE, OSCAR RESTREPO, ANEESH PRABHAKARAN, Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, Belgium — Gold nanoparticles condensed on the surface of organic materials induce large ion yield enhancements in secondary ion mass spectrometry, using atomic projectiles. Here, we first show that the interest of surface metallization extends to MeV-SIMS and to UV laser desorption/ionization, in which the energy of the primary beam is deposited through the electronic subsystems (but not to keV-cluster-SIMS). For the three methods, gold nanoislands induce at least a ten-fold increase of the characteristic fragment and molecular ion yields, making surface metallization an interesting approach for imaging MS of organic surfaces. In the second part of this report, we discuss the underlying physics. For instance, using molecular dynamics simulations, we explain why 10 keV atomic projectiles interacting with metallized organic surfaces desorb more molecules, and why it is not the case with cluster projectiles such as C_{60} and Au_{400}. For the other regimes of irradiation, arguments involving photon absorption and electronic effects are proposed.

3:06PM L21.00004 Surface characterization at the spatial resolution limit with Individual Cluster Impacts[1] , FRANCISCO FERNANDEZ-LIMA, MICHAEL J. ELLER, JOHN D. DEBORD, STANISLAV V. VERKHOTUROV, Texas A&M University, SERGE DELLA-NEGRA, IPN, Orsay, EMILE A. SCHWEIKERT, Texas A&M University — The use of cluster bombardment (e.g. C_{60} and Au_{400}) for surface analysis and characterization has shown significant advantages due to enhanced emission of molecular ions, low damage cross section, and reduced molecular fragmentation. At temporally and spatially discrete cluster impacts, the small impacted volume (10^3 nm^3) and ionized ejecta are ideal candidates for surface molecule interrogation. In the present talk, recent measurements of co-emitted photons, electrons and secondary ions from individual cluster impacts for several projectile-target combinations will be presented. Inspection of the photon and electron emissions show that the emission profiles are correlated with the target structure/composition at the nanometer level, with the particularity that co-emitted photons, electrons and secondary ion pairs can be used as indicators of the surface content and homogeneity. Examples of surface mapping of intact molecules via electron emission microscopy combined with secondary ion detection will be shown.

[1]This work was supported by the National Science Foundation (Grant CHE-0750377). F. A. F-L acknowledges the National Institute of Health support (Grant No. 1K99RR030188-01).

3:18PM L21.00005 Electronic response of dielectric covered metal surfaces to highly charged ions[1]

, R.E. LAKE, Clemson University, J.M. POMEROY, National Institute of Standards and Technology, C.E. SOSOLIK, Clemson University — The strong Coulombic perturbation on a solid target from a highly charged ion (HCI) initiates a complex many-body response from target electrons that can produce novel effects such as potential energy sputtering, nanofeature formation and huge secondary electron yields. Far above the surface, HCIs reach a critical electron capture distance and neutralization proceeds via resonant charge transfer over the vacuum barrier [1]. Motivated by recent experiments [2], we detail the onset of charge transfer between a HCI and a metal covered with a dielectric thin film (Co with 1.5 nm Al_2O_3) to determine the film's effect on the critical distance. Surprisingly, we find that the first captured electrons are pulled through the exposed dielectric and come from the underlying metal. Additionally, the Al_2O_3 film lowers the effective work function of the target and extends the critical distance compared to a clean metal. I will discuss how the experimental parameters (thin film material/thickness and ion charge state/velocity) can be tuned to allow the ion to interact with electrons in either the metal or thin film.

[1] Phys. Rev. A **44**, 5674 (1991).
[2] J. Phys.: Condens. Matter **22**, 084008 (2010).

[1]We acknowledge support from NIST and NSF-CHE-0548111.

3:30PM L21.00006 Extraordinary sensitivity of nanoscale infrared spectroscopy demonstrated on Graphene and thin SiO_2

, GREG ANDREEV, Z. FEI, UCSD, W. BAO, Z. ZHAO, C.N. LAU, UC Riverside, L.M. ZHANG, Boston U, M. FOGLER, G. DOMINGUEZ, M. THIEMENS, UCSD, F. KEILMANN, Max Planck, Garching, D. BASOV, UCSD — Infrared Spectroscopy is a powerful tool for characterizing materials by their vibrational mode fingerprint and/or electron conductivity. Its application to nanoscale resolved studies is highly desirable but remained challenging mainly for two reasons: a suitable source of intense, broadband infrared illumination was not widely available and the spatial resolution of conventional microscopes was limited by diffraction. We have resolved both issues by utilizing tunable External Cavity Quantum Cascade Lasers (EC-QCLs) as an intense illumination source for a scattering Scanning Near Field Optical Microscope (s-SNOM), capable of <10nm spatial resolution. With this combination of EC-QCLs + s-SNOM we demonstrate <10nm resolution imaging and spectroscopy of extremely thin materials: Silicon oxide layers (SiO_2) as thin as 2nm and even single atomic layers of Carbon (Graphene). The spectra register contrasts for volumes as small as 20x20x1nm^3 = 400 yoktoliters of SiO_2, and about 70 yl of Graphene over a broad spectral range: 1065-2250cm^{-1}. We explain the origins of this extraordinary sensitivity with an improved theoretical framework for calculating the near field response of a multilayer system.

3:42PM L21.00007 Mesoscopic metal-insulator transitions at twin domain walls in improper ferroelastic VO_2[1]

, ALEXANDER TSELEV, Oak Ridge National Laboratory — Appearance of unusual phenomena at interfaces of different materials due to symmetry breaking and atomic, electronic, or spin reconstructions is well established area of intensive research. Domain walls in ferroic materials also can show unusual behavior due to symmetry discontinuities. VO_2 is a strongly-correlated-electron material, which exhibits a metal-insulator phase transition with a structural, lattice symmetry-lowering transformation making this material an improper ferroelastic. We observe mesoscopic metal-insulator transitions at the ferroelastic domain walls in the lower-symmetry phase of VO_2 that occur at temperatures as much as 10-12 °C below the bulk transition, resulting in the formation of metallic channels in the semiconducting material. The experiments are made using AFM-based scanning near-field microwave microscopy, which allows simultaneous accurate imaging of topography and the low-frequency dielectric function with a special resolution as high as 50 nm. The latter is possible due to a relatively high frequency used (in a few GHz range), when the sample-probe capacitive coupling becomes sufficiently strong and the electric current path is complete by displacement currents between the sample, probe tip, and the probe shield electrode. Density functional calculations indicate that ferroelastic domain walls of this type possess metallic character at low temperatures, which can be ascribed to elevated structural symmetry at the domain walls. The observed behavior, linked as well to the strain inhomogeneity inherent to ferroelastic materials, is generally relevant to symmetry-lowering phase transitions in other material systems.

[1]Research at ORNL's CNMS was sponsored by the Division of Scientific User Facilities, Office of Basic Energy Sciences, U.S. DOE.

4:18PM L21.00008 Simulation of Non-contact Atomic Force Microscopy for Structural Analysis

, JAMES CHELIKOWSKY, TZU-LIANG CHAN, University of Texas at Austin, C.Z. WANG, KAI-MING HO, Ames Laboratory of US DOE, Iowa State University — A powerful probe of materials centers on the use of atomic force microscopy (AFM). However, an analysis of AFM images can be complex and problematic. We will present an efficient scheme to simulate non-contact AFM images by employing a first-principles self-consistent potential from the sample as the essential input. This scheme does not require an explicit modeling of the AFM tip. Our method will be illustrated by applying it to various types of semiconductor surfaces including Si(111) (7x7), TiO2 (110) (1x1), Ag/Si(111)- ($\sqrt{3} \times \sqrt{3}$) R30^o and Ge/Si(105) (1x2) surfaces. We obtain good agreement with experimental results and previous theoretical studies by using this scheme. The method can quickly and efficiently aid in identifying different models for surface structures.

4:30PM L21.00009 Synchrotron X-ray Enhanced Scanning Tunneling Microscopy[1]

, VOLKER ROSE, JOHN FREELAND, Argonne National Laboratory — Proper understanding of complex phenomena occurring in nanostructures requires tools with both the ability to resolve the nanometer scale as well as provide detailed information about chemical, electronic, and magnetic structure. Scanning tunneling microscopy (STM) achieves the requisite high spatial resolution; however, direct elemental determination is not easily accomplished. X-ray microscopies, on the other hand, provide elemental selectivity, but currently have spatial resolution only of tens of nanometers. We present a novel and radically different concept that employs detection of local synchrotron x-ray interactions utilizing a STM that provides spatial resolution, and x-ray absorption directly yields chemical, electronic, and magnetic sensitivity. If during tunneling the sample is simultaneously illuminated with monochromatic x-rays, characteristic absorption will arise. Electrons that are excited into unoccupied levels close to the Fermi level modulate the tunneling current giving rise to elemental contrast.

[1]This work was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under contract DE-AC02-06CH11357.

4:42PM L21.00010 Frequency comb generation in a tunneling junction by intermode mixing of ultrafast laser pulses

, MARK HAGMANN, NewPath Research L.L.C., DZMITRY YAROTSKI, ANATOLY EFIMOV, ANTOINETTE TAYLOR, Los Alamos National Laboratory — Nonlinear interaction of electromagnetic radiation with tunneling electrons results in a number of peculiar physical phenomena, such as frequency mixing and imaging of insulating surfaces with scanning tunneling microscopy (STM). Arguably, the most promising among them is coupling of femtosecond laser pulses to the STM for material dynamics observation at nm/ps scales. However, the underlying physics is still poorly understood and the majority of existing studies of nonlinear mixing have been restricted to the use of CW lasers in a narrow range. Here, we present a new method for the hyper-spectral characterization of the nonlinear effects in tunneling junction. We use a 10-fs laser pulses at a nominal repetition rate of 74.25 MHz to generate a frequency comb in the tunneling current with frequencies up to 1 GHz. The typical output power at the fundamental (repetition) frequency is -120 dBm, and decreases for higher harmonics. The observed magnitude and square-law dependence of the signal power on the tunneling current and incident laser power are in good agreement with theoretical predictions.

4:54PM L21.00011 First principles computation of dynamical structure factor in real and momentum space in cuprates , YUNG JUI WANG, B. BARBIELLINI, HSIN LIN, TANMOY DAS, SUSMITA BASAK, Northeastern Univ. (NU), P. E. MIJNARENDS, Delft Univ. of Tech. and NU, S. KAPRZYK, NU and AGH (Poland), R. S. MARKIEWICZ, A. BANSIL, NU — We present a method for efficient, accurate first-principles calculations of the dynamical structure factor $S(\mathbf{q},\omega)$ in periodic systems, using products of real space Green functions and fast Fourier transforms (FFT). We further invert $S(\mathbf{q},\omega)$ via Fourier transformation [1] to reconstruct the propagator of electron density $X(\mathbf{x},t)$ in real space and time domain, thereby visualising spatially the dynamics of an electron doped cuprate system in real time. The present method is useful for many-body perturbation theories of excitations based on Density Function Theory (DFT) and modeling of various highly resolved spectroscopies going beyond the standard LDA [2-5]. Some illustrative examples will be presented. Work supported by the US DOE.

[1] P. Abbamonte *et al.*, Phys. Rev. Lett. **92**, 237401 (2004).
[2] Susmita Basak *et al.*, Phys. Rev. B **80**, 214520 (2009).
[3] J. Nieminen *et al.*, Phys. Rev. B **80**, 134509 (2009).
[4] R. S. Markiewicz *et al.*, Phys. Rev. B **77**, 094518 (2008).
[5] G. Stutz *et al.*, Phys. Rev. B **60**, 7099 (1999).

5:06PM L21.00012 Beam self-focusing in the near field emission scanning electron microscopy , FUXIANG LI, ARTEM ABANOV — Recent experiment on the near field emission scanning electron microscopy shows an unexpectedly high lateral and vertical resolution. We show that these effects can be explained by the beams self-focusing. We derive the equations for the beam propagation and solve them numerically. Our results are in a very good agreement with the experiment.

5:18PM L21.00013 Enhancing the spatial resolution in PEEM beyond 30nm using diamondoid surface coating , HITOSHI ISHIWATA, Stanford University, HENDRIK OHLDAG, Stanford Synchrotron Radiation Lightsource, ZHI-XUN SHEN, NICK MELOSH, Stanford University, ANDREAS SCHOLL, Advanced Light Source — The spatial resolution in Photoemission Electron Microscopy typically does not allow imaging features smaller than 30nm. PEEM resolution is limited by chromatic and spherical aberrations of the electrostatic lenses in the microscope column in combination with a wide angular and energy distribution of the secondary electrons to make these aberrations significant. Diamondoids have recently been shown to act as a monochromator for secondary electrons, thus reducing chromatic aberration in PEEM. In addition to improving the resolution of the microscope the diamondoid coating will also enhance the image intensity since now more secondary electrons will be accepted by the aperture. At 10kV the spatial resolution of PEEM3 is of the order of 150-200nm so that the magnetic domains can hardly be recognized anymore without the diamondoid coating. However, they become visible on the sample that was coated with diamondoids, indicating that the coating improved the spatial resolution by monochromatizing the secondary electrons. We also find that the image intensity is enhanced by a factor of 2-3 with the diamondoid coating. These initial findings on samples with relatively large domains of 150nm are very encouraging and we are therefore convinced that we can push the resolution limit below 30nm studying samples with smaller domains at higher acceleration voltages of 20kV.

Tuesday, March 22, 2011 2:30PM - 5:18PM –
Session L22 DCMP GMAG: URu2Si2 D163

2:30PM L22.00001 Quantification of U f-valence in URu_2Si_2 from 3D Bulk Fermi Surface Topology[1] , JONATHAN DENLINGER, O. KRUPIN, Lawrence Berkeley Natl Lab, J.W. ALLEN, U. of Michigan, B.J. KIM, Argonne Natl Lab, K. HAULE, KYOO KIM, G. KOTLIAR, Rutgers U., J.L. SARRAO, Los Alamos Natl Lab, N.P. BUTCH, U. of Maryland, M.B. MAPLE, UC San Diego — The three-dimensional bulk Fermi surface (FS) topology of paramagnetic-phase URu_2Si_2, as measured by photon-dependent angle-resolved photoemission spectroscopy of UHV-cleaved surfaces, is presented and discussed. Complete characterization of silicon-terminated surface states using spatial dependence, surface adsorption and theoretical surface slab calculations, allows identification of the bulk electronic band structure. The bulk FS topology is shown to be distinctly different from those of both localized $ThRu_2Si_2$-like f-core LDA calculations (U^{4+}) and fully itinerant LDA calculations. Key experimental FS topologies can be matched to itinerant LDA contours with suitable Fermi energy shifts that may mimic strong correlation effects not well treated in LDA. The intermediate-sized FS band topologies point to a mixed valent f-occupation between those of the two LDA calculations, $n_f \approx 2.2$ (f-core) and $n_f \approx 2.6$ (f-itinerant).

[1]Supported by U.S. DOE at the Advanced Light Source (DE-AC02-05CH11231), at UM (DE-FG02-07ER46379) and UCSD (FG02-04ER46105 & FG02-04ER46178), and by NSF at UCSD (DMR08-02478).

2:42PM L22.00002 Band renormalization at the hidden order transition in URu_2Si_2 , T. DURAKIEWICZ, G. DAKOVSKI, Y. LI , G. RODRIGUEZ, J.J. JOYCE, E.D. BAUER, P.H. TOBASH, Los Alamos National Laboratory, P.M. OPPENEER, Uppsala University, P.S. RISEBOROUGH, Temple University — The temperature-dependent evolution of the band structure in the hidden order (HO) system URu_2Si_2 was investigated by angle-resolved photoemission(ARPES) and time-resolved photoemission (trARPES) methods. The band structure changes with temperature, and the two dominant effects set the scale for the observed variations near the Fermi level. A hybridization gap is opening at around 70K, and the smaller gap forms below the HO transition temperature. The quasiparticle dynamics across the transition is measured with trARPES. The 3D nature of the electronic structure results in differences obtained by ARPES performed at different photon energies. We show how three different experiments, performed at 7eV, 21.2eV and 34eV can be reconciled with one model when the 3D electronic structure is taken into account.

2:54PM L22.00003 Complete mapping of dynamic spin correlations in the Hidden Order phase of URu_2Si_2[1] , H. BARATH, Johns Hopkins University, Z. YAMANI, W.J.L. BUYERS, CNBC, National Research Council, Canada, T. WILLIAMS, G. LUKE, McMaster University, Canada, J. RODRIGUEZ, J. LEAO, NIST Center for Neutron Research, D. GARRETT, McMaster University, Canada, K.J. MCCLELLAN, E.D. BAUER, J.L. SARRAO, LANL, USA, C. BROHOLM, Johns Hopkins University — URu_2Si_2 is a heavy fermion compound which undergoes a phase transition at 17.5 K to a "Hidden Order (HO) phase". We use inelastic neutron scattering to investigate spin correlations in the HO and paramagnetic phases and find them to be qualitatively different. While the normal state response has sharp features in Q but not in energy, consistent with an itinerant magnet, a distinct spectral gap develops in the HO phase. These results are consistent with previous measurements [1]. Here we present a full measurement of the scattering function, $S(\mathbf{Q},\omega)$, for energy transfers, $\hbar\omega < 11$ meV throughout the [H 0 L] plane. The data shows qualitatively different dispersion within, and perpendicular to, the tetragonal basal plane and provides information about the Fermi surface and its reconstruction upon entering the HO phase.

[1] C.R. Wiebe *et. al.*, Nature Physics, **3**, 96-100 (2007).

[1]Supported by DOE grant number DoE BES DE-FG02-08ER46544

3:06PM L22.00004 Broken Rotational Symmetry in the Hidden Order Phase of URu_2Si_2 , T. SHIBAUCHI, R. OKAZAKI, H.J. SHI, Department of Physics, Kyoto University, Y. HAGA, T.D. MATSUDA, E. YAMAMOTO, JAEA, Y. ONUKI, JAEA and Osaka University, H. IKEDA, Y. MATSUDA, Department of Physics, Kyoto University — The nature of the so-called 'hidden order' phase transition at $T_h = 17.5$ K in the heavy fermion compound URu_2Si_2 has posed a long-standing mystery, because despite 25 years of study it remains unidentified what symmetry is broken in this ordered phase. We report the emergence of an in-plane anisotropy of the magnetic susceptibility below T_h, which breaks four-fold rotational symmetry in tetragonal URu_2Si_2. Two-fold oscillations in the magnetic torque, which is measured in magnetic ?elds rotating precisely within the ab plane, are sensitively detected in small pure crystals for the first time. The amplitude of the two-fold oscillations onsets precisely at T_h, indicating its close link to an order parameter of the hidden order phase. Our findings uncover that the hidden order phase is an electronic 'nematic' phase, a translationally invariant metallic phase with spontaneous breaking of rotational symmetry.

3:18PM L22.00005 Optical evidence of Fermi liquid scattering in URu_2Si_2 , THOMAS TIMUSK, JESSE HALL, SARAH PURDY, TRAVIS WILLIAMS, GRAEME LUKE, McMaster University, TOOMAS RÕÕM, TAANIEL ULEKSIN, URMAS NAGEL, Natl-. Inst. of Chem Phys, & Biophys., Tallinn, Estonia, RICARDO LOBO, ESPCI-Paris-Tech, Paris France, P. LEJAY, Inst. Neel, Grenoble, France, CHRISTOPHER HOMES, Brookhaven Natl. Lab. Upton, N.Y. — We present new high resolution, low noise, data that demonstrates that in the coherent heavy Fermion state of URu_2Si_2 the conductivity is due to heavy ($m \approx 50m_e$) quasiparticles with a self energy that is dominated by Fermi liquid scattering according to $1/\tau(T,\omega) = A(\omega^2 + (\pi T)^2)$ where the coefficient $A = 0.23\ \mu\Omega\text{cmK}^{-2}$. We use this property to develop a new method of reducing the noise in the low frequency reflectance spectra of this material. In the hidden order state the spectra show evidence of anisotropy of the hidden order gap parameter with $2\Delta_{max} = 6.0$ meV and $2\Delta_{min} = 4.6$ meV.

3:30PM L22.00006 Signature of Hidden Order in URu_2Si_2 in the c-axis Optical Conductivity , JESSE HALL, SARAH PURDY, TRAVIS WILLIAMS, GRAEME LUKE, THOMAS TIMUSK, McMaster University, TOOMAS RÕÕM, TAANIEL ULEKSIN, URMAS NAGEL, Natl-. Inst. of Chem Phys & Biophys., Tallinn, Estonia, RICARDO LOBO, ESPCI-Paris-Tech, Paris France — We present high quality c-axis far infrared optical data for the heavy fermion compound URu_2Si_2. In particular, we compare the signature of the as yet poorly understood 'hidden order' state along the a- and c-axes of the tetragonal structure. The results presented here demonstrate the presence of the hidden order in the ac plane along the c- direction, although there is a very pronounced difference from the absorption at 5 meV seen along the a-axis. We present an assessment of the nature and significance of the a-c anisotropy of the hidden order signature.

3:42PM L22.00007 Cyclotron resonance of ultra-clean URu_2Si_2 single crystals in the hidden order and superconducting states , SHO TONEGAWA, KEN-ICHIRO HASHIMOTO, YAO-HAN LIN, RYO KATSUMATA, KOUSUKE IKADA, Department of Physics, Kyoto University, YOSHINORI HAGA, TATSUMA MATSUDA, ETSUJI YAMAMOTO, Advanced Science Research Center, Japan Atomic Energy Agency, YOSHICHIKA ONUKI, Graduate School of Science, Osaka University, TAKASADA SHIBAUCHI, YUJI MATSUDA, Department of Physics, Kyoto University — The cyclotron resonance is a powerful probe to detect the effective mass and scattering time of the electron, but there is few example of the report in the heavy fermion compounds. We succeeded in observing cyclotron resonance in the heavy fermion superconductor URu_2Si_2 not only in the hidden ordered state, but also in the superconducting state. In the hidden ordered state, we observe the missing heavy band which has not been detected by de Haas van Alphen (dHvA) measurements. In the superconducting state, the resonance lines exhibit an unexpected sharpening below the transition temperature, suggesting the realization of quasiparticle Bloch state in the vortex lattice state. We will compare our data to the dHvA measuments and discuss the possible electronic structure of the hidden order state.

3:54PM L22.00008 Neutron Scattering Study of $URu_{1.9}Re_{0.1}Si_2$: Driving Hidden Order Towards Quantum Criticality , TRAVIS WILLIAMS, McMaster University, N.P. BUTCH, University of Maryland, G.M. LUKE, McMaster University, M.B. MAPLE, University of California San Diego, Z. YAMANI, W.J.L. BUYERS, Chalk River Laboratories — We report inelastic neutron scattering measurements in the hidden order state of $URu_{1.9}Re_{0.1}Si_2$. We have fit the data to a resolution convolved simple harmonic oscillator model, plus a continuum extending to 10meV. We observe that towards the Quantum Critical Point (QCP) induced by Re-doping, the gapped incommensurate fluctuations are fairly robust, being nearly identical to the parent material. The gap at the commensurate point (1 0 0) is driven down as the doped system approaches the QCP. The response of this commensurate spin fluctuation associated with the hidden order acquires substantial damping. The particle-hole spectrum of nested fermions [1] can be fitted to the energy and damping of the excitations, but there is no evidence for the static charge density wave that the model implies [2], in agreement with STM [3]. We conclude that Re-doping weakens, but does not destroy, the hidden order on approaching the QCP transition to ferromagnetism.
[1] Balatsky et al. Phys. Rev. B 79 (2009) 214413
[2] Su et al. arXiv/cond-mat:1010.0767 (2010)
[3] Schmidt et al. Nature 465 (2010) 570
Research at UCSD supported by U.S. DOE Grant #DE-FG02-04ER46105.

4:06PM L22.00009 Fano resonance and the hidden order in URu_2Si_2 probed by quasiparticle scattering spectroscopy* , W. K. PARK, L. H. GREENE, Univ. of Ill. at Urbana-Champaign, E. D. BAUER, P. H. TOBASH, F. RONNING, X. LU, J. L. SARRAO, J. D. THOMPSON, Los Alamos Nat. Lab. — The nature of the hidden order transition occurring at 17.5 K in URu_2Si_2remains puzzling despite intensive investigations over the past two and half decades. Recent experimental and theoretical developments render it a timely subject to probe the hidden order state using quasiparticle tunneling and scattering techniques. We report on the Fano resonance in pure and Rh-doped URu_2Si_2 single crystals using point-contact spectroscopy. The conductance spectra reproducibly reveal asymmetric double peak structures slightly off-centered around zero bias with the two peaks merging well above the hidden order transition temperature. An analysis using the Fano resonance model in a Kondo lattice [1] shows that the conductance peaks arise from the hybridization gap opening. Our estimated gap size agrees well with those reported from other measurements. We will present experimental results over a wide parameter space including temperature and doping dependences and discuss their underlying physics. [1] M. Maltseva, M. Dzero, and P. Coleman, Phys. Rev. Lett. **103**, 206402 (2009). *The work at UIUC is supported by the U.S. DOE under Award Nos. DE-FG02-07ER46453 and DE-AC02-98CH10886, and the work at LANL is carried out under the auspices of the U.S. DOE, Office of Science.

4:18PM L22.00010 Tunneling into clean Heavy Fermion Compounds: Origin of the Fano Lineshape[1] , PETER WOLFLE, Institute for Theory of Condensed Matter and Center for Functional Nanostructures, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany, YONATAN DUBI, ALEXANDER BALATSKY, Los Alamos National Lab — Recently observed tunneling spectra on clean heavy fermion compounds show a lattice periodic Fano lineshape similar to what is observed in the case of tunneling to a Kondo ion adsorbed at the surface. We show that the translation symmetry of a clean surface in the case of *weakly correlated* metals leads to a tunneling spectrum given by the superposition of the local weighted density of states of all energy bands involved, which does not have a Fano lineshape. In particular the spectrum will show any hybridization gap present in the band structure. By contrast, in a *strongly correlated* heavy fermion metal the heavy quasiparticle states will be broadened by interaction effects. The broadening grows as one moves away from the Fermi surface, up to a value of the order of T_K , the Kondo scale. We show that the hybridization gap is completely filled in this way, and an ideal Fano lineshape of width T_K results, similar to the impurity case. We also discuss the possible influence of the tunneling tip on the surface, in (i) leading to additional broadening of the Fano line, and (ii) enhancing the hybridization locally, hence adding to the impurity type behavior. The latter effects depend on the tip-surface distance.

[1]This work was supported by US DoE , LDRD and BES at Los ALamos.

4:30PM L22.00011 A Γ_5 composite density wave model for the hidden order of URu_2Si_2[1] , PIERS COLEMAN, PREMALA CHANDRA, Rutgers University, REBECCA FLINT, Massachusetts Institute of Technology — Motivated by recent experiments on URu_2Si_2[1-4], we propose a theory for the hidden order in this material in which the hidden order parameter is a composite density wave formed formed between conduction electrons and a Γ_5 $5f^2$ doublet. In this theory, two-channel quadrupole fluctuations in the $Gamma_5$ proceed via virtual fluctuations into a $5f^1$ Kramer's doublet with Γ_7 symmetry. Hybridization in these two channels is described by a Schwinger boson which condenses in both the hidden order and the magnetic phase. In the magnetic phase, the hybridization develops in the up or down channels, whereas in the hidden order phase, it develops with equal amplitude in both channels. Our theory can account for the development of an anomalous $\Delta\chi_{xy}$ as a consequence of the composite order. It also predicts the formation of a tiny orbital moment aligned along the xy axis in the basal plane of the crystal that should be observable in neutron scattering experiments.

[1]Work supported by DOE grant DE-FG02-99ER45790 (PC) and the Simons (RF).

4:42PM L22.00012 Hybridization wave as the "Hidden Order" in URu_2Si_2[1] , JONATAN DUBI, ALEXANDER BALATSKY, Los Alamos National Lab — A phenomenological model for the hidden order transition in the heavy Fermion material URu_2Si_2 is introduced. The model assumes an incommensurate, momentum-carrying hybridization between the light hole band and the heavy electron band, appearing after a Fano hybridization takes place. The hybridization wave is identified as the "Hidden Order" order parameter. The model, simplified to one dimension, qualitatively reproduces numerous experimental results obtained from e.g. neutron scattering and scanning tunneling microscopy, and mainly the gap-like features in the density of states and the appearance of features at an incommensurate vector $Q^* \sim 0.6\pi/a_0$. Finally, the model allows us to make various predictions which are amenable to current experiments.

[1]This work was supported by LDRD and in part, by grant No. DE-AC52-06NA25396 and UCOP-TR-01.

4:54PM L22.00013 Hexadecapolar Kondo effect in URu_2Si_2? , ANNA TOTH, GABRIEL KOTLIAR — Motivated by recent findings on the electronic structure of URu_2Si_2 , we derive the coupling of a localized hexadecapolar mode to itinerant fermionic quasiparticles in tetragonal crystal field, and show how it maps onto the two-channel Kondo (2CK) model. Channel symmetry is a consequence of time-reversal symmetry, and a 2CK regime can be observed if the crystal field splitting is less than the Kondo temperature. Corollary to the derivation, for an f^2-configuration in tetragonal environment, a relevant crystal field splitting is always present in addition to the 2CK interaction–even if the local degrees of freedom are a Γ_5 doublet. Solving the coupling by the numerical renormalization group, we are able to fit the susceptibility and the specific heat of the dilute system, $Th_{1-x}U_xRu_2Si_2$, in magnetic field and place the measurements on the verge of the local moment and the 2CK regimes.

5:06PM L22.00014 Electronic structure and multipolar fluctuations in URu2Si2 , HIROAKI IKEDA, Department of Physics, Kyoto University, RYOTARO ARITA, Department of Applied Physics, University of Tokyo, TETSUYA TAKIMOTO, Asia Pacific Center for Theoretical Physics, POSTECH — The intriguing phase transition at 17.5K in URu_2Si_2 was discovered by Palstra in 1985. In spite of intensive research studies over a quarter century, the order parameter remains still unknown; so-called "hidden order" phase. Many recent experimental data indicate that the magnetic and electronic properties can be easy to understand from the viewpoint of the itinerant picture rather than the localized picture. Thus, to elucidate the complicated electronic structure will be our important first step to comprehend the nature. Recently, by using a state-of-the-art *ab initio* downfolding, we have succeeded to construct the Wannier orbitals and to obtain the tight-binding Hamiltonian in terms of these basis set. Adding on-site Coulomb interactions between f orbitals, we obtain a multi-band Anderson lattice model, including full f orbitals. We here analyze the model Hamiltonian within the random phase approximation, and investigate magnetic fluctuations and multipolar fluctuations in URu_2Si_2. From these results, we discuss possible order parameters in the "hidden order" phase.

Tuesday, March 22, 2011 2:30PM - 5:30PM –

Session L23 DMP: Focus Session: Search for New Superconductors II: Towards Theoretical Design D165

2:30PM L23.00001 Spectral Weight Transfer in a Multi-Orbital Mott System , WEI-CHENG LEE, PHILIP PHILLIPS, Department of Physics, University of Illinois at Urbana-Champaign — One of the unique properties in a single band Hubbard model is the spectral weight transfer upon doping. Unlike in a Fermi liquid the redistribution of the spectral weights occurs predominantly near the chemical potential, a significant amount of spectral weights can be transferred from the high energy scales (upper Hubbard band) down to the chemical potential as a Mott insulator is doped. In this talk, we analyze the spectral weight transfer in a multi-orbital Mott system. We find that the spectral weights transferred from the high energy scales are greatly increased due to the multi-orbital structure, leading to a reduction of the critical doping level exhibiting zero thermopower. We argue that this indicates a suppression of the pseudogap phase and also predict the existence of new branches of charge 2e bosons carrying spin 1 at low energy in a multi-orbital Mott system. Relevant experimental consequences will be discussed.

2:42PM L23.00002 Electron-electron interaction in superconducting Lithium under pressure[1] , AMANDEEP KAUR, ERIK YLVISAKER, University of California, Davis, DEYU LU, YAN LI, Brookhaven National Laboratory, GIULIA GALLI, WARREN PICKETT, University of California, Davis — Lithium is known to exist in different phases and to uperconduct under pressure (P). We investigate the screened electron-electron interaction in Li as a function of P by analyzing the dielectric band structures of several phases. These band structures are obtained by iterative diagonalization[2] of the dielectric matrix as a function of wave vector and frequency. Even though the superconductivity in lithium is electron-phonon mediated, lithium is a good test system to study the screened e-e interaction more generally, which might be a primary mechanism for the superconductivity in high T_c nitrides of the form MNCl (M=Ti,Zr,Hf).

[1]Work supported by Grant # DE-FC02-06ER25777.

[2]H.Wilson, F.Gygi and G.Galli, Phys. Rev. B, 78,113303 (2008); Hugh F. Wilson, Deyu Lu, Francois Gygi Phys. Rev. B. 79, 245106 (2009).

2:54PM L23.00003 An investigation of non-superconducting PuPt2In7 , HAHNBIDT RHEE, WARREN PICKETT, UC Davis, Dept of Physics, FILIP RONNING, Los Alamos National Lab, MPA-CMMS, JIAN-XIN ZHU, Los Alamos National Lab, Theoretical Division, ERIC BAUER, Los Alamos National Lab, MPA-CMMS — $PuPt_2In_7$, like the heavy-fermion 115s, is member of a family of systems that are made up of RM_3 (R=Ce, Pu, ...; M=In, Ga, ...) building blocks. Superconductivity is observed in many of these materials, and it is understood to arise from an unconventional pairing mechanism due to antiferromagnetic spin fluctuations. Experiments discover that $PuPt_2In_7$, however, is an enhanced Pauli paramagnet with a Sommerfeld coefficient of $\sim$250 mJ/mol K^2. Here we present a DFT (Density Functional Theory) study of its electronic structure, with direct comparisons made to superconducting $PuCoGa_5$ and $PuCoIn_5$. Fermi surfaces, orbital decomposition of density of states, and band structures reveal many similarities between the two compounds. Our goal is to understand why we observe superconductivity in one but not the other.

3:06PM L23.00004 Why positive hole carriers and negatively charged planes are conducive to high temperature superconductivity , J.E. HIRSCH, University of California San Diego — The vast majority of superconducting materials have positive Hall coefficient in the normal state, indicating that hole carriers dominate the normal state transport. This was noticed even before BCS theory, and has been amply confirmed by materials found since then: the sign of the Hall coefficient is the strongest normal state predictor of superconductivity. In the superconducting state instead, superfluid carriers are always electron-like, i.e. negative, as indicated by the fact that the magnetic field generated by rotating superconductors is always parallel, never antiparallel, to the body's angular momentum ("London moment"). BCS theory ignores these facts. In contrast, the theory of hole superconductivity, developed over the past 20 years (papers listed in http://physics.ucsd.edu/∼jorge/hole.html) makes charge asymmetry the centerpiece of the action. The Coulomb repulsion between holes is shown to be smaller than that between electrons, thus favoring pairing of holes, and this fundamental electron-hole asymmetry is largest in materials where the conducting structures have *excess negative charge*, as is the case in the cuprates, arsenides and MgB_2. Charge asymmetry implies that superconductivity is driven by lowering of kinetic energy, associated with expansion of the carrier wavefunction and with *expulsion of negative charge* from the interior to the surface of the material, where it carries the Meissner current. This results in a macroscopic electric field (pointing outward) in the interior of superconductors, and a macroscopic spin current flowing near the surface in the absence of external fields, a kind of macroscopic zero point motion of the superfluid (spin Meissner effect). London's electrodynamic equations are modified in a natural way to describe this physics. It is pointed out that a dynamical explanation of the Meissner effect *requires* radial outflow of charge in the transition to superconductivity, as predicted by this theory and not predicted by BCS. The theory provides clear guidelines regarding where new higher T_c superconductors will and will not be found.

3:42PM L23.00005 The Possibility of Phonon-Mediated Superconductivity in an Iron-Based Material , SHEENA SHAH, ELENA ROXANA MARGINE, ALEKSEY KOLMOGOROV, University of Oxford — We have identified a synthesizable candidate FeB4 material with a potential for conventional superconductivity at 15-20 K [1,2]. The strong electron-phonon coupling in the proposed material is unexpected as the recently discovered iron-based superconductors are considered to display an unconventional pairing mechanism. The new nonmagnetic ground state crystal structure has been predicted with an ab initio evolutionary search [3] and shown to be marginally stable at ambient pressures.

[1] A. N. Kolmogorov, S. Shah, E. R. Margine, A. F. Bialon, T. Hammerschmidt, R. Drautz, Phys. Rev. Lett. 105, 217003 (2010).
[2] A. F. Bialon, T. Hammerschmidt, R. Drautz, S. Shah, E. R. Margine, A. N. Kolmogorov (submitted)
[3] A. N. Kolmogorov, MAISE (http://maise-guide.org)

3:54PM L23.00006 A DFT (LDA+U) study of the electronic properties of layered, square-planar coordinated, copper monoxide structures , PAUL M. GRANT, IBM Research Staff Member Emeritus, San Jose, CA 95120 USA — It is now 25 years and two months since Georg Bednorz observed the onset of high temperature superconductivity in copper oxide perovskites, and yet today its origin remains still largely unresolved. However, it quickly became evident the phenomenon was restricted to those structures possessing a common feature – square planar coordinated "sheets," or "layers" of copper monoxide, and thus now thought to be essential to effect superconductivity in this family of materials. We examine the structural stability and electronic properties of these 2D approximations to the layered CuO compounds as a function of Hubbard U within the DFT (LDA+U) framework, especially for those particular values yielding metallic band formation, and their subsequent fermiology and electron/hole-phonon coupling properties. Although such particular 2D embodiments do not, as yet, exist, we consider their study via DFT as valuable proxies[1] to aid eventual understanding of that flavor of superconductivity revealed by the Bednorz-Mueller breakthrough.

[1]P. M. Grant, Journal of Physics: Conference Series **129** (2008) 012042.

4:06PM L23.00007 Design Algorithms for Novel High Temperature Superconductors[1] , O. PAUL ISIKAKU-IRONKWE, The Center for Superconductivity Technologies(TCST), EMEKA OGUZIE, UKO OFE, TCST — A grand challenge in superconductivity is to develop a "materials specific" theory that enables us to design superconductors from the Periodic Table. Using the Periodic Table properties of electronegativity, valence electrons, formula weight and atomic number, we have been able to quantitatively describe all superconductors in terms of those parameters. We have observed specific correlations with various families of superconductors that enable us to reverse engineer those superconductors. We have developed simple equations, maps and algorithms that facilitate the design of superconductors and predict their approximate transition temperatures. Our design method does not employ density functional theory, even though DFT can be used to verify it. In this paper, we provide many examples of predicted "materials specific" novel high temperature superconductors that should test the authenticity of our design algorithms. We also propose a design for possible room temperature superconductivity.

[1]Research support from Dr. M.J. Schaffer, General Atomic, San Diego CA.

4:18PM L23.00008 Ionic Plasma Screening and Long-Range Electron Correlations in Quasi-One-Dimensional Conductors[1] , YURI GARTSTEIN, ANVAR ZAKHIDOV, University of Texas at Dallas — In quasi-one-dimensional systems with the intercalation-type doping, the dynamical response of dopant ions can substantially affect the interplay of density-wave and superconducting instabilities. We study a generic model of the system of Coulombically coupled Luttinger-liquid chains modified by the Coulomb interaction with displacements of dopant ions. Our interest is in the macroscopic, long wave-length, effects of the ionic response. This three-dimensional electron-ion model system is exactly solvable in the forward-scattering channel allowing us to find the resulting system excitations and electron correlations. For a jellium-like ion response, the effect of the bare electron-electron repulsion on the long- range correlations is essentially canceled by the ions with the effective electron-electron interactions now exhibiting regions of shorter-range repulsion and longer-range attraction. This picture is clarified and reproduced within the macroscopic dielectric function framework. If the system also features a non-polarizational interaction with another optical phonon mode, superconducting correlations are developed already due to the forward-scattering only.

[1]The support of the AFOSR grant FA9550-09-1-0384 is greatly acknowledged.

4:30PM L23.00009 Phase transitions in a three dimensional $U(1) \times U(1)$ lattice London superconductor: Metallic superfluid and charge-4e superconducting states[1] , EGIL HERLAND, Norwegian University of Science and Technology, EGOR BABAEV, Amherst University, ASLE SUDBO, Norwegian University of Science and Technology — We consider a three-dimensional lattice $U(1)\times U(1)$ and $[U(1)]^N$ superconductors in the London limit, with individually conserved condensates. The $U(1)\times U(1)$ problem, generically, has two types of intercomponent interactions of different characters. First, the condensates are interacting via a minimal coupling to the same fluctuating gauge field. A second type of coupling is the direct dissipationless drag represented by a local intercomponent current-current coupling. We study phase transitions and two types of competing paired phases which occur: (i) a metallic superfluid phase, (ii) a composite superconducting phase where there is order in the phase sum of the order parameters which has many properties of a single-component superconductor but with a doubled value of electric charge.

[1]This work was supported by the Wallenberg Foundation and by the Research Council of Norway

4:42PM L23.00010 Exact calculations of phase separation instabilities and pairing in two-dimensional Betts nanoclusters , ARMEN KOCHARIAN, Department of Physics, California State University, Los Angeles, GAYANATH FERNANDO, KUN FANG, Department of Physics, University of Connecticut, Storrs — The energy eigenvalues and eigenstates of the Hubbard model with nearest and next nearest neighbor hoppings are calculated by exact diagonalization and Lanczos (algorithm) techniques in isotropic Betts nanoclusters with the square symmetry and periodic boundary conditions. The electron pairing instabilities and quantum critical points for one hole off half filling are evaluated by monitoring the charge and spin pairing gaps and level crossings instabilities in the ground state and at finite temperatures. The calculated spin and charge energy gaps and quantum critical points in optimized 8 and 10 site Betts clusters of square symmetry pertain universal critical behavior and are fully consistent with the exact results obtained for an "elementary" bipartite square geometry [Kocharian et al., Phys. Rev. B 78, 075431 (2008)]. We found the strong particle-hole assymetry effect in the electron pairing instability due to the presence of the next nearest neighbor hopping term. Correlated lectrons in various contrasting bipartite and non-bipartite two- and three- dimensional cluster topologies display a number of inhomogeneous, coherent and non-coherent nanoscale phases seen by scanning tunneling microscopy in high Tc cuprates, iron pnictides, manganites, etc.

4:54PM L23.00011 Electromagnetic Interactions between Electrons moving in the Layered Conductors with a Dielectric Interlayer , KENJI TANAHASHI, Hokkaido Institute of Technology — Electromagnetic interactions between two electrons moving in the two layered conductors separated with a dielectric interlayer have been estimated. We assume a simple situation in which the two electrons in the layered conductors move with the constant velocity in the same direction. The electric and magnetic fields of a moving electron are derived from the scalar and the vector potentials in the non-relativistic frame. The total electromagnetic force exerted between two electrons is obtained by the Lorentz expression, and the force depends on the velocity of the moving electrons. With increasing the velocity of the electrons, the magnetic force increases and the magnetic attractive force exceeds the electric repulsive force, when $v/c \geq 1/\sqrt{\varepsilon_r \mu_r}$, where v is the velocity of the two electrons moving parallel in the same direction, c is the speed of light, andε_r is the relative dielectric constant in the direction of the perpendicular to the plane of the layers, andμ_r is the in-plane permittivity of the conduction layers. In vacuum the magnetic interaction between moving electrons never surpasses the electric interaction. However, in the highly anisotropic structures in conductivity, the magnetic interaction between moving electrons should be taken into consideration to investigate the behavior of the electrons.

5:06PM L23.00012 Electrodynamics of Nearly Ferroelectric Superconductors in the non-local Pippard limit[1] , UPALI APARAJITA, City College, CUNY and Queensborough Community College, CUNY, JOSEPH BIRMAN, City College, CUNY — We report the structure of the magnetic field and secular current in a Nearly Ferroelectric Superconducting (NFE-SC) thin film. It was shown that unlike in conventional superconducting films, the external radiation causes alternating pattern of current strips. The strength of the innermost current torrents is governed by the laser field intensity as well as resonance with the ferroelectric component. The latter is modeled by secular reflection and random scattering in the Pippard non-local limit. Our calculations suggest that corresponding magnetic field pattern affects vortex formation in such material.

[1]We acknowlege support from FRAP-PSC-CUNY.

5:18PM L23.00013 Planar-coordinated nickelates, isoelectronic to overdoped cuprates: an LDA+DMFT comparison , CHUCK-HOU YEE, GABRIEL KOTLIAR, KRISTJAN HAULE, Rutgers University — We show the Ni-O planes in the bilayer and trilayer T'-type nickelates, recently synthesized by Poltavets, *et al.* [1], are electronically analogous to the Cu-O planes in overdoped superconducting cuprates. The density of states, Fermi surface, nickel valence and mass renormalization, computed using LDA+DMFT, are in good agreement with available experiment, and indicate that the compounds are well-described by multilayer Hubbard physics. Significant interlayer coupling generates bonding-antibonding Fermi surfaces, similar to those seen in the cuprates. We investigate the possibility that interlayer coupling can explain the presence of a phase transition with $R \log 2$ entropy in the trilayer, and the absence of such a transition in the bilayer.

[1] Poltavets, *et al.*, Phys. Rev. Lett. **104**, 206403 (2010).

Tuesday, March 22, 2011 2:30PM - 5:18PM –

Session L24 DCOMP: Focus Session: Quantum Transport Simulations and Computational Electronics – GNRs and QDs D167

2:30PM L24.00001 Numerical simulation of time-dependent transport in graphene , DHARMENDAR REDDY, PRIYAMVADA JADAUN, LEONARD F. REGISTER, SANJAY K. BANERJEE, The University of Texas at Austin — We present a numerical method for modeling time-dependent quantum transport in graphene. The time-dependent Schrodinger equation is solved with a pi-orbital-based atomistic tight-binding Hamiltonian. A novel variation of an alternating-direction semi-implicit scheme is employed on the hexagonal tight-binding lattice to maintain stability and conserve probability while achieving computational efficiency. Open boundaries including source terms to allow time-dependent non-equilibrium Green's function (NEGF) calculation of graphene devices will be discussed.

2:42PM L24.00002 ABSTRACT WITHDRAWN –

2:54PM L24.00003 Current-Voltage Characteristics of Graphane Nanoribbon Transistors[1] , JUN-QIANG LU, DANIEL VALENCIA, University of Puerto Rico at Mayaguez — Using first-principles transport calculations, we investigate current-voltage characteristics of transistors made by graphane nanoribbons (or hydrogenated graphene nanoribbons). Our results show that transistors made by graphane nanoribbons can achieve better performance than those made by graphene nanoribbons because of the intrinsic large band gap presented in graphane.

[1]JQL acknowledges start-up support from the Institute for Functional Nanomaterials, University of Puerto Rico.

3:06PM L24.00004 Switching Behavior of Carbon Chains Bridging Graphene Nanoribbons: Effects of Uniaxial Strain , BRAHIM AKDIM, RUTH PACHTER, Air Force Research Lab — Recently, several experiments [1,2] demonstrated the stability of chain-like carbon nanowires bridged between graphene nanoribbons, paving the way for potential applications in nano-devices. On the basis of density functional tight-binding calculations, we demonstrated switching for chains terminated with a five-membered ring under an applied strain, serving as a model for morphological changes in realistic materials. Electron transport calculations showed an increase of up to 100% in the output current, achieved at a reverse bias-voltage of 2V and an applied strain of just 1.5%. Structural analysis suggested that the switching is driven by conformational changes, in our case triggered by the formation and annihilation of a five-membered ring at the interface of the chain-graphene edge. In addition, we showed that a five-membered ring can easily be formed at the interface under a source-drain bias or through a gate voltage. This mechanism can serve as an explanation of experimentally observed conductance for the materials.

[1] Jin, C.; Lan, H.; Peng, L; Suenaga, K.; Iijima S. *Phys. Rev. Lett.* **2009**, 102, 205501.
[2] Chuvilin, A.; Meyer, J. C.; Algara-Siller, G.; Kaiser, U. *New J. Phys.* **2009**, 11, 083019

3:18PM L24.00005 Giant Mechanoelectrical Switching in Ferromagnetic Graphene Nanoribbons , HONG LI, RUI QIN, JING ZHOU, QIHANG LIU, ZHENGXIANG GAO, JING LU, State Key Laboratory of Mesoscopic Physics and Department of Physics, Peking University, Beijing 100871, P. R. China, WAI-NING MEI, R.F. SABIRIANOV, Department of Physics, University of Nebraska at Omaha, Omaha, Nebraska 68182-0266, USA — Giant mechanoelectrical effect is observed when twisting a ferromagnetic zigzag-edged graphene nanoribbon (ZGNR) with collinear spin configuration from ab initio quantum transport calculations. The resulting switch ratio is up to 10^{10}% when the ZGNRs are overturned once and can be even enhanced to over 10^{14}% via multiply overturnings. We find such a switch equivalent to a spin valve without resort to an external magnetic field. Furthermore, consideration under Noncollinear situation is aslo in progress.

3:30PM L24.00006 Transport in Carbon Nanotubes: 2LSU(2) regime reveals subtle competition between Kondo and Intermediate Valence states , G. MARTINS, C. BUSSER, E. VERNEK, P. ORELLANA, G. LARA, E. KIM, A. FEIGUIN, E. ANDA — Three different numerical techniques are used to study the two-level SU(2) regime, obtained from an SU(4) Hamiltonian by orbital mixing via coupling to the leads. SU(4) Kondo physics has been experimentally observed, and studied in detail, in Carbon Nanotube Quantum Dots. Adopting a two molecular orbital basis, the Hamiltonian is rewritten, such that one of the molecular orbitals decouples from the charge reservoir, although still interacting capacitively with the other molecular orbital. This basis transformation explains in a clear way how the charge transport in this system turns from double- to single-channel when it transitions from the SU(4) to the 2LSU2 regime. The charge occupancy of these molecular orbitals displays gate-potential-dependent occupancy oscillations that arise from a competition between the Kondo and Intermediate Valence (IV) states. The determination of whether the Kondo or the IV state is more favorable, for a specific value of gate potential, is assessed by the definition of an energy scale T_0, which is calculated through DMRG. We speculate that the calculation of T_0 may provide experimentalists with a useful tool to analyze correlated charge transport in many other systems. For that, a current work is underway to improve the numerical accuracy of its DRMG calculation and explore different definitions.

3:42PM L24.00007 Scattering matrix approaches for dissipative quantum transport , DAVID FERRY, Arizona State University — The Usuki method, which is closely related to both the scattering matrix approach and recursive Green's functions provides a stable numberical method for the simulation of quantum transport in semiconductors. It has major advantage over the Green's function method for self-consistent simlations in that the electron density involves integrals in the contacts where the distribution is near equilibrium, rather than throughout the active area. Various applications of this approach have been studied, and we discuss primarily ballistic transport in quantum dots and dissipative transport in gated quantum wire transistors. Dissipation is introduced via a proper self-energy determined in the mode representation, which is then transformed to the site representation used in the recursive approach.

4:18PM L24.00008 Electron hopping between Wurtzite CdSe Quantum Dots Linked by Molecules[1] , IEK-HENG CHU, Dept of Physics and QTP, Univ of Florida, MARINA RADULASKI, Dept of Physics, Univ of Belgrade, Serbia, NENAD VUKMIROVIC, Lawrence Berkeley National Lab, HAI-PING CHENG, Dept of Physics and QTP, Univ of Florida, LIN-WANG WANG, Lawrence Berkeley National Lab — Recent experimental results show that the transport properties of quantum dot (QD) arrays will be tremendously improved after attached by cross-linking molecules. Here, we present an *ab initio* study on the electron hopping rates between wurtzite CdSe QDs connected by Sn_2S_6 molecules. The conduction band minima (CBM) transports among connected QDs are calculated. The charge patching method (CPM) is used to construct the charge density of the QDs and the connected systems. The folded spectrum method (FSM) was applied to find the band edge states and the electronic coupling between the neighboring QDs. Electron-phonon couplings are calculated to yield the reorganization energy. The electron hopping rate is then calculated by Marcus theory and its corresponding quantum treatments. Hopping rates for three different sizes of QDs, and two different types of molecular attachments are also presented here for comparison.

[1]Supported by DOE/BES-DE-FG02-02ER45995, DOE/BES-DE-AC02-05CH11231 and NSF/DMR-0804407, and computers from NERSC.

4:30PM L24.00009 Coulomb Drag in Open Quantum Dots[1] , CANRAN XU, MAXIM VAVILOV, University of Wisconsin - Madison — We investigate the Coulomb drag effect in a system of two open quantum dots, in the presence of interdot and intradot Coulomb interactions. We present an analytical expression for the drag current at the low temperature limit obtained in the random-phase approximation. We show that the non-zero current arises from the asymmetry of electronic states with respect to the Fermi level. This asymmetry originates due to fluctuations of the transmission amplitudes in the chaotic quantum dots described by a random-matrix theory, and therefore the drag current exhibits interesting sample-to-sample mesoscopic fluctuations.

[1]Supported by NSF Grant No. DMR-0955500 and Petroleum Research Fund

4:42PM L24.00010 Nonequilibrium quantum many-body transport in multiple lead quantum dot devices[1] , JONG HAN, SUNY at Buffalo — Recently proposed imaginary-time formalism of steady-state nonequilibrium is extended to three reservoir systems and discuss their interference effects. We first consider a quantum dot coupled to three non-interacting leads in the context of the Anderson impurity model driven by source-drain bias. We discuss the difference between the two and three reservoir systems. We then consider the system of interacting leads, used as a prototype for two-channel Kondo model in quantum dot device.[2] We rewrite the charging interaction on the large dot via a gauge transformation to a correlated tunneling and perform quantum Monte Carlo simulation for equilibrium and nonequilibrium using the Matsubara-voltage formalism. We discuss the cross-over from local Fermi liquid to non-Fermi liquid as a function of the Coulomb parameter in the large dot in the electron self-energy and the magnetic susceptibility. We discuss the nonequilibrium spectral evolution of local Fermi liquid.

[1]This work has been supported by NSF with the grant number DMR-0907150.
[2]R. M. Potok et al, Nature **446**,167 (2007)

4:54PM L24.00011 Continuous measurements of electron tunneling through a quantum dot by a quantum point contact , HSI-SHENG GOAN, National Taiwan University — The time-resolved charge detection through a quantum dot (QD) by a nearby quantum point contact (QPC) detector, each coupled to its own independent electrodes and gates, has been demonstrated. The conditional counting statistics of electron transport in this QD-OPC system has also been measured [1]. The conditional counting statistics that is the statistical current fluctuations of one system given the observation of a particular current in the other system could be substantially different from their unconditional counterparts. We provide a thorough analysis on the QD-QPC system. We use the stochastic master equation (or quantum trajectory) approach to describe the conditional dynamics of the QD under continuous measurements by a QPC. We simulate in each single experimental realization the observed QPC current which reveals the real time information of single-electron tunneling events through the QD. We then use the n-resolved master equation approach to calculate the conditional counting statistics through the QD (QPC) conditioned on the observed current in QPC (QD). Our investigation goes beyond the analysis presented in Ref.[1] in which they neglected, in the noise power(second cumulant) of the QPC, the QPC shot noise as compared to the telegraph noise contribution induced by the single-electron tunneling events through the QD.
[1] E.V.Sukhorukov et. al, Nature Physics, **3**, 243 (2007).

5:06PM L24.00012 Designer switches: Effect of contact geometry on the transient current of a strongly correlated quantum dot[1] , ALI IHSAN GOKER, Bilecik University, ZHIYONG ZHU, UDO SCHWINGENSCHLOGL, AURELIEN MANCHON, King Abdullah University of Science and Technology — The time-dependent non-crossing approximation is utilized to investigate the influence of the geometry of contacts made of gold on time dependent current through a quantum dot suddenly shifted into the Kondo regime via a gate voltage. For an asymmetrically coupled system, instantaneous conductance exhibits complex fluctuations. We identify the frequencies participating in these fluctuations and they turn out to be proportional to the separation between the sharp features in the density of states and the Fermi level. Increasing ambient temperature or bias quenches the amplitude of these fluctuations. This suggests that the interference between the emerging Kondo resonance and the van Hove singularities in the density of states is the underlying microscopic mechanism for these fluctuations. Based on these observations, we predict that using different electrode geometries would give rise to drastically different transient currents which can be accessed with state-of-the-art ultrafast pump-probe techniques.

[1]King Abdullah University of Science and Technology

Tuesday, March 22, 2011 2:30PM - 4:54PM –
Session L25 DCMP: Superconductivity: Vortex Phenomena II D166

2:30PM L25.00001 Vortex Pinning in MoGe Thin Films Containing Periodic Hole Arrays , MICHAEL LATIMER, Northern Illinois University, ZHILI XIAO, WAI-KWONG KWOK, ALEXANDRA JOSHI-IMRE, Argonne National Laboratory, CASTRO ABUGHAYADA, Northern Illinois University — Resistivity measurements on MoGe thin films containing periodic hole arrays were carried out to study the effects of the lattice symmetry and the size of the pinning centers. Thin films of MoGe were prepared with holes drilled using focused-ion-beam milling to create pinning sites for the vortex lattice. We investigate periodic arrays with hexagonal, square and triangular geometry to determine the change in transport properties with varying magnetic fields. Hole sizes from 50nm to 100nm were tested determine the effects of single and multiple vortices in a single pinning site.

2:42PM L25.00002 Flux dynamics across MoGe bridges in the parallel field orientation[1] , MILIND KUNCHUR, MANLAI LIANG, University of South Carolina, ALEXANDER GUREVICH, Florida State University — We have investigated flux motion in amorphous molybdenum-germanium (MoGe) film bridges with the magnetic field B parallel to the film plane but perpendicular to the current direction. In a temperature range close to the transition temperature Tc we observe an exponential dependence of the Ohmic resistance R on B at low values of the current I, and a nonlinear R(I) at higher currents. In this regime, the diameter of the vortex is approximately equal to the film thickness and the applied magnetic field is comparable to the lower critical field for the parallel field orientation. Dissipation presumably occurs by thermally activated flux jumps over the thickness of the film involving nucleation and expansion of vortex kinks.

[1]This work was supported by the U. S. Department of Energy under Grant No. DE-FG02-99ER45763.

2:54PM L25.00003 Vortex instability in molybdenum-germanium superconducting film[1] , MANLAI LIANG, MILIND KUNCHUR, University of South Carolina — We studied the high driving force regime of the current-voltage transport response in the mixed state of amorphous molybdenum-germanium (MoGe) superconducting films to the point where the flux flow becomes unstable. The observed nonlinear response conforms with the classic Larkin-Ovchinikov picture with a quasiparticle energy-relaxation rate dominated by the quasiparticle recombination process. The measured energy relaxation rate was found to have a magnitude and temperature dependence in agreement with theory.

[1]This work was supported by the U. S. Department of Energy under Grant No. DE-FG02-99ER45763.

3:06PM L25.00004 Small Angle Neutron Scattering Studies of the Vortex Lattice in $CeCoIn_5$ with $H \perp c$, M.R. ESKILDSEN, P. DAS, University of Notre Dame, IN, USA, A.T. HOLMES, E.M. FORGAN, University of Birmingham, UK, A.D. BIANCHI, Universite de Montreal, Canada, J.S. WHITE, S. GERBER, M. KENZELMANN, J.L. GAVILANO, M. ZOLLIKER, Paul Scherrer Institute, Switzerland, C. WANG, E.D. BAUER, J.L. SARRAO, Los Alamos Natl. Lab., NM, USA, C. PETROVIC, Brookhaven Natl. Lab., NY, USA — We report on small-angle neutron scattering measurements on the vortex lattice (VL) in the mixed state of $CeCoIn_5$ with the magnetic field (H) along [100] and [110]. For both field orientations a distorted hexagonal VL is observed, reflecting the penetration depth anisotropy of the screening current plane. With $H \parallel [100]$ the VL is oriented with Bragg reflections along the [001]-axis at all fields. For $H \parallel [110]$ the same VL orientation is observed at low fields, followed by a 90° first-order reorientation transition as H is increased. We attribute this behavior to Fermi surface anisotropy coupled with non-local effects. For $H \parallel [100]$ we obtain the field dependence of the form factor ($|F|^2$) both within (50 mK) and outside (350 mK) the magnetic Q-phase. At both temperatures $|F|^2$ varies with H in a manner similar to $H \parallel [001]$ [J.S. White *et al.*. New J. Phys. **12**, 023026 (2010)], due to the competition between Pauli paramagnetism and the antiparallel spin alignment of d-wave pairing giving rise to "magnetized" VL cores.

3:18PM L25.00005 Low temperature enhancement of the remanent magnetization in $CeCoIn_5$, C.F. MICLEA, Los Alamos National Laboratory, Los Almos, USA, M. NICKLAS, A.C. MOTA, F. STEGLICH, Max-Planck-Inst. for Chemical Physics of Solids, Dresden, Germany, M.M. ALTARAWNEH, N. HARRISON, Los Alamos National Laboratory, Los Almos, USA, I. VEKHTER, Louisiana State Univ., Baton Rouge, USA, J.D. THOMPSON, R. MOVSHOVICH, Los Alamos National Laboratory, Los Alamos, USA — We investigated the vortex dynamics together with RF penetration depth measurements in the heavy fermions compound $CeCoIn_5$ down to 50 mK. No strong pining is observed and the relaxation curves are logarithmic as expected from Kim-Anderson theory. The temperature dependence of the relaxation rate, S, with a small but finite residual value indicate that quantum tunneling plays a role in the vortex creep only at very low temperatures. Remarkably, a new phase transition marked by a strong increase in the remnant magnetization, M_{rem} is observed around $T = 0.3$ K in very low magnetic fields. M_{rem} increases roughly by a factor of two at 50 mK and we discuss if this can be caused solely by the change in the vortex lattice symmetry or underling magnetism has to play a role. Moreover, this anomaly is corroborated by the RF measurements at very low fields. We extended the vortex dynamics investigation to Pb irradiated $CeCoIn_5$. While the defects created by irradiation have a clear effect on the relaxation rates the enhancement of M_{rem} still takes place at the same temperature.

3:30PM L25.00006 Vortex Core Size Measurements in YNi_2B_2C and $TmNi_2B_2C$, P. DAS, C. RASTOVSKI, K. SCHLESINGER, M.R. ESKILDSEN, University of Notre Dame, IN, USA, J.M. DENSMORE, Army Research Laboratory, Aberdeen, MD, USA, S.L. BUD'KO, P.C. CANFIELD, Ames Laboratory and Iowa State University, IA, USA — The vortex core size in type-II superconductors is typically determined from measurements of a related quantity combined with a theoretical model, with the best known example being the upper critical field and the GL-result: $\xi = \sqrt{\phi_0/2\pi H_{c2}}$. However, for many non-conventional superconductors such an approach is problematic, as for example in the case of $TmNi_2B_2C$ and $CeCoIn_5$ where H_{c2} is suppressed by coexistence with magnetism. In such instances a direct, model independent determination of the vortex core is desirable, and can be obtained by small-angle neutron scattering (SANS) measurements of the vortex lattice (VL) if a sufficient number of reflections are recorded [J. M. Densmore *et al.*, Phys. Rev. B **79**, 174522 (2009)]. Here we report on VL SANS studies on two members of the borocarbide superconductors, YNi_2B_2C and $TmNi_2B_2C$. Non-magnetic Y1221 measurements at 0.2 and 0.5 T show clear evidence of a vortex squeezing effect. In magnetic Tm1221 the vortex core size was found to be $\xi = 10.8$ nm, roughly a factor of two smaller than the value estimated by the measured H_{c2} (21 nm). Supported by NSF award no. DMR-0804887 (Notre Dame) and DOE BES contract No. DE-AC02-07CH11358 (Ames).

3:42PM L25.00007 ABSTRACT WITHDRAWN –

3:54PM L25.00008 Revealing the effect of edge contamination on vortex matter structure in a Nb single crystal with neutron diffraction techniques[1] , HELEN HANSON, XI WANG, MICHAEL LUK, JING SHI[2], XINSHENG LING, Brown University, BRIAN MARANVILLE, CHARLES MAJKRZAK, NIST Center for Neutron Research — The vortex matter of type II superconductors provides a model system to study the effect of quenched random disorder on an elastic lattice, particularly in the framework of Bragg glass theory. Neutron scattering techniques are used to examine the structure of the vortex matter and to quantify the phase diagram. After measuring various thermal-magnetic histories, our data provided evidence for the edge contamination model in a Nb single crystal. Since surface oxidation is known to suppress the Bean-Livingston Surface barrier and the inhomogeneous distribution of surface impurities in Nb, we oxidize our sample surface and repeat our measurements. By comparing the data, we are able isolate the dynamic impact of the edge disorder from the static influence of bulk pinning. We discuss the various experimental obstacles in measuring the predicted Bragg glass state. We also report on Reverse Monte Carlo Refinement simulations modeling possible structures of our vortex matter.

[1]This research was supported by the U.S. DOE under grant DE-FG02 – 07ER46458.
[2]Permenant Address: Wuhan University

4:06PM L25.00009 Exploring the vertical variation of the flux line lattice angular orientation using a novel neutron diffraction technique[1] , XI WANG, HELEN HANSON, JING SHI[2], XINSHENG LING, Brown University, BRIAN MARANVILLE, CHARLES MAJKRZAK, NIST, MARK LAVER, PSI, UWE KEIDERLING, MARGARITA RUSSINA, HZB — We use a slicing neutron diffraction technique, employing neutron reflectometry collimation, to study the orientational order of the flux line lattice in a Nb single crystal. We are able to reveal the spatial variation of the different orientation distributions along the length of the flux lines. The results are strongly dependent on the magnetic history of the vortex matter, suggesting various interactions with the disorder in the system. After thermally annealing the different initial states, memory of the growth procedure is removed from the data and a possible ground state is reached. In this final state, the novel vertical slicing reveals the persistence of a domain splitting. We suggest that this domain splitting is due to the quenched disorder in the underlying Nb atomic lattice. We believe that this new insight will be instrumental in growing a true Bragg glass, the theoretically predicted ground state with topological order.

[1]This research is supported by the US DOE under the grant DE-FG02 - 07ER46458.
[2]Permanent address:Wuhan University, Wuhan 430072, PRC

4:18PM L25.00010 Vortex activation energy in high-Tc superconductors from transport measurements: new systematics[1] , YURI L. ZUEV, JOHN SINCLAIR, JAMES R. THOMPSON, University of Tennessee, SUNG HUN WEE, CLAUDIA CANTONI, DAVID K. CHRISTEN, Oak Ridge National Laboratory — From electrical transport measurements on thin films of YBCO with and without nano-precipitate "columnar defects," we extract information about the activation energy for vortex creep. We also obtain new scaling between temperature, critical current density J_C, and the power law index n describing the voltage-current relation $V \propto I^n$. This scaling occurs in the range of field and temperature where J_C decays as a power-law of magnetic field. In this regime the n-value can unexpectedly increase as applied field increases. We will discuss implications of these observations and compare systems with and without such scaling.

[1]Work at ORNL supported by the US DOE.

4:30PM L25.00011 Comparison of free flux flow in two single crystals of V_3Si with slightly different pinning strengths[1] , OZARFAR GAFAROV, ALBERT A. GAPUD, SUNHEE MORAES, University of South Alabama, JAMES R. THOMPSON, University of Tennessee Knoxville and Oak Ridge National Laboratory, DAVID K. CHRISTEN, Oak Ridge National Laboratory, ARNEIL P. REYES, National High Magnetic Field Laboratory — Results of recent measurements on two very clean, single-crystal samples of the A15 superconductor V_3Si are presented. Magnetization and transport data confirm the "clean" quality of both samples, as manifested by: (i) high residual resistivity ratio, (ii) low critical current densities, and (iii) a "peak" effect in the field dependence of critical current. The (H,T) phase line for this peak effect is shifted in the slightly "dirtier" sample, which also has higher critical current density J_c(H). High-current Lorentz forces are applied on mixed-state vortices in order to induce the highly ordered free flux flow (FFF) phase, using the same methods as in previous work. A traditional model by Bardeen and Stephen (BS) predicts a simple field dependence of flux flow resistivity ρ_f(H), presuming a field-independent flux core size. A model by Kogan and Zelezhina (KZ) takes core size into account, and predicts a deviation from BS. In this study, ρ_f(H) is confirmed to be consistent with predictions of KZ, as will be discussed.

[1]Funded by Research Corporation and the National Science Foundation.

4:42PM L25.00012 Magnetic-field-induced stripe order and a 2D vortex glass phase in $La_{1.905}Ba_{0.095}CuO_4$[1] , JOHN TRANQUADA, JINSHENG WEN, QING JIE, SU JUNG HAN, QIANG LI, MARKUS HUECKER, ZHIJUN XU, LIYUAN ZHANG, GENDA GU, Brookhaven Natl Lab, M.V. ZIMMERMANN, HASYLAB, D.K. SINGH, NCNR — We have measured the resistivity parallel and perpendicular to the CuO_2 planes in $La_{1.905}Ba_{0.095}CuO_4$ ($T_c = 32$ K) as a function of perpendicular magnetic field. We have discovered a significant regime of field and temperature where the perpendicular resistivity is finite (and large) but the parallel resistivity is zero. This regime appears to correspond to a quasi-two-dimensional vortex glass phase, a state that theory predicts cannot exist at finite temperature. It seems to be stabilized by field-induced charge and spin stripe order, which we have detected with x-ray and neutron diffraction, respectively.

[1]Supported by Office of Basic Energy Sciences, US DOE, under Contract No. DE-AC02-98CH10886.

Tuesday, March 22, 2011 2:30PM - 5:30PM –
Session L26 DMP DCOMP: Focus Session: Iron Based Superconductors – ARPES D162/164

2:30PM L26.00001 ABSTRACT WITHDRAWN –

2:42PM L26.00002 Angle-resolved photoemission spectroscopy study of $Ba(Fe_{1-x}Ru_x)_2As_2$, TIAN QIAN, NAN XU, PIERRE RICHARD, YINGBO SHI, GUANGHAN CAO, ZU'AN XU, HONG DING, INSTITUTE OF PHYSICS, CHINESE ACADEMY OF SCIENCES COLLABORATION, ZHEJIANG UNIVERSITY COLLABORATION — Ru-doped $BaFe_2As_2$ compounds were discovered recently to show superconductivity at a relatively wide doping range. We will present angle-resolved photoemission spectroscopy results of electronic structure and Fermi surface of $Ba(Fe_{1-x}Ru_x)_2As_2$, and discuss implications to its superconductivity.

2:54PM L26.00003 Chiral orbital angular momentum and warping effect in topological insulator Bi2Te3 , WON SIG JUNG, Y.K. KWAN, B.Y. KIM, Yonsei University, Seoul, Korea, J.Y. KIM, B.K. CHO, Dept of Materials Science and Engineering, GIST, Korea, C. KIM, Yonsei University, Seoul, Korea — The spin of a topologically protected metallic surface state on topological insulators has a chiral state. The Spin chiral state is aligned with orbital angular momentum of the electron in the surface states. We observe orbital angular momentum direction by using angle resolved photoemission (ARPES) with circularly polarized lights.

3:06PM L26.00004 Pseudogap in non-superconducting pnictides, $CaFe_2As_2$ and $EuFe_2As_2$, K. MAITI, G. ADHIKARY, N. SAHADEV, D.N. BISWAS, R. BINDU, N. KUMAR, A. THAMIZHAVEL, S.K. DHAR, Dept of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Homi Bhabha Road, Colaba, Mumbai - 400 005, India — Superconductivity in Fe-pnictides are studied extensively recently as they provide a non-cuprate domain to study unconventional superconductivity via doping induced suppression of magnetism. In order to study the role of magnetic interactions in the electronic structure and its implication in superconductivity, we probed the electronic structure of the parent compounds $CaFe_2As_2$ and $EuFe_2As_2$ using high resolution photoemission spectroscopy. Single crystalline samples were prepared by flux method. Photoemission measurements were carried out using a Gammadata Scienta analyzer R4000 and monochromatic photon sources. The high resolution spectra exhibit signature of a pseudogap above the spin density wave (SDW) transition temperature in both $CaFe_2As_2$ and $EuFe_2As_2$. The intensity at the Fermi level show a sudden decrease across the SDW transition indicating more prominent pseudogap. An additional gap opens up in $EuFe_2As_2$ across the antiferromagnetic transition temperature as expected. Interestingly, $CaFe_2As_2$ also exhibit signature of another gap opening at low temperatures although no phase transitions observed in this temperature range.

3:18PM L26.00005 Unconventional superconducting gap in $NaFe_{0.95}Co_{0.05}As$ observed by ARPES , PIERRE RICHARD, Institute of Physics, Chinese Academy of Sciences, Z.-H. LIU, Renmin University, K. NAKAYAMA, Tohoku University, G.-F. CHEN, Renmin University, S. DONG, J.-B. HE, D.-M. WANG, T.-L. XIA, Renmin University, K. UMEZAWA, T. KAWAHARA, S. SOUMA, T. SATO, T. TAKAHASHI, Tohoku University, T. QIAN, Y. HUANG, N. XU, Y. SHI, H. DING, Institute of Physics, Chinese Academy of Sciences, S.-C. WANG, Renmin University — The size, the symmetry and the temperature evolution of the superconducting (SC) gap in a given material are directly related to the SC pairing mechanism. The momentum-resolution capability of angle-resolved photoemission spectroscopy (ARPES) allows precise determination of these key parameters, even for complex multi-band systems such as the iron-based superconductors. We performed an ARPES study of $NaFe_{0.95}Co_{0.05}As$. The fermiology of this electron-doped 111-pnictide is similar to that of other pnictides. Similarly, the measured SC gaps are nearly isotropic and their size indicates that the system is in the strong coupling regime. Surprisingly, the SC gaps show little change upon increasing temperature towards T_c, while coherence vanishes.

3:30PM L26.00006 Studies on the orbital characters and quasi-particle dynamics of LiFeAs , YEONGKWAN KIM, B.Y. KIM, CHUL KIM, D.J. SONG, W.S. KYUNG, C. KIM, Institute of Physics and Applied Physics, Yonsei University, Seoul 120-749, Korea, B.S. LEE, K.H. KIM, FPRD, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea — Since the discovery, iron-based superconductors have been intensively and extensively studied by using various techniques including angle resolved photoelectron spectroscopy (ARPES). So far, most of ARPES studies have been performed on 122-compounds and 1111-compounds. However, 122-phase materials do not have neutral cleavage surfaces and have 3-dimensional band structures. These traits of 122- and 1111-phase make the spectral shape generally broad and do not allow investigation of the intrinsic electronic structures in detail. In that respect, LiFeAs is an ideal material with neutral cleavage surfaces and quasi-2 dimensional band structures. In this presentation, our recent ARPES work on the electronic structure of LiFeAs will be presented. We investigated the orbital character of each band by ARPES with various polarizations of the photon. Since the main valence band of LiFeAs comes from iron d-orbitals, pin-pointing the characters of bands should be an important starting point. In addition, we analyzed details of the spectral function in regard to the quasi-particle dynamics..

4:18PM L26.00008 Nodeless superconductivity in the stoichiometric superconductor LiFeAs , HYUNSOO KIM, MAKARIY A. TANATAR, RUSLAN PROZOROV, Ames Laboratory, Ames, IA 50011, USA, YOO JANG SONG, YONG SEUNG KWON, Department of Physics, Sungkyunkwan University, Suwon, Gyeonggi-Do 440-746, Republic of Korea — The in- and out-of-plane London penetration depths were measured in single crystals of the intrinsic LiFeAs superconductor using a tunnel diode resonator (TDR) down to $0.03T_c$. This compound appears to be in the clean limit with a residual resistivity of $\rho_0 \approx 5$ $\mu\Omega$·cm and $RRR = 65$; it can be placed at a slightly overdoped value when compared to the charge-doped pnictides. The low-temperature region of the penetration depth, which is sensitive to the superconducting gap symmetry, is exponentially flat implying a nodeless gap. The superfluid density is well described by the self-consistent two-gap γ-model, where the larger gap is $\Delta_1/T_c \sim 2$ and the smaller gap is $\Delta_2/T_c \sim 1$. Together with the previous data, our results support the $s_\pm$ symmetry that evolves from nodeless to a nodal gap structure upon departure from optimal doping in Fe-based superconductors. We also conclude that pairbreaking scattering plays an important role in the deviations of the low-temperature behavior from exponential in $\lambda(T)$ of Fe-based compounds.

4:30PM L26.00009 Superfluid Density in the 111 Fe Pnictide Superconductors , C. J. ARGUELLO, T. GOKO, J.P. CARLO, Y.J. UEMURA, Columbia University, A.A. ACZEL, T.J. WILLIAMS, G.M. LUKE, McMaster University, C.Q. JIN, Beijing IoP — We performed muon spin relaxation studies in two kinds of '111' iron pnictides, $Li_{1.1}FeAs$ and $Li_{0.9}FeP$. The zero field spectra of the latter show a fast relaxation in a small volume fraction (approximately 13%) due probably to magnetism. In the case of the arsenide, the zero field spectra show a completely paramagnetic state. Below Tc, an applied transverse field allowed us to measure the superfluid density (via relaxation rate σ) for both compounds. We found that both of them have very high superfluid density and low Tc: $\sigma(T = 2K) \simeq 1.8\mu s^{-1}$ with Tc$\simeq$18K for $Li_{1.1}FeAs$, and $\sigma(T = 2K) \simeq 2.0\mu s^{-1}$ with Tc$\simeq$4K for $Li_{0.9}FeP$.

4:42PM L26.00010 Spin lattice relaxation rate measurements in $Ba_{0.69}K_{0.31}Fe_2As_2$ by nuclear magnetic resonance[1] , SANGWON OH, ANDREW MOUNCE, WILLIAM HALPERIN, Northwestern University, CHENGLIN ZHANG, PENGCHENG DAI, University of Tennessee, ARNEIL REYES, PHILIL KUHNS, National High Magnetic Field Lab — Magnetic impurities have been a problem with NMR measurements of single crystals in the K doped Ba-122 system because of extremely wide linewidth that can be more than 1MHz at low temperature [1]. We have a high quality single crystal of $Ba_{0.69}K_{0.31}Fe_2As_2$ (T_c = 34K) for which the NMR linewidth does not significantly increase at low temperatures and at very large external magnetic fields. In this sample we measure the spin-lattice relaxation rate, $1/T_1$, from 300 K to 4 K at various magnetic fields 6.4 T, 13 T, and 16 T. The rapid increase of $1/T_1T$ down to T_c on cooling can be attributed to spin fluctuations above T_c. In the superconducting state, $1/T_1$ has a kink around 20 K, and below this temperature in a field of 13 T it exhibits a power law dependence, \varpropto T^3. This behavior can be explained by an impurity effect in a superconductor with extended s-wave symmetry [2].

[1] S. Mukhopadhyay *et al.* New J. Phys. **11**, 055002 (2009)
[2] Y. Bang *et al.* Phys. Rev. B **79**, 054529 (2009)

[1]This work is supported by DOE/BES: DE-FG02-05ER46248 and the NHMFL by NSF and the State of Florida.

4:54PM L26.00011 Frustrated proximity effects between s and $s_\pm$ superconductors , VALENTIN STANEV, ALEXEI E. KOSHELEV, Materials Science Division, Argonne National Laboratory — The nature of the superconducting order parameter (OP) in iron pnictides and chalcogenides is a hotly debated issue. It was theoretically proposed that the OP has opposite signs on the hole and the electron bands, i.e., it belongs to the unconventional class of $s_\pm$ (or extended s)-wave. There are, however, very few experiments that can directly distinguish this state from the ordinary s-wave OP. One way to address this problem is to study the proximity effects in a sandwich composed of conventional and iron pnictide superconductors (SC). If the pnictides indeed have the $s_\pm$ OP this system is intrinsically frustrated. In the case of strong frustration, a time-reversal symmetry-breaking (TRSB) SC state emerges, in which the OP phases in different bands are tilted at an angle, different from π, and controlled by the coupling strength. Observation of such state in the iron-based SC materials would give definite evidence for the $s_\pm$ OP. We present a microscopic, fully self-consistent approach to this problem, based on Usadel equations. We have studied the conditions for existence of the TRSB state and its experimental signatures.

5:06PM L26.00012 Doping dependence of $Ba(Fe_{1-x}Co_x)_2As_2$ thin films by the THz conductivity measurement , D. NAKAMURA, F. NABESHIMA, Y. IMAI, A. MAEDA, Dept. of Basic Science, the University of Tokyo, T. KATASE, Materials and Structures Laboratory, Tokyo Institute of Technology, H. HIRAMATSU, ERATO-SORST, Japan Science and Technology Agency, H. HOSONO, Materials and Structures Laboratory, Tokyo Institute of Technology — We investigated the THz conductivity for thin films of Fe-based superconductor, $Ba(Fe_{1-x}Co_x)_2As_2$ with different Co concentrations. For the optimally doped sample, we found a structure corresponding to superconductivity gap, 2 Δ, whose magnitude is 2.8 meV at lowtemperatures, leading to 2 Δ/k_BT_c = 4.1[1]. This value is in good agreement with the smaller gap found in an ARPES measurement[2]. For the underdoped sample in which the coexistence of antiferromagnetic ordering with superconductivity was observed, we found the strong suppression of the carrier lifetime around the antiferromagnetic phase transition temperature ($T \sim$ 40 K). However, the real part of the complex conductivity did not be clearly suppressed in this temparature regigon. This behavior may be related to the responce of carriers at the Dirac cone, which observed in $BaFe_2As_2$[3]. Details will be discussed in the presentation.

[1] D. Nakamura *et al.*, arXiv: 0912.4351.
[2] K. Terashima *et al.*, PNAS 106 (2009) 7330.
[3] P. Richard *et al.*, Phys. Rev. Lett. 104 (2010) 137001.

5:18PM L26.00013 Pair breaking in iron-based superconductors , KEVIN KIRSHENBAUM, SHANTA SAHA, TYLER DRYE, STEVEN ZIEMAK, JOHNPIERRE PAGLIONE, University of Maryland at College Park — The relative ease of crystal growth combined with the range of elements available for chemical substitution, especially on the transition metal site, has allowed for numerous studies of different iron-based superconductors. There are, however, remaining questions about the pairing symmetry in this system. We present transport scattering rate data for optimally-doped single crystals from several superconducting 122 materials and discuss the relationship between superconducting transition temperature and transport scattering rate in the context of pair breaking.

Tuesday, March 22, 2011 2:30PM - 5:30PM –

Session L28 DCOMP DMP: Focus Session: Computational Materials Design - Property Optimization C156

2:30PM L28.00001 Computational Design of Microstructures , LONG-QING CHEN, Penn State University — Many important engineering materials are designed by controlling their phase transformations and microstructure evolution. Examples include the improvement of mechanical properties through solid state precipitation reactions in alloys such as Ni-based superalloys and age-hardened Al-alloys, the useful dielectric properties and electro-mechanical coupling effects by manipulating the phase transitions in ferroelectric crystals, the memory effect of shape-memory alloys by utilizing martensitic transformations. In this presentation, recent effort on integrating the phase-field approach with other computational methods such as first-principles calculations and CALPHAD will be discussed. A number of examples of coupling phase-field simulations and experimental measurements will be presented. It will be demonstrated that one can use the phase-field method to not only help interpreting experimental observations but also provide guidance to achieve desirable transition temperatures and specific domain/microstructure structures. The possibility to directly obtain the effective responses of a microstructure under an applied field from phase-field simulations, and thus the evolution of effective mechanical and transport properties will also be discussed.

3:06PM L28.00002 Phase-field model and its numerical solution for coring and microstructure evolution studies in alloys[1] , PATRICE E. A. TURCHI, JEAN-LUC FATTEBERT, MILO R. DORR, MICHAEL E. WICKETT, JAMES F. BELAK, Lawrence Livermore National Laboratory — We describe an algorithm for the numerical solution of a phase-field model (PFM) of microstructure evolution in alloys using physical parameters from thermodynamic (CALPHAD) and kinetic databases. The coupled system of PFM equations includes a local order parameter, a quaternion representation of local crystal orientation and a species composition parameter. Time evolution of microstructures and alloy composition is obtained using an implicit time integration of the system. Physical parameters in databases can be obtained either through experiment or first-principles calculations. Application to coring studies and microstructure evolution of Au-Ni will be presented.

[1]Prepared by LLNL under Contract DE-AC52-07NA27344

3:18PM L28.00003 High Temperature Thermal Conductivity from First Principles , CHRISTIAN CARBOGNO, Materials Department, University of California Santa Barbara / Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, RAMAMURTHY RAMPRASAD, University of Connecticut, Storrs / Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — In spite of significant research efforts, little is yet known about the atomistic details and mechanisms that underlie peculiarly low (or high) thermal conductivities, especially at elevated pressures and temperatures. Under such extreme conditions, systematic experimental measurements are hard to perform; conventional theoretical approaches typically fail to capture significant physical aspects of the problem, since these methods are either inherently limited to (a) low temperatures and/or (b) to perfect crystals. A recently developed *ab initio* simulation strategy [1] allows to overcome the latter limitation, but the assessment of the high temperature regime remains an unsolved challenge. Within this work, we present efficient strategies to overcome this serious restriction and show their applicability for zirconia based ceramics - a material typically used in high temperature applications, for instance in thermal barrier coatings [2].
[1] T. M. Gibbons, and S. K. Estreicher, *Phys. Rev. Lett.* **102**, 255502 (2009).
[2] D. R. Clarke, and C. G. Levi, *Annu. Rev. Mat. Res.* **33**, 383 (2003).

3:30PM L28.00004 First Principles Studies of the Thermoelectric Figure of Merit of Zintl Compounds $Ca_{14}AlSb_{11-x}As_x$, TRINH VO, PAUL VON ALLMEN, JEAN-PIERRE FLEURIAL, Jet Propulsion Lab, CalTech — We present predictions for the thermoelectric Figure of merit (ZT) of zintl compounds $Ca_{14}AlSb_{1-x}As_x$ obtained from Density Functional Theory calculations. The Seebeck coefficient, S, was obtained using the Boltzmann transport equation in the relaxation time approximation and first principles electronic structure calculations. We found that the Seebeck coefficient changes dramatically when one or more Sb atoms in the zintl compound $Ca_{14}AlSb_{11}$ are replaced with one or more As atoms, and that the difference in S between the original $Ca_{14}AlSb_{11}$ and the substituted one, $Ca_{14}AlSb_{11-x}As_x$, depends strongly on the positions of substituting As atoms.

3:42PM L28.00005 First-principles model of absolute band shifts induced by (001) biaxial strain in group IIIA-VA semiconductors , EUGENE KADANTSEV, PAWEL HAWRYLAK, IMS NRC — A new model for the evolution of conduction and valence bands of IIIA-VA (InAs, GaAs, InP) semiconductors under (001) biaxial strain is developed. The model is based on ab initio calculations which take into account finite strain dependent relaxation of the reference levels. It is shown that in type I heterostructures subjected to (001) compressive biaxial strain, the confinement of holes can be reduced as compared to some existing models of biaxial strain.

3:54PM L28.00006 Possible calcium centers for hydrogen storage applications: An accurate many-body study by AFQMC calculations with large basis sets[1] , WIRAWAN PURWANTO, HENRY KRAKAUER, SHIWEI ZHANG, YUDISTIRA VIRGUS, College of William and Mary — Weak H_2 physisorption energies present a significant challenge to first-principle theoretical modeling and prediction of materials for H storage. There has been controversy regarding the accuracy of DFT on systems involving Ca cations. We use the auxiliary-field quantum Monte Carlo (AFQMC) method[2] to accurately predict the binding energy of Ca^+-$4H_2$. AFQMC scales as $N^3_{\rm basis}$ and has demonstrated accuracy similar to or better than the gold-standard coupled cluster CCSD(T) method. We apply a modified Cholesky decomposition to achieve efficient Hubbard-Stratonovich transformation in AFQMC at large basis sizes. We employ the largest correlation consistent basis sets available, up to Ca/cc-pCV5Z, to extrapolate to the complete basis limit. The calculated potential energy curve exhibits binding with a double-well structure.

[1]Supported by DOE and NSF. Calculations were performed at OLCF Jaguar and CPD.
[2] S. Zhang and H. Krakauer, Phys. Rev. Lett. **90**, 136401 (2003); W. A. Al-Saidi, S. Zhang and H. Krakauer, J. Chem. Phys. **124**, 224101 (2006).

4:06PM L28.00007 Theoretical modification of WO_3 for water splitting , PREDRAG LAZIC, MARIA K. CHAN, RICKARD ARMIENTO, YABI WU, GERBRAND CEDER, Massachusetts Institute Of Technology — Using the sun's energy to produce hydrogen from water through photocatalytic process has been a dream since its first demonstration by Fujishima and Honda 40 years ago. Since then significant effort has been made to find a suitable material for this purpose but so far efficiency of the available materials is too low to be commercially interesting. However there are some promising candidates that have some very desirable properties for solar water splitting and their other properties are believed to be improvable by some changes in the material. One of such candidates is WO_3 which shows a very good light absorption and very high stability in aqueous environment. Unfortunately it also has a position of conduction band minimum slightly too low to support H^+/H_2 reaction of hydrogen evolution and also has a relatively large gap which prevents it from using a large part of solar spectrum and thus yielding a low efficiency for water splitting. We have tried to remedy those two problems by substitutions and codoping in the pure WO_3 material within the density functional theory. For some of the modifications we see improved material properties.

4:18PM L28.00008 Ab initio investigations of complex oxides , ALTYNBEK MURAT, JULIA E. MEDVEDEVA, Missouri University of Science & Technology — We employ *ab-initio* density functional approach to investigate the structural, optical and electronic properties of twelve complex oxides with layered structure $RAMO_4$, R=In or Sc, A=Al, Ga, M=Ca, Cd, Mg, and/or Zn. We find that presence of the light metal (e.g., Al, Ca, Mg and Sc) oxides significantly affects the optical band gap which varies from 0.64 eV ($InGaCdO_4$) to 4.35 eV ($ScAlMgO_4$). At the same time, the electron effective mass remains nearly isotropic in all oxides, and both structurally and chemically distinct layers are expected to participate in charge transport once the materials are degenerately doped. Further, for a comparative systematic investigation of carrier generation mechanisms in complex oxides, we calculated the electronic properties of fluorine doped (F_O) and oxygen-reduced $RAMO_4$ materials as well as their single-cation constituents in various phases. We determine most preferable spatial distribution of the F impurity and the oxygen defect in the layered structure of each material and find that the dopant/vacancy site locations correlate with the formation energy of the single-cation oxides. The results allow us to draw conclusions on the role played by each constituent oxide and to predict how the properties of multicomponent materials can be controlled via chemical composition, crystal structure and carrier generation.

4:30PM L28.00009 Tuning of Metal-Metal Bonding by Counterion Size in Hypothetical AETiO2 Compounds , XIAODONG WEN, ROALD HOFFMANN, Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY — The structures and electronic properties of a number of real and hypothetical ABX2 compounds sharing (or evolving from) a single P4/mmm structural type are examined utilizing first principle calculations. These include the known CaCuO2 and SrFeO2 phases. A number of variations of this P4/mmm ABX2 framework, some obvious, some exotic, all with a chemical motivation, were investigated: A=alkali metal, alkaline earth metal or La, B= Ti, Fe, Cu or Pt, and X=C, O, S, C2, H2 or F. Careful attention was given to the d-orbital splitting patterns and magnetic states (ferromagnetic or antiferromagnetic) of these compounds, as well as their stability gauged by phonon dispersions and energetics. The most interesting as yet unmade compounds that emerged was an AETiO2 (AE = alkaline earth metal, Be, Mg, Ca, Sr and Ba) series, with Ti-Ti bonding, part σ, part π, tuned by the AE2+ cation size. The Ti-Ti bonding in 3D AETiO2 structures has a unique electronic feature of 1D metal chain. These AETiO2 (M=Ca, Sr and Ba) structures are calculated to be thermodynamically and dynamically stable. Experimentally, the high temperature method fails so far. Perhaps a low temperature method offer a better pathway to synthesize the AETiO2 (M=Ca, Sr and Ba) structures.

4:42PM L28.00010 Rational Band Structure Engineering of TiO_2 for Photoelectrochemical Water Splitting , SU-HUAI WEI, WAN-JIAN YIN, YANFA YAN, National Renewable Energy Lab — The search for new semiconducting materials or the engineering of existing semiconductors for commercially viable photoelectrochemical (PEC) water splitting has been extremely challenging. Meeting that challenge requires the discovery of a semiconductor with several tightly coupled material property criteria such as appropriate band gap (1.6 – 2.2 eV), efficient visible light absorption, high carrier mobility, and correct band edge positions that straddle the water redox potentials. However, previous searches/modifications of semiconducting materials for PEC water splitting application have often focused on a particular individual criterion such as band gap, neglecting the possible detrimental consequence to other important criteria. In this talk, general strategies for the rational design of semiconductors such as TiO_2 to simultaneously meet all of the requirements for a high efficiency solar-driven PEC water splitting device are discussed. Density-functional theory calculations reveal that with appropriate donor-acceptor co-incorporation, heavily doped anatase TiO_2 hold great potential to satisfy all of the criteria for a viable PEC device. Other approaches to modify the band structure of TiO_2, such as the application of strain, will also be discussed.

4:54PM L28.00011 Structural and Electronic Properties of $LaTiO_2N$ with O/N Disorder[1] , WEI KANG, MARK S. HYBERTSEN, Center for Functional Nanomaterials, Brookhaven National Lab — $LaTiO_2N$ is an attractive candidate photo-catalyst for water-splitting, showing strong absorption in the visible range with an optical gap about 2.1 eV and catalytic activity for hydrogen and oxygen evolution in the presence of auxiliary co-catalysts. It is also a good prototype suitable for theoretical study. It has a small unit cell while exhibiting several key characteristics found in the more complex oxides and oxynitrides synthesized in the search for improved photo-catalysts. This includes the reduced band gap and the disorder in one of the components, the O/N anion sublattice. We study the structural properties using a first-principles cluster expansion method. Our results reveal that at the temperatures characteristic of synthesis and annealing conditions, the occupation of O/N in $LaTiO_2N$ is intrinsically disordered. However the structure retains residual long-range order, in agreement with anion site occupancies measured in powder neutron diffraction. Short-range order in the O/N occupation is also observed. We use many-body perturbation theory to study the electronic and optical properties for some low-energy structures. The fundamental gap is found about 0.5 eV lower than the apparent absorption edge observed in experiments.

[1]This work is supported by the DOE

5:06PM L28.00012 The Se effect on the oxygen reduction reaction on the Se/Ru electrocatalysts. Insight from first principles. , SERGEY STOLBOV, University of Central Florida — Rational search for new efficient low-cost electrocatalysts for oxygen reduction reaction (ORR) on the hydrogen fuel cell cathodes focuses on varying the material composition to modify the local densities of electronic states (LDOS) of the surface atoms, in order to tune the surface-adsorbate electronic state hybridization and hence binding energies of the ORR intermediates. My calculation results for the Se/Ru electrocatalysts suggest an alternative way of tuning the binding energies. The Se atoms deposited on the Ru surface are found not to change Ru LDOS noticeably, however, Se atoms are negatively charged due to ionic Se-Ru bonding. As a result, they repeal electrostatically the adsorbed negatively charged O and OH intermediates, and this way reduce their binding energies. Since for the Ru case, reduction of the O and OH binding energies makes ORR energetically favorable, Se deposition dramatically improve the ORR rate on Ru. The ORR rate can thus be enhanced by changing coverage of the deposited halchogen atoms or by tuning the charge transfer to those by modifying the substrate composition.

5:18PM L28.00013 First principles studies of the oxygen reduction reaction on Se-Ru nanostructures , SEBASTIAN ZULUAGA, SERGEY STOLBOV, University of Central Florida — Experiments show an enhanced rate of the oxygen reduction reaction (ORR) on Se-Ru nanostructures (NS) in hydrogen fuel cell cathodes. We use first principles methods to study Ru and Se-Ru NS of approximate 1.2 nm size and shine some light on how the Se affects the O and OH adsorption, which is the bottle neck of the power delivered by the fuel cell. Experiments shows that the Se-Ru NS have a Ru core but is not clear how the Se is distributed on the surface. Our calculation shows that the Se atom adsorbs on the Ru surface with a binding energies in the range 5.7 to 7.1 eV with electronic charge transfer from the Ru atoms. Due to repulsion between negatively charged Se atoms, they tend to spread uniformly over the the Ru NS rather than form islands on its surface. We have also found that, in contrast to the flat Ru surface, the Se bond to the low coordinated Ru atoms have significant covalent component. Our calculation shows how the presence of Se atoms affects the adsorption of the ORR intermediates on the NS. In particular, we show that the electrostatic repulsion between charged Se and O or OH reduces the binding energy of the latters.

Tuesday, March 22, 2011 2:30PM - 5:30PM –
Session L29 GQI: Quantum Entanglement C148

2:30PM L29.00001 Entanglement entropy between two coupled Tomonaga-Luttinger liquids , SHUNSUKE FURUKAWA, YONG BAEK KIM, Dept. of Physics, University of Toronto — We consider a system of two coupled Tomonaga-Luttinger liquids (TLL) on parallel chains and study the Rényi entanglement entropy S_n between the two chains. The limit $n \to 1$ corresponds to the von Neumann entanglement entropy. The system is effectively described by two-component bosonic field theory with different TLL parameters in the symmetric/antisymmetric channels. We argue that in this system, S_n is a linear function of the length of the chains followed by a universal subleading constant γ_n determined by the ratio of the two TLL parameters. We derive the formulae of γ_n for integer $n \geq 2$ using (a) ground-state wave functionals of TLLs and (b) conformal boundary states, which lead to the same result. These predictions are checked in a numerical diagonalization analysis of a hard-core bosonic model on a ladder. Although our formulae of γ_n are not analytic in the limit $n \to 1$, our numerical result suggests that the subleading constant in the von Neumann entropy is also universal.

2:42PM L29.00002 Entanglement from Charge Statistics: Exact Relations for Many-Body Systems , FRANCIS SONG, Yale University, CHRISTIAN FLINDT, Universite de Geneve, STEPHAN RACHEL, Yale University, ISRAEL KLICH, University of Virginia, KARYN LE HUR, Yale University — We present exact formulas for the entanglement and Rényi entropies generated at a quantum point contact (QPC) in terms of the statistics of charge fluctuations, which we illustrate with examples from both equilibrium and non-equilibrium transport. The formulas are also applicable to groundstate entanglement in systems described by non-interacting fermions in any dimension, which in one dimension includes the critical spin-1/2 XX and Ising models where conformal field theory predictions for the entanglement and Rényi entropies are reproduced from the full counting statistics. These results may play a crucial role in the experimental detection of many-body entanglement in mesoscopic structures and cold atoms in optical lattices.

2:54PM L29.00003 Quantum Monte Carlo Calculation of the Topological Entanglement Entropy in a Kagome Spin Liquid , ROGER MELKO, Waterloo, SERGEI ISAKOV, ETH Zurich, ANN KALLIN, Waterloo, MATTHEW HASTINGS, Microsoft Research and Duke — We develop a quantum Monte Carlo procedure to compute the Renyi entanglement entropy of interacting quantum many-body systems at nonzero temperature. We illustrate the method by calculating the topological entanglement entropy in a featureless Mott Insulating phase of a Bose-Hubbard model on the kagome lattice. The topological entanglement entropy displays a characteristic finite-temperature crossover behavior discussed previously in the context of the toric code. At zero-temperature it becomes the log of the quantum dimension of the topological order, confirming the existence of a Z2 spin liquid phase in the groundstate of this model.

3:06PM L29.00004 Entanglement entropy and boundary operators in quantum impurity systems , ERIK ERIKSSON, HENRIK JOHANNESSON, University of Gothenburg — Entanglement in quantum impurity systems can be studied analytically using boundary conformal field theory (BCFT). In particular, the effect from an impurity on the entanglement entropy of a surrounding region is governed by the boundary operator content of the model. We present general results for the corrections to scaling of the Rényi entanglement entropies when perturbing the BCFT with boundary operators [arXiv:1011.0448]. These results are then used to predict the asymptotic large-block behavior of the impurity contribution to the entanglement entropy in various Kondo systems.

3:18PM L29.00005 Global quantum correlations in the spin-1 bilinear-biquadratic chain , ROMAN ORUS, University of Queensland and Max Planck Institute of Quantum Optics, TZU-CHIEH WEI, University of British Columbia — We investigate global properties of the ground state of the spin-1 bilinear-biquadratic quantum spin chain in the thermodynamic limit, focusing on the geometric entanglement and fidelity diagram. The two quantities are computed via iTEBD and they appear to be capable of detecting the various well-known phase transitions in the system, including a Kosterlitz-Thouless one. The two quantities also behave distinctively at other points in the phase diagram. In particular, this is the case for the fidelity diagram at $\theta \approx 1.34\pi$ (around a possible transition to a spin nematic phase), and also for the geometric entanglement at the integrable gapped point $\theta = 3\pi/2$, where we conjecture an infinite entanglement length in the system.

3:30PM L29.00006 Definitions of entanglement entropy of spin systems in the valence-bond basis[1] , YU-CHENG LIN, Applied Physics, National Chengchi University, ANDERS SANDVIK, Physics, Boston University — The valence-bond structure of spin-1/2 Heisenberg antiferromagnets is closely related to quantum entanglement. We investigate definitions of entanglement entropy based on individual valence bonds connecting two subsystems, as well as shared loops of the transposition graph (overlap) of two valence-bond states [1]. We reformulate a previously used definition based on valance bonds in the wave function as a true ground state expectation value, and find that its scaling for the Heisenberg chain agrees with an exact result. The loop-based entanglement entropy of the two-dimensional Heisenberg model is shown to satisfy the area law (with an additive logarithmic correction), unlike single-bond definitions (which exhibit multiplicative logarithmic corrections).

[1] Y.-C. Lin and A.W. Sandvik, arXiv:1005.0821.

[1]Supported by NSC(Taiwan) Grant No. 98-2112-M-004-002-MY3, and NSF Grant No. DMR-0803510

3:42PM L29.00007 ABSTRACT WITHDRAWN –

3:54PM L29.00008 General relation between energy spectrum and entanglement spectrum , XIAOLIANG QI, Stanford University, HOSHO KATSURA, Gakushuin Univeristy, Tokyo, Japan, ANDREAS LUDWIG, University of California, Santa Barbara — We demonstrate that the bipartite density matrix, arising from a spatial bipartitioning of a gapped topological state which possesses gapless edge modes in the form of a conformal field theory (CFT) (when terminated against a topologically trivial state/vacuum), such as e.g. a general quantum Hall state, is the density matrix of a the chiral edge state CFT at a finite temperature. We obtain this result by applying a physical instantaneous cut of the gapped system, and by viewing the cutting process as a sudden "quantum quench" into a CFT, using the tools of boundary conformal field theory. In particular, we obtain a general relation between the Hamiltonian spectrum of gapless theories and the entanglement spectrum of the gapped theory obtained from coupling two gapless theories.

4:06PM L29.00009 The entanglement spectrum of perturbed Chern-Simons theories[1] , THOMAS JACKSON, ISRAEL KLICH, University of Virginia — Topological field theories — theories insensitive to the metric of the space they live on — have been shown to be applicable to a remarkable variety of condensed matter systems. A natural and important question is how perturbations relevant for real systems (interactions, etc.) deform these topological structures. In this work, we consider perturbations of Chern-Simons theory by a small Yang-Mills term, which breaks topological symmetry by introducing local bulk degrees of freedom in the form of massive gluons. We consider the behavior of the entanglement spectrum (the eigenvalues of the reduced density matrix) of this theory under this perturbation. We argue that the act of taking the partial trace may be viewed as adding a chemical potential gradient for the gluons near the boundary of the space, with a length scale determined by the gluon mass — or, colloquially, a "hot edge."

[1]Supported by NSF grant DMR 0956053

4:18PM L29.00010 Entanglement, Dissipation and the Casimir effect , ISRAEL KLICH, University of Virginia — The role of dissipation in the Casimir force between metals or dielectric has a been discussed in many works and is an important part of the Casimir theory, where puzzles about the finite temperature corrections to the effect are still being worked out. Here, we study the contribution of dissipation in creating distance dependent entanglement between materials, and on the meaning of the corresponding entropy.

4:30PM L29.00011 Entanglement Entropy Scaling of 2D Critical Wave Functions , MICHAEL ZALETEL, JENS BARDARSON, JOEL MOORE, UC Berkeley — While CFT calculations have revealed a variety of universal predictions for the entanglement spectrum of critical 1+1D field theories, much less is known about higher-dimensional systems. CFT methods can be extended to a class of 2+1D theories characterized by a $z = 2$ critical point, the so-called Rokhsar-Kivelson wave functions. The entanglement entropy of RK-type critical wave functions contains a universal logarithmic contribution $\gamma \log(L)$ for some geometries arising from a trace anomaly in the corresponding CFT. We first re-examine the free boson, where the existence of order-unity contributions that depend on the boson compactification radius has been discussed in several recent papers (Hsu et al., Stéphan et al., Oshikawa). We find analytically and numerically that the logarithmic contribution exists with the coefficient predicted by Fradkin and Moore and is independent of the compactification. However, it appears that their conjecture that general CFTs show the same dependence of γ on central charge as the free boson is incorrect. We present arguments and numerical evidence for this conclusion in $c = 1/2$ and $c = 1$ lattice models.

4:42PM L29.00012 Entanglement spectra of Hofstadter and related models , ZHOUSHEN HUANG, DANIEL AROVAS, University of California, San Diego — We compute the bipartite entanglement spectra for the Hofstadter model on various two-dimensional lattices. The behavior of the entanglement eigenstates in the vicinity of a partition boundary is investigated in detail. We also investigate the formation of entanglement edge states as one tunes through a topological phase transition in Haldane's honeycomb lattice model and other related systems.

4:54PM L29.00013 Entanglement Spectrum In Condensed Matter[1] , B. ANDREI BERNEVIG, Princeton University — I will review the information that entanglement spectra give for a wide range of systems in condensed matter physics, such as fractional quantum hall effect, quantum spin chains, topological insulators, and disordered systems. (the results are based on a series of works performed in collaboration with N. Regnault, R. Thomale, A. Chandran, A Sterdyniak, M. Hermanns, Z. Papic, T.L. Hughes, E. Prodan, D.P. Arovas)

[1] NSF

5:06PM L29.00014 Simultaneous generation of multiple quadripartite continuous-variable cluster states in the optical frequency comb of a single optical parametric oscillator , MATTHEW PYSHER, University of Virginia, YOSHICHIKA MIWA, University of Tokyo, REIHANEH SHAHROKHSHAHI, RUSSELL BLOOMER, OLIVIER PFISTER, University of Virginia — We report the experimental generation of multiple, four-mode, continuous-variable cluster states from a single optical parametric oscillator (OPO) operating below threshold. We use a PPKTP crystal phasematching two concurrent nonlinear interactions to entangle the optical frequency comb formed by the OPO cavity. Four independent entanglement witnesses (a.k.a. infinitesimal operators of stabilizers, or "nullifiers") display squeezing in each cluster state, and we utilize the large phase-matching bandwidth of the nonlinear interactions to display the simultaneous creation of several such cluster states using only a single pump frequency. A slightly more sophisticated version of this experimental method, using a crystal with three nonlinear interactions and 15 pump frequencies, has theoretically shown the ability to produce arbitrarily large square-grid cluster states suitable for universal one-way quantum computing.

5:18PM L29.00015 Multipartite entanglement in the optical frequency comb of a depleted-pump optical parametric oscillator , REIHANEH SHAHROKHSHAHI, OLIVIER PFISTER — The optical frequency comb (OFC) of a single optical parametric oscillator (OPO) has been shown to be a very interesting candidate for scaling the size of quantum entangled states. In sophisticated OPOs below threshold, square-grid cluster states of very large size can in principle be generated. Here, we study a very simple OPO well above threshold, in the linearized fluctuation approximation, and investigate the effect of pump depletion on multiple, simultaneously resonant, signal-mode pairs. We find that the depleted quantum pump mediates quantum correlations between the signal fields. These correlations lead in turn to inseparability of these fields, as evidenced by the well-known van Look-Furusawa entanglement criteria. Due to its simplicity and its scalability, this fully inseparable multipartite entangled state could used as a resource in quantum information protocols.

Tuesday, March 22, 2011 2:30PM - 5:30PM –

Session L30 DCMP: Graphene: Thermal Conduction and Phonons C147/154

2:30PM L30.00001 Thermal transport in suspended and supported monolayer graphene grown by chemical vapor deposition , WEIWEI CAI, Xiamen University, ARDEN MOORE, SHANSHAN CHEN, YANWU ZHO, Univ. of Texas at Austin, LI SHI, RODNEY S. RUOFF, Univ. of Texas at Austin — Although electron transport in graphene has been studied extensively and graphene is predicted to have very high thermal conductivity near room temperature, there is only limited experimental data in the literature on phonon transport in graphene because of experimental challenges. We report results based on micro-Raman spectroscopy for the measurement of the thermal conductivity of large-area, monolayer graphene grown by CVD on copper and subsequently suspended over a circular hole. The obtained optical absorption is measured directly by measuring the transmission through the graphene covered hole. Based on the thermal interface conductance of (28+2.8/-3.8) MW/m^2 K, the contact thermal resistance is determined to be considerably smaller than the measured thermal resistance of the suspended graphene. The obtained thermal conductivity of the supported graphene is (370 +490/-300) W/m K, which is considerably smaller than that of suspended graphene in agreement with recent measurements of mechanically exfoliated graphene supported on SiO_2.

2:42PM L30.00002 Surprising Effects of Substrate on Thermal Transport in Supported Graphene , ZHUN-YONG ONG, Physics Department, University of Illinois at Urbana-Champaign, ERIC POP, ECE Department, University of Illinois at Urbana-Champaign — We study thermal transport in graphene "supported" on SiO2 using molecular dynamics (MD) simulations. We find that coupling to the substrate leads to an order of magnitude decrease in the apparent thermal conductivity (TC), explaining recent experiments [1]. This reduction is due to the substrate damping of flexural acoustic (ZA) phonons, which implies that the high TC of isolated graphene is due to the large mean free path of long-wavelength ZA modes [2]. However, we find that by increasing the strength of the interfacial interaction, the apparent TC is enhanced by up to a factor of four. Using a continuum model [3], we relate the apparent TC enhancement to the ZA modes coupling with the substrate Rayleigh waves. In the weak coupling limit, the ZA modes have a quadratic dispersion and small group velocities at long wavelengths; in the strong coupling limit, the hybridized interfacial modes have a linear dispersion and larger group velocities. This finding suggests that the TC of supported graphene may be tunable through interfacial interaction.

[1] J. H. Seol et al., Science 328, 213 (2010)
[2] L. Lindsay et al., PRB 82, 115427 (2010).
[3] B. N. J. Persson et al., EuroPhys. Lett. 91, 56001 (2010)

2:54PM L30.00003 Two Dimensional Phonon Transport in Graphene , INSUN JO, Department of Physics, The University of Texas at Austin, JAE HUN SEOL, ARDEN L. MOORE, MICHAEL T. PETTES, Department of Mechanical Engineering, The University of Texas at Austin, LUCAS LINDSAY, Department of Physics - Boston College, NATALIO MINGO, Laboratoire d'Innovation pour les Technologies des Energies Nouvelles et les Nanomatériaux, Commissariat à l'Énergie Atomique Grenoble, DAVID BROIDO, Department of Physics - Boston College, ZHEN YAO, Department of Physics, The University of Texas at Austin, LI SHI, Department of Mechanical Engineering, The University of Texas at Austin — We present thermal conductivity measurements of monolayer graphene exfoliated on a silicon dioxide substrate at different temperatures. A nanofabricated resistance thermometer device is developed to measure the thermal conductance of graphene and supporting 300nm thick SiO_2 layer, which allows us to extract the thermal conductivity of graphene while supported on this layer. The measured value is as high as 600 W/mK near room temperature, which is lower than that of suspended graphene, 1500-5800 W/mK, but still higher than those of metal interconnects. Theoretical calculations show that the strong interface-scattering of flexural modes across the graphene-oxide interface is responsible for the decreased value.

3:06PM L30.00004 Influence of Polymeric Residue on the Thermal Conductivity of Suspended Bi-Layer Graphene[1] , MICHAEL PETTES[2], Department of Mechanical Engineering, The University of Texas at Austin, Austin, Tx, INSUN JO[3], ZHEN YAO, Department of Physics, The University of Texas at Austin, Austin, Tx, LI SHI[4], Department of Mechanical Engineering, The University of Texas at Austin, Austin, Tx — The thermal conductivity (κ) of two bi-layer graphene samples suspended between two micro-resistance thermometers was measured to be close to 600 W m^{-1} K^{-1} at room-temperature and exhibits a $\kappa \propto T^{1.5}$ behavior at temperature (T) between 50 – 125 K. The lower thermal conductivity than the basal plane values of graphite and the temperature dependence are attributed to scattering of phonons in the bi-layer graphene by a residual polymeric layer that was clearly observed by transmission electron microscopy.

[1]This work was supported by the U.S. Department of Energy award DE-FG02-07ER46377 and the National Science Foundation Graduate Research Fellowship Program (M.T.P.).

[2]These authors contributed equally.

[3]These authors contributed equally.

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3:18PM L30.00005 Phonon thermal conductivities of multi-layered graphene , LUCAS LINDSAY, Department of Physics, Computer Science, and Engineering, Christopher Newport University, Newport News, VA 23606, USA, DAVID BROIDO, Department of Physics, Boston College, Chestnut Hill, MA 02467, USA — Using an exact numerical solution of the phonon Boltzmann equation, we show that the intrinsic lattice thermal conductivities, κ, of N-layer graphene (N=1-5) are dominated by contributions from out-of-plane, flexural (ZA) phonon modes contrary to previous theories based on the relaxation time approximation, which assumed this contribution to be negligible [1, 2]. We find a reduction of κ with increasing N due to interlayer coupling, which: 1) lifts the degeneracy of the flexural acoustic mode frequencies, 2) makes the ZA phonon branch become linear near the zone-center, and 3) breaks a selection rule for anharmonic phonon-phonon scattering in two-dimensional systems.

[1] P. G. Klemens and D. F. Pedraza, Carbon vol. 32, pp. 735-741 (1994).
[2] B. D. Kong, S. Paul, M. B. Nardelli and K. W. Kim, Phys. Rev. B 80, 033406 (2009).

3:30PM L30.00006 Thermal properties of novel 2D hybrid graphene-BN nanostructures , NIKHIL MEDHEKAR, Monash University, JUN SONG, Brown University — Graphene, a 2D honeycomb carbon crystal of one-atom thickness, has been widely recognized as a very promising material for next generation optoelectronic and NEMS applications. Recent developments have shown that it is possible to obtain hybrid 2D structures by combining sp2-graphene lattice with sp2-lattice of non-carbon materials such as hexagonal Boron Nitrides. The atomically thin sheets containing both hexagonal-Boron Nitride and graphene can result in new materials with properties complementary to their individual properties and further enrich the potential applications. Here, using molecular dynamics simulations, we elucidate the characteristics of thermal transport in 2D hybride h-BN and graphene materials. We find the thermal conductivity of the hybrid material is a strong function of the relative domain widths, interface type (e.g., zigzag and armchair) as well as the interface quality. Our results provide crucial insights on the role of the interfaces and defects in phonon scattering in the hybrid material and can potentially provide means to tailor its thermal properties.

3:42PM L30.00007 Thermal Expansion in Graphene and Graphane: Role of Anharmonic and Harmonic Effects , ARUNIMA SINGH, RICHARD G. HENNIG, Department of Materials Science and Engineering, Cornell University — As the practical application of graphene nears realization, knowledge of effects of temperature on mechanical properties of graphene becomes important. In this study we use empirical potentials and density-functional perturbation theory (DFPT) to determine the thermal expansion of free-standing graphene, graphene on substrates, and its hydrogenated derivative graphane. Comparisons of MD simulations with calculations using the quasi- harmonic approximation using an empirical potential show that anharmonic effects are negligible at temperatures below 2200K. In contrast to the DFPT calculations using the quasi-harmonic approximation, MD results show that free-standing graphene has a positive thermal expansion coefficient above 600K. For graphene on a substrate our DFPT results agree with those of Jiang et. al [1] and show that the substrate suppresses the negative thermal expansion coefficient with increasing strength of the substrate- graphene interaction. We also investigate the thermal expansion of the thermodynamically stable conformers of graphane using DFPT.

[1] J. W. Jiang, J. S. Wang, B. Li, Phys. Rev. B 80, 205429 (2009).

3:54PM L30.00008 Observation of coherent G-mode phonon oscillations in graphene films , J.-H. KIM, Chungnam National University, M.H. JUNG, B.H. HONG, Sungkyunkwan University, E.H. HAROZ, J. KONO, Rice University, K.J. YEE, Chungnam National University — We have observed coherent G-mode lattice vibrations in three stacked-mono layer and multi-layer graphene films by using ultrashort pulses from a Ti:Sapphire laser. The degenerated E_{2g}modes were excited through the impulsive stimulated Raman scattering process, and detected through induced reflectivity modulations. The G-mode frequency from the stacked-mono layer graphene is shifted toward higher energy compared with that of the multi-layer graphene. A dephasing time of abound 0.6 ps for the stacked-mono layer graphene was found to be shorter than that of semiconducting single-walled carbon nanotubes (1.48 ps) and slower than that of metallic single-walled carbon nanotubes, due to stronger electron-phonon interactions, where the phonon energy can be dissipated by exciting electrons between a linear bands of graphene. Through the strong polarization dependence of coherent G-mode lattice vibrations, we confirmed that the $E_{2g}^{(2)}$ symmetry is dominant.

4:06PM L30.00009 Theory of coherent phonons in graphene[1] , G.D. SANDERS, Universiy of Florida, C.J. STANTON, University of Florida, J.-H. KIM, K.-J. YEE, Chungnam National University, M.H. JUNG, B.H. HONG, Sungkyunkwan University, E.H. HAROZ, J. KONO, Rice University — We develop a theory for the generation and detection of coherent phonons in graphene. Coherent phonons are generated via the deformation potential electron-phonon interaction with photogenerated carriers. In our theory the electronic states are treated in a third nearest neighbor extended tight binding formalism which gives a good description of the states over the entire graphene Brillouin zone while the phonon states are treated in a valence force field model. The equations of motion for the coherent phonon amplitudes are obtained in a density matrix formalism and we find that the coherent phonon amplitudes satisfy driven oscillator equations for each value of the phonon wavevector. Comparison is made with recent experimental measurements.

[1]Supported by NSF through grants OISE-0530220 and DMR-0706313 and the ONR through grant ONR-00075094, and the Robert A. Welch Foundation through grant No. C-1509.

4:18PM L30.00010 Coherent phonon spectroscopy of the shearing mode in bilayer and few-layer graphene , DAVIDE BOSCHETTO, Department of Physics, Columbia University and Laboratoire d'Optique Appliquée, ENSTA/Ecole Polytechnique, Palaiseau, LENADRO MALARD, CHUN HUNG LUI, KIN FAI MAK, HUGEN YAN, Department of Physics, Columbia University, ZHIQIANG LI, TONY F. HEINZ, Department of Physics and Electrical Engineering, Columbia University — The interlayer shearing vibration in graphite, a low-energy optical phonon, is known to consist of adjacent atomic planes moving laterally in opposite directions with respect to one another. We have applied coherent phonon spectroscopy, based on a sensitive femtosecond pump-probe measurement, to investigate the corresponding mode in few-layer graphene samples down to bilayer thickness. Here we report on the evolution of the frequency and lifetime of this mode with thickness. To model the expected behavior, we have analyzed a model of identical nearest-neighbour couplings. We find that this model predicts most of the observed reduction in frequency with decreasing layer thickness. We consider to the remaining deviations between the model and our experimental data in terms of a slight increase in the interlayer spacing, leading to a reduced restoring force, with decreasing graphene layer thickness. This decrease in lattice spacing with thickness is expected for layered materials governed by van der Waals forces. We also show experimentally that the shearing mode frequency is robust against external perturbations, such as different substrates and the presence of adlayers.

4:30PM L30.00011 Tuning the Kohn Anomaly in the Phonon Dispersion of Graphene by Interaction with the Substrate and by Doping , LUDGER WIRTZ, CNRS - IEMN, Lille, France, ADRIEN ALLARD, CNRS - IEMN, Lille, CLAUDIO ATTACCALITE, CNRS, Institut Neel, Grenoble, MICHELE LAZZERI, CNRS - IMPMC, Paris, FRANCESCO MAURI, ANGEL RUBIO, ETSF/Univ. Basque Country, San Sebastian, Spain — The phonon dispersion of graphene displays two strong Kohn Anomalies (kinks) in the highest optical branch (HOB) at the high-symmetry points G and K. The slope of the HOB around K is a measure of the electron-phonon coupling (EPC) and determines the dispersion of the Raman D and 2D lines as a function of the laser energy. We show that the EPC can be strongly modified both due to interaction with a metallic substrate and due to doping. For graphene grown on a Ni(111) surface, a total suppression of the Kohn anomaly occurs: the HOB around K becomes completely flat. This is due to the strong hybridization of the graphene p-bands with the Nickel d-bands which lifts the linear crossing of the p-bands at K. From experimental phonon dispersions one can therefore draw conclusions about the interaction strength between graphene and its different substrates. Furthermore, we present a new way to tune the EPC in graphene through electron/hole doping. We show that for the highest optical branch at K, the EPC is strongly dependent on the doping level. This dependency influences the dispersion of the Raman D and 2D lines and makes it possible to measure the charge state of graphene via resonant Raman spectroscopy.

4:42PM L30.00012 Thermoelectric effect in high mobility single layer epitaxial graphene[1] , XIAOSONG WU, YIKE HU, MING RUAN, NERASOA K. MADIOMANANA, CLAIRE BERGER, WALT A. DE HEER, School of Physics, Georgia Tech — The thermoelectric response of high mobility single layer epitaxial graphene on silicon carbide substrates as a function of temperature and magnetic field have been investigated. For the thermopower, a strong deviation from the Mott relation, i.e. a quardratic correction to the linear temperature dependence, has been observed even when the carrier density is high. In the quantum Hall regime, the amplitude of the TEP peaks is lower than a quantum value predicted by theories, despite the high mobility of the sample. A systematic reduction of the amplitude with decreasing temperature suggests that the suppression of the TEP is intrinsic to Dirac electrons in graphene.

[1]This work was supported by NSF grant DMR-0820382 and the W. M. Keck Foundation.

4:54PM L30.00013 Thermoelectric transport in graphene with tunable mobility[1] , XINFEI LIU, Physics Deaprtment, UC Riverside, DEQI WANG, JING SHI, Physics Department, UC Riverside — Thermoelectric transport properties of single layer graphene have recently been studied both experimentally and theoretically. The unique band structure of graphene leads to unusual thermoelectric properties which are very sensitive to the carrier mobility. However, all previous experiments were carried out in graphene devices with different mobility values and comparisons were drawn among different devices. Recently, we have shown that by controlling the charge state of the ligand-bound nanoparticles on graphene it is possible to tune the mobility of the same graphene device over a wide range, e.g. 5000-19000cm^2/Vs. In this work, we adopted this method and successfully tuned the mobility of graphene while systematically studied the Seebeck and Nernst effects in a magnetic field up to 14 Tesla for each fixed mobility value. Our results show that at zero magnetic field, the width of the transition region near the Dirac point decreases sharply and the diverging behavior in the Seebeck coefficient becomes more pronounced as the mobility is tuned from low to high. At high magnetic fields, the Seebeck coefficient in the high mobility state clearly reveals additional features that are related to the splitting of the zeroth Landau level near the Dirac point. Moreover, we demonstrate that the Nernst peak height at the Dirac point depends linearly on the carrier mobility in graphene.

[1]This work was supported in part by a DOE grant.

5:06PM L30.00014 Thermoelectric Properties of Graphene Ribbons[1] , ENRIQUE MUNOZ, Instituto de Fisica, Pontificia Universidad Catolica de Valparaiso, Chile — Several theoretical and experimental studies have been recently concerned with electric and thermal transport in graphene layers and ribbons, where propagation of electrons [1] and phonons [2] seems to be dominated by a ballistic mechanism. Of particular interest in this context is the identification and characterization of thermoelectric effects [3], which represent a promising alternative for energy recovery in technological applications. In the present work, the effect of the electron- phonon interaction over a predominantly ballistic transport mechanism in graphene ribbons is studied in the context of thermoelectricity. Theoretical estimations of the thermopower S, and the corresponding figure of merit ZT, are presented for this system as a function of temperature.

[1] K. Saito, J. Nakamura, and A. Natori, "Ballistic thermal conductance of a graphene sheet," Phys. Rev. B 76, 115409 (2007).
[2] E. Munoz, J. Lu, and B. I. Yakobson, "Ballistic thermal conductance of graphene ribbons," Nano Lett. 10, 1652 (2010).
[3] Y. Ouyang and J. Guo, "A theoretical study on thermoelectric properties of graphene nanoribbons," Appl. Phys. Lett. 94, 263107 (2009).

[1]I acknowledge financial support from the grant Fondecyt de Iniciacion 11100064.

5:18PM L30.00015 Theromelectricity in Graphene: Effects of a gap and magnetic fields[1] , SUBROTO MUKERJEE, Indian Institute of Science, Bangalore India, AAVISHKAR PATEL, Indian Institute of Technology, Kanpur India — We calculate the thermopower of monolayer graphene in various circumstances. First we show that experiments on the thermopower of graphene can be understood quantitatively with a very simple model of screening in the semiclassical limit. We can calculate the energy dependent scattering time for this model exactly. We then consider acoustic phonon scattering which might be the operative scattering mechanism in free standing films, and predict that the thermopower will be linear in any induced gap in the system. Further, the thermopower peaks at the same value of chemical potential (tunable by gate voltage) independent of the gap. Finally, we show that in the semiclassical approximation, the thermopower in a magnetic field saturates at high field to a value which can be calculated exactly and is independent of the details of the scattering. This effect might be observable experimentally.

[1]The authors acknowledge support from the Department of Science and Technology of the Government of India

Tuesday, March 22, 2011 2:30PM - 5:30PM –

Session L31 DMP GSCCM DCOMP: Focus Session: Materials at High Pressure III: Electronic Transitions C145

2:30PM L31.00001 Pressure Induced Metal Insulator Phase Transition in $Eu_2Ir_2O_7$, FAZEL FALLAH TAFTI, JUN ISHIKAWA, YO MACHIDA, ALIX MCCOLLAM, SATORU NAKATSUJI, STEPHEN JULIAN — The metal to insulator phase transition of the pyrochlore iridate $Eu_2Ir_2O_7$ has been studied by means of resistivity measurements under pressure in the range 2 to 12 GPa. At ambient pressure, the system is a "metal" at high temperatures with a non-metallic rise of resistivity with decreasing temperature followed by a metal-insulator phase transition at T_{MI} below which it becomes insulating. With increasing pressure, a cross-over from non-metallic to metallic appears in the resistivity curves at a temperature $T^* > T_{MI}$. As the pressure is further increased T^* rises, T_{MI} drops and the low temperature insulating phase melts into a metallic phase through a continuous transition at P $\sim$ 7.8 GPa. The high pressure metallic phase is rather curious and exhibits two characteristic features of Kondo metals: a minimum resistivity and a logarithmic rise of resistivity at low temperatures. We will show that there is a remarkable correspondence between the resistivity curves measured at various pressures and those obtained by successively replacing the R site of the $R_2Ir_2O_7$ family by larger rare earth atoms.

2:42PM L31.00002 Pressure-induced Metallization of Carbon Disulfide[1] , RANGANATH DIAS, Institute for Shock Physic, Dept. of Physics, Washington State University, Pullman, WA 99164 , MATHEW DEBESSAI , Institute for Shock Physic, Washington State University, Pullman, WA 99164 , CHOONG-SHIK YOO, Institute for Shock Physics, Dept. of Chemistry, Washington State University, Pullman, WA 99164 — We will report high pressure electrical resistivity measurements on solid CS_2 in diamond anvil cell to 60GPa. The result shows a steady decrease in resistivity to that of metal at around 55GPa. Its visual appearance of CS_2 also supports its insulator-metal transition: the initially transparent CS_2 becomes opaque and eventually reflective with increasing pressure. We will also present a plausible mechanism for the observed metallization.

[1]The work has been supported by NSF (DMR-0854618) and DTRA (HDTRA1-09-1-0041).

2:54PM L31.00003 Electrical resistance measurement of optimal doped YBCO under pressure , TAKAKI MURAMATSU, TcSUH, University of Houston, DUC PHAM TEAM, CHING-WU CHU TEAM — High pressure effect on nearly optimal doped high T_C cuprate superconductor $YBa_2Cu_3O_{7-x}$ was studied by the electrical resistance measurements up to about 30 GPa. Superconducting phase of $YBa_2Cu_3O_{7-x}$ in pressure-temperature phase diagram was confirmed. T_C has the broad maximum at about 8 GPa and then decreases with pressure and disappears at the pressure between 23 GPa and 25 GPa. In higher pressure region, the resistance shows upturn below about 60 K, indicating the possibility of crossover on $YBa_2Cu_3O_{7-x}$ from superconductor to semiconductor at about 24 GPa

3:06PM L31.00004 Pressure induced phase transition in FeGa alloys , CHRISTOPHER DEVREUGD, Virginia Tech University, MUHTAR AHART, Carnegie Institution of Washington, PETER GEHRING, NIST Center for Neutron Research, DWIGHT VIEHLAND, Virginia Tech University, RUSSELL HEMLEY, Carnegie Institution of Washington — Giant magnetostriction in Fe– x Ga alloys (15 – x - 27) offers potential for future generations of sensors and actuators. A maximum in the magnetostrictive strain is found at Ga content of about 19 percent, which is ten times higher than that of pure alpha-Fe. To investigate the behavior of FeGa alloys under pressure, we chose a slow cooled alloy of FeGa-19 as our sample and performed x-ray diffraction experiments in a diamond anvil cell up to 45 GPa. Diffraction pattern shows powder rings associated with (110), (200), and (211) Bragg reflections from expected bcc structure of iron below 24 GPa. We also observed the intensity increases along the powder rings associated with the crystal structure of Galfenol. Considering the (110) Bragg peak splits into three peaks above 24 GPa, our results indicate that FeGa alloy undergoes a bcc cubic to a hexagonal transition around 24 GPa. When the pressure is decreased, the hcp phase transforms back to the bcc phase. The transition mechanism can be understood by using the analogy to the bcc-hcp phase transition in pure iron under pressure. The transition in iron is a martensitic or displacive one. The hcp structure can be derived from the bcc structure through a relatively minor distortion of the bcc structure.

3:18PM L31.00005 High Pressure Studies of UO_3[1] , ZSOLT JENEI, MAGNUS LIPP, JAE-HYUN KLEPEIS, BRUCE BAER, HYUNCHAE CYNN, WILLIAM EVANS, Lawrence Livermore National Laboratory, CHANGYONG PARK, DIMITRI POPOV, HPCAT, Advanced Photon Source, Argonne National Laboratory — It has been reported that upon compression t ambient temperature δ-UO3 becomes amorphous at 2.2 GPa. (Journal of Alloys and Compounds 315 p59–61). We studied the properties of γ-UO3 in diamond anvil cell up to 75 GPa. Powder diffraction experiments performed at HPCAT/Advanced Photon Source show the crystalline uranium trioxide transforms to an amorphous solid between 12 and 14 GPa and remains amorphous up to 75 GPa. The transition has been confirmed by Raman spectroscopy as well. In this paper we'll present our findings on the amorphous transition together with the equation of state of both the crystalline phase and the amorphous phase.

[1]This work performed under the auspices of the US DOE by LLNL under Contract DE-AC52-07NA27344 HPCAT is supported by CIW, CDAC, UNLV and LLNL through funding from DOE-NNSA, DOE-BES and NSF. APS is supported by DOE-BES, under Contract No. DE-AC02-06CH11357.

3:30PM L31.00006 High-pressure equation of state of U_3O_8[1] , JAE-HYUN KLEPEIS, ZSOLT JENEI, MAGNUS LIPP, WILLIAM EVANS, Lawrence Livermore National Laboratory, DMITRY POPOV, HPCAT, APS, Argonne National Laboratory, CHANGYONG PARK, HPCAT APS Argonne National Laboratory — We will present experimental studies at high pressures of the equation of state of U_3O_8. Isothermal pressure-volume measurements of U_3O_8 were made at ambient/elevated (600 K) temperatures in the pressure range of 1 atm $\sim$ 80 GPa (10 $\sim$ 70 GPa). Angle dispersive X-ray diffraction patterns at ambient temperature indicate that the A-centered orthorhombic structure of U_3O_8 transforms to the face centered cubic (fcc) structure above 9 GPa. Both the orthorhombic and cubic phases co-exist between 9 GPa and 30 GPa. As the temperature is increased at 10 GPa, we find that U_3O_8 also transforms to the fcc structure. As the pressure is increased at 600 K, the fcc structure undergoes a phase transition to the body centered tetragonal structure. Since the uranium in U_3O_8 is the dominant x-ray scatterer, the behavior of the oxygen at the phase transitions was measured using Raman spectroscopy.

[1]This work was performed under the auspices of the US DOE by LLNL under Contract DE-AC52-07NA27344. HPCAT is supported by CIW, CDAC, UNLV and LLNL through DOE-NNSA, DOE-BES and NSF. APS is supported by DOE-BES, under Contract DE-AC02-06CH11357.

3:42PM L31.00007 High pressure x-ray diffraction of uranium oxide formed by natural oxidation of uranium[1] , HYUNCHAE CYNN, WILLIAM J. EVANS, BRUCE J. BAER, Lawrence Livermore National Laboratory, SIMON MACLEOD, Atomic Weapons Establishment, MAGNUS J. LIPP, ZSOLT JENEI, J.H. PARK KLEPEIS, Lawrence Livermore National Laboratory, YUE MENG, STANISLAV SINOGEIKIN, HP-CAT, APS — Naturally oxidized uranium has been compressed using a diamond anvil cell. Although X-ray diffraction shows the anisotropic nature in the pressure dependent changes to the lattice parameters of pure uranium as previously recorded, uranium oxide appears stable at high pressure in the fluorite structure with no clear evidence of a phase transition observed above the transition pressure previously measured for bulk uranium oxide. The lattice parameters of uranium oxide formed by natural surface oxidation have been determined along with those of the underlying pure uranium employing Rietveld refinement. We will discuss the seemingly unexpected findings about uranium oxide.

[1]Work performed under the auspices of the US DOE by LLNL under Contract DE-AC52-07NA27344. Diffraction studies were performed at HPCAT (Sector 16), APS/ANL. HPCAT is supported by CIW, CDAC, UNLV and LLNL through funding from DOE-NNSA, DOE-BES and NSF. APS

3:54PM L31.00008 Uranium hydride (UH_3) and deuteride (UD_3) under conditions of high pressure and temperature , MAGNUS LIPP, ZSOLT JENEI, JAE HYUN PARK KLEPEIS, BRUCE BAER, HYUNCHAE CYNN, WILLIAM EVANS, DON FUJINO, Lawrence Livermore National Laboratory, BLAKE NOLAN, JOE WERMER, Los Alamos National Laboratory, CHANGYONG PARK, DMITRY POPOV, HPCAT, Advanced Photon Source, Argonne National Laboratory — Uranium hydrides are currently being evaluated as fuels in new reactor designs. They also serve as sources for very clean hydrogen by decomposing when heated at ambient pressure. We have examined their behavior over a large pressure and temperature range by placing small quantities and a pressure marker in a diamond anvil cell for angle dispersive x-ray diffraction. Neon was chosen as pressure transmitting medium to ensure the best possible hydrostatic conditions. We'll discuss crystal structures, the equation of state, the bulk modulus and the phase diagram. Work performed under the auspices of the US DOE by LLNL under Contract DE-AC52-07NA27344. Diffraction studies were performed at HPCAT (Sector 16), APS/ANL. HPCAT is supported by CIW, CDAC, UNLV and LLNL through funding from DOE-NNSA, DOE-BES and NSF. APS is supported by DOE-BES, under Contract No. DE-AC02-06CH11357.

4:06PM L31.00009 Structural Stabilities and Electronic Properties of Cobalt Hydrides , YASUYUKI MATSUURA, TATSUYA SHISHIDOU, ADSM, Hiroshima University, TAMIO OGUCHI, ISIR, Osaka University, ADSM, Hiroshima University — Cobalt forms ferromagnetic hydrides CoH_x at high pressures of hydrogen [1]. As the hydrogen pressure increases at temperatures 250-350°C, the concentration of hydrogen in the hcp phase monotonically increases, and reaches $x \sim 0.6$ at 7 GPa. At higher pressures, an fcc-based hydride with $x \sim 1.0$ is formed. At ambient pressure and 120 K, hydrogen atoms in the solution with $x \leq 0.26$ are randomly distributed over octahedral interstitial sites [2]. In the solution with $x = 0.34$ ($x \geq 0.38$), hydrogen atoms occupy every third (second) layer. The magnetic moments of the hcp-based hydrides are oriented to the c-axis, and are decreased with increasing hydrogen concentration at a rate of about 0.36 μ_B per hydrogen atom. In this study, we optimize the structural parameters for several structures, and investigate the structural stabilities and related electronic properties by using first-principles calculations. The full-potential linearized augmented plane wave method with the generalized gradient approximation is adopted.

[1] V. E. Antonov, J. Alloys Compd. **330-332**, 110 (2002).
[2] V. K. Fedotov, V. E. Antonov, T. E. Antonova, E. L. Bokhenkov, B. Dorner, G. Grosse, and F. E. Wagner, J. Alloys Compd. **291**, 1 (1999).

4:18PM L31.00010 Formation of collapsed tetragonal phase in $EuCo_2As_2$ under high pressure[1] , MATTHEW BISHOP, University of West Georgia (UWG), Carrollton, GA 30118, USA, WALTER UHOYA, GEORGIY TSOI, YOGESH VOHRA, University of Alabama at Birmingham (UAB), Birmingham, AL 35294, USA, ATHENA SEFAT, BRIAN SALES, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN 37831, USA — The structural properties of $EuCo_2As_2$ have been studied up to 35 GPa, through the use of x-ray diffraction in a diamond anvil cell at a synchrotron source. At ambient conditions, $EuCo_2As_2$ ($I4/mmm$) has a tetragonal lattice structure with a bulk modulus of 48 $\pm$ 4 GPa. With the application of pressure, the $a$axis exhibits negative compressibility with a concurrent sharp decrease in c-axis length. The anomalous compressibility of the $a$axis continues until 4.7 GPa, at which point the structure undergoes a second-order phase transition to a collapsed tetragonal (CT) state with a bulk modulus of 111 $\pm$ 2 GPa. We found a strong correlation between the ambient pressure volume of 122 parents of superconductors and the corresponding tetragonal to collapsed tetragonal phase transition pressures.

[1]MB acknowledges support from the National Science Foundation (NSF) Research Experiences for Undergraduates (REU)-site under grant no. NSF-DMR-06446842.

4:30PM L31.00011 The behavior of semi-metal Bi_4Te_3 under pressure , JASON JEFFRIES, Lawrence Livermore National Laboratory, A.L. LIMA SHARMA, Sandia National Laboratory and San Jose State University, P.A. SHARMA, C.D. SPATARU, Sandia National Laboratory, S.K. MCCALL, Lawrence Livermore National Laboratory, J.D. SUGAR, Sandia National Laboratory, S.T. WEIR, Lawrence Livermore National Laboratory, Y.K. VOHRA, University of Alabama, Birmingham — As a member of the $(Bi_2)_m(Bi_2Te_3)_n$ adaptive series, Bi_4Te_3 exhibits identical crystallographic symmetry and similar electronic properties to the archetypal thermoelectric material Bi_2Te_3. The extra Bi atoms in Bi_4Te_3 serve to increase the electronic density of states, making Bi_4Te_3 a semi-metal, as opposed to semiconducting Bi_2Te_3, at ambient pressure. We will report the results of high-pressure structural and magnetotransport characterization of Bi_4Te_3, focusing on the interplay between structural parameters and the underlying electronic properties. Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration under Contract DE-AC52-07NA27344.

4:42PM L31.00012 Theoretical X-ray Spectroscopy for Strongly Correlated Materials at High Pressure[1] , ADAM P. SORINI, CHENG-CHIEN CHEN, SHIBING WANG, WENDY L. MAO, THOMAS P. DEVEREAUX, Stanford Institute for Materials and Energy Science, CHI-CHANG KAO, SSRL, SLAC National Acclererator Laboratory — We present theoretical x-ray spectra for correlated d- and f-electron materials under extreme conditions. We use exact-diagonalization to study small clusters of atoms including ligand charge-transfer and atomic-multiplet effects. These techniques allow us to extract information from spectroscopic measurements regarding phase transitions in strongly correlated materials as a function of pressure. We show recent results for hematite (Fe2O3) which undergoes a variety of phase transitions (structural, spin, metal/insulator) near 50 GPa, which have been observed using hard x-ray quadrupolar absorption. We also apply our models to the correlated f-electron "volume collapse" systems which show complex behavior under pressure.

[1]DOE Grant No. DE-AC02-76SF00515 and No. DE-FG02- 08ER46540

4:54PM L31.00013 Fermi surface of SnO under pressure , NIELS CHRISTENSEN, AXEL SVANE, Aarhus University — Tin monoxide undergoes a pressure induced insulator-metal transition around 5 GPa. The pressure effects on the electronic band structure, the Fermi surface (FS) and its nesting properties of SnO in the metallic phase have been derived from ab initio calculations within the local density (LDA) and quasiparticle selfconsistent GW (QSGW) approximations. It is found that the topologies of the FS determined by the two approaches are very similar. Nesting occurs between two different sheets of the FS, most pronounced via (1,1,0) Q- vectors connecting the outer electron surface with the hole surface The present study was motivated by recent observation of superconductivity in SnO under pressure [1].

[1] M.K. Forthaus el al., Phys. Rev. Lett. **105**, 157001 (2010).

5:06PM L31.00014 Dynamic response of Cu46Zr54 metallic glass to high-strain-rate shock loading: Plasticity, spall, and atomic-level structures , BEDRI ARMAN, Texas A&M, SHENG-NIAN LUO, TIMOTHY GERMANN, Los Alamos National Laboratory, TAHIR CAGIN, Texas A&M — Dynamic response of Cu46Zr54 metallic glass under adiabatic planar shock wave loading with molecular dynamics simulations was investigated. We analyzed the Hugoniot (shock) states up to 60 GPa, shock-induced plasticity and dynamic spall strengths. Especially, the spall strengths likely represent the limiting values achievable in experiments such as laser ablation. To characterize local deformation and structure at various stages of shock, release, tension and spallation, the local von Mises shear strain and Voronoi tessellation analyses were used. Modeled glass showed plasticity as localized shear transformation zones rather than thermal origin. Nucleation of voids occurred preferentially at the highly shear-deformed regions. Our simulations through the Voronoi and shear strain analyses suggest that the atoms having different local structures are of different shear resistances that lead to shear localization.

5:18PM L31.00015 Single Crystal X-ray Diffraction at Megabar Pressures and Temperatures of Thousands Degrees , LEONID DUBROVINSKY, NATALIA DUBROVINSKAIA, MARCO MERLINI, MICHAEL HANFLAND — The most reliable information about crystal structures and their response to changes in pressure and temperature is obtained from single crystal diffraction experiments. We have developed a methodology to perform single crystal X-ray diffraction experiments in laser-heated diamond anvil cells and demonstrate that structural refinements and accurate measurements of the thermal equation of state of metals, oxides, silicates from single crystal intensity data are possible in a pressures ranging up to megabars and temperatures of thousands degrees. New methodology was applied to solve *in situ* high-pressure high-temperature structure of iron oxide and study structural variations of iron and aluminum bearing silicate perovskite at conditions of the Earth lower mantle.

Tuesday, March 22, 2011 2:30PM - 5:30PM –

Session L32 DMP: Focus Session: Nano-Optics, Semiconductor and Metal Nanostructures C144

2:30PM L32.00001 Linear Optical and SERS Study on Metallic Membranes with Subwavelength Complementary Patterns , QINGZHEN HAO, YONG ZENG, LASSE JENSEN, DOUGLAS WERNER, VINCENT CRESPI, TONY JUN HUANG, Pennsylvania State University, INTERDEPARTMENTAL COLLABORATION — An efficient technique is developed to fabricate optically thin metallic films with subwavelength patterns and their complements simultaneously. By comparing the spectra of the complementary films, we show that Babinet's principle nearly holds in the optical domain. A discrete-dipole approximation can qualitatively describe their spectral dependence on the geometry of the constituent particles and the illuminating polarization. Using pyridine as probe molecules, we studied surface-enhanced Raman spectroscopy (SERS) from the complementary structure. Although the complementary structure posses closely related linear spectra, they have quite different near-field behaviors. For hole arrays, their averaged local field gains as well as the SERS enhancements are strongly correlated to their transmission spectra. We therefore can use $\cos^4\theta$ to approximately describe the dependence of the Raman intensity on the excitation polarization angle θ, while the complementary particle arrays present maximal local field gains at wavelengths generally much bigger than their localized surface plasmonic resonant wavelengths.

2:42PM L32.00002 Optically controlled patchy modification of metal nanoparticles , STEFAN STOIANOV, JASON RIDLEY, BRANDON THORPE, WEBSTER SANTOS, HANS ROBINSON, Virginia Polytechnic Institute and State Univeristy — It is well known that that metal nanostructures strongly concentrate light intensity at hot spots located at sharp corners or in narrow gaps, either due to plasmonic resonances or the lightning-rod effect. This is exploited a several important applications, such as surface enhanced Raman spectroscopy (SERS) and apertureless NSOM. We propose using this phenomenon to induce photochemical reaction on the surface of metal nanoparticles, leading to differential, or patchy, functionalization of the particles. We have functionalized gold and silver nanoparticles fabricated using nanosphere lithography with ligands that contain o-nitrobenzyl functional groups. Upon absorption of a photon, these compounds cleave off, leaving behind a modified surface. Differential functionalization will be demonstrated by comparing the rate of photoreactions at the hotspots (measured with SERS) to the average cleavage rate (measured with FTIR).

2:54PM L32.00003 ABSTRACT WITHDRAWN –

3:06PM L32.00004 TDDFT studies of plasmonic excitations in small transition metal-doped gold chains[1] , NEHA NAYYAR, ALAMGIR KABIR, Department of Physics Univ. of Central Florida, VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Department of Physics and NSTC Univ. of Central Florida — We apply a TDDFT approach to study the absorption spectra of pure Au chains and those doped with transition metal (TM) atoms (Ni, Rh, Fe) up to 24 atoms. We find that for gold chains with more than 10 atoms a collective plasmon mode is formed whose intensity grows with the number of atoms. The plasmon energy approaches asymptotically a value of 0.6eV when the number of atoms is about 20. However, in the chains with odd number of atoms, an additional low-energy excited state close to the plasmonic peak is found which can be related to an excitation at the chain edge. Doping with TM atoms also leads to the formation of additional plasmon peaks close in energy to the main one, especially pronounced in the case of Ni- doped chains. We compare the results for the optical absorption spectrum of the system in the case of doping by different TM atoms and the role of the d-electron states of these atoms in formation of the additional plasmon peaks.

[1]Work supported in part by DOE Grant No. DOE-DE-FG02-07ER46354

3:18PM L32.00005 ABSTRACT WITHDRAWN –

3:30PM L32.00006 Ultrafast photoconductive response of $LaAlO_3/SrTiO_3$ nanoscale photodetectors[1] , YANJUN MA, CHENG CEN, University of Pittsburgh, CHUNG WUNG BARK, CHAD M. FOLKMAN, CHANG-BEOM EOM, University of Wisconsin-Madison, JEREMY LEVY, University of Pittsburgh — Conducting AFM lithography can be used to create nanoscale field effect transistors at the $LaAlO_3/SrTiO_3$ interface.[2,3] Such devices exhibit gatable photoconductive response, which spans from visible to near-infrared regime.[4] By implementing the pump-probe measurement with a home-built femtosecond laser, we observe an ultrafast nonlinear optical response of these nanoscale photodetectors. We explore the feasibility of these devices for molecular-scale THz spectroscopy applications.

[1]This work was supported by NSF DMR-0704022 (J.L.), DARPA W911NF-09-10258 (J.L.), the Fine Foundation (JL), NSF DMR-0906443 (C.B.E.) and David and Lucile Packard Fellowship (C.B.E.)

[2]C. Cen et al., Nature Material, 7, 2136(2008)

[3]C.Cen et al., Science, 323, 1026 (2009)

[4]P.Irvin et al., Nature Photonics advanced online publication, 14 Nov.2010 (DOI 10.1038/nphoton.2010.238)

3:42PM L32.00007 Infrared and Terahertz Nanoscopy , RAINER HILLENBRAND, CIC nanoGUNE Consolider — During the last years, near-field microscopy based on elastic light scattering from atomic force microscope tips (scattering-type scanning near-field optical microscopy, s-SNOM [1]) has become a powerful tool for nanoimaging of local dielectric material properties [2-5] and optical near fields of photonic nanostructures [6-8]. After an introduction of s-SNOM, I will discuss recently developed applications in materials sciences and nanophotonics. I will focus particularly on IR and THz imaging at wavelengths λ around 10 and 118 μm, where we typically achieve a wavelength-independent resolution better than 40 nm, corresponding to $\lambda/250$ and $\lambda/3000$, respectively [3]. Using metal-coated tips, the strong field enhancement at the tip apex probes the local dielectric properties of a sample, allowing for the simultaneous recognition of materials and free-carrier concentration in semiconductor nanodevices [3] and nanowires [5]. Quantitative free-carrier mapping is enabled by near-field plasmon-polariton spectroscopy, which can be also applied to study strain-induced changes of carrier concentration and mobility [4]. Nanoscale imaging of strain and nanocracks in ceramics can be achieved by near-field infrared phonon-polariton spectroscopy [4]. I will also discuss the capability of s-SNOM to image the vectorial near-field distribution of photonic nanostructures. In this application, a dielectric tip scatters the near fields at the sample surface. I will discuss how the amplitude and phase-resolved measurement of different near-field components allows for mapping of the polarization state in nanoscale antenna gaps [8], of near-field modes in loaded infrared gap antennas [7] and of mid-infrared energy transport in nanoscale transmission lines.

[1] F. Keilmann, R. Hillenbrand, Phil. Trans. R. Soc. Lond. A 362, 787 (2004).
[2] R. Hillenbrand et al., Nature 418, 159 (2002).
[3] A. Huber et al., Nano Lett. 8, 3766 (2008).
[4] A. Huber et al., Nature Nanotech. 4, 153 (2009).
[5] J.M. Stiegler et al., Nano Lett. 10, 1387 (2010).
[6] T. Taubner et al. Science 313, 1595 (2006).
[7] M. Schnell et al., Nature Photon., 3, 287 (2009).
[8] M. Schnell et al., Nano Lett., 10, 3524 (2010).

4:18PM L32.00008 Single GaN nanowire polariton luminescence , AYAN DAS, MARC JANKOWSKI, WEI GUO, PALLAB BHATTACHARYA, University of Michigan, Ann Arbor — Polariton emission from a single GaN nanowire in the strong coupling regime has been investigated in the temperature range of 200-300 K. GaN nanowires grow in the wurtzite structure with the c-axis along the growth direction. The polariton dispersion characteristics are determined from angle-resolved reflectivity measurements. The light emission characteristics measured as a function of incident optical power density reveal a distinct non-linear behavior and threshold, accompanied by a sharp decrease in linewidth over an order of magnitude and a small blue-shift that is ascribed to polariton-polariton interactions. Angle-resolved photoluminescence measurements above threshold indicate polariton cooling to the bottom of the lower polariton branch, triggered by the onset of stimulated scattering which is characterized by a fast relaxation time as obtained from time resolved photoluminescence measurements. Emission above threshold is linearly polarized. Second order correlation measurements and interferomtery indicate significant bunching below threshold and a coherent emission above threshold. These measurements indicate a coherent emission. Photon lasing due to carrier population inversion is observed at higher pump power densities.

4:30PM L32.00009 Photoreflectance spectroscopy of single GaAs/GaP Core-shell Nanowires[1] , A. WADE, M. MONTAZERI, M.A. FICKENSCHER, H.E. JACKSON, L.M. SMITH, University of Cincinnati, J.M. YARRISON-RICE, Miami University, J.H. KANG, Q. GAO, H.H. TAN, C. JAGADISH, Australian National University — We present a direct observation of the light hole (lh) and heavy hole (hh) valence band splitting in highly strained GaAs/GaP core/shell nanowires obtained by photoreflectance (PR) from a single nanowire. The NWs were prepared by Au nanoparticle (100 nm) catalyst-assisted MOCVD growth with two different shell thicknesses, where the induced strain is controlled varying the core/shell ratio. They were then dispersed on silicon for the PR measurement. The spectra show a $\sim$140eV splitting of the lh and hh bands for two different wires. Raman spectroscopy was carried out on the same growths in order to measure the hydrostatic and shear strain [1]. From the measured strain we calculate the hh and lh splitting and find them to be in reasonable agreement with PR.

[1] M. Montazeri, et. al., Nano Letters 10, 880-886 (2010).

[1]Supported by the NSF (0701703, 0806700, 0806572) and the Australian Research Council.

4:42PM L32.00010 Photoreflectance measurements of single wurtzite InP nanowires , M. MONTAZERI, A. WADE, S. PERERA, K. PEMASIRI, L.M. SMITH, H.E. JACKSON, University of Cincinnati, J.M. YARRISON-RICE, Miami University, S. PAIMAN, Q. GAO, H.H. TAN, C. JAGADISH, Australian National University — We have carried out photoreflectance measurements from a single semiconductor nanowire for the first time to our knowledge. We show that photoreflectance is an easy, quick and nondestructive technique which could be used to study the electronic band structure of a single semiconductor nanowire at both room and low temperatures. We have used photoreflectance to study electronic band structure of single wurtzite InP nanowires at room and low temperatures. Nanowires were grown by MOCVD using 100nm Au-nanoparticle catalysts. Derivative like features in the photoreflectance spectrum around the fundamental gaps allow us to extract energies of 1.50eV, 1.53eV and 1.70eV for A, B and C excitons of wurtzite an InP nanowire at low temperature. These values are compared to values obtained by photoluminescence-excitation and photocurrent measurements. Supported by the NSF (#0701703, #0806700 and #0806572) and the Australian Research Council.

4:54PM L32.00011 Investigation of Electronic Structure in Wurtzite InP Nanowires , SARANGA PERERA, K. PEMASIRI, M. FICKENSCHER, A. WADE, L.M. SMITH, H.E. JACKSON, University of Cincinnati, J.M. YARRISON-RICE, University of Miami, Oxford OH, S. PAIMAN, Q. GAO, H. TAN, C. JAGADISH, Australian National University — We use photoluminescence excitation (PLE), time-resolved photoluminescence (PL), and CW photoluminescence to investigate the electronic structure of wurtzite InP nanowires (NWs) as a function of diameter (30, 50, 100 nm) at 10 K. The NWs were prepared by Au catalyst-assisted MOCVD growth with a 420°C growth temperature and a V/III ratio of 700. A tunable Titanium-Sapphire laser was used to excite the nanowire sample. PL from the NWs show a dominant defect line near 840nm (1.475eV) that obstructs the view of the free exciton line which should be around 824nm (1.504eV). PLE was performed by measuring the intensity of the defect emission as a function of the excitation laser. The laser was polarized parallel and perpendicular to the nanowire and the PL was collected with circular polarization. PLE spectra show three peaks for the A, B and C hole bands (*APL* **97**, 023106-2010). Polarization measurements may probe optical selection rules. Support for this work was provided by the NSF (0701703, 0806700 and 0806572) and the Australian Research Council.

5:06PM L32.00012 Photoluminescence in Strain-Engineered Si/SiGe Three Dimensional Nanostructures , NIKHIL MODI, New Jersey Institute of Technology, ECE Department, Newark NJ 07102 USA, LEONID TSYBESKOV, New Jersey Institute of Technology, ECE Department, Newark NJ 07102, USA, DAVID LOCKWOOD, XIAO WU, JEAN-MARC BARIBEAU, National Research Council, Institute for Microstructural Sciences, Ottawa ON, Canada — The effect of strain on the degeneracy of energy band minima in composition-controlled Si/SiGe nanostructures with high germanium content ($\sim$ 50%) is studied by low temperature photoluminescence (PL) spectroscopy, ultra-high resolution transmission electron microscopy and energy dispersive X-ray spectroscopy measurements. PL spectra obtained from selective excitation of the multilayered nanostructures show a reduction in the strained-silicon fundamental energy bandgap and a splitting of energy levels presumably associated with partial removal of two-fold degeneracy of the SiGe valence band. PL kinetics recorded using different excitation wavelengths show dramatically different PL lifetimes, ranging from $\sim$ 2 μs to $<$ 10 ns. We show that it is possible to obtain high quantum efficiency luminescence at 1.3-1.6 μm.

5:18PM L32.00013 State filling dependent tunneling in hybrid InAs/GaAs-InGaAs/GaAs dot-well structures , VITALIY DOROGAN, YURIY MAZUR, EUCLYDES MAREGA JR., MOURAD BENAMARA, GEORGIY TARASOV, Department of Physics, University of Arkansas, Fayetteville, AR 72701, USA, CHRISTOPH LIENAU, Institute of Physics, Carl von Ossietzky University, 26129 Oldenburg, Germany, GREGORY SALAMO, Department of Physics, University of Arkansas, Fayetteville, AR 72701, USA — A strong dependence of quantum dot (QD) - quantum well (QW) tunnel coupling on the energy band alignment is established in hybrid InAs/GaAs - $In_xGa_{1-x}As$/GaAs dot-well structures by changing the QW composition to shift the QW energy through the QD wetting layer (WL) energy. Due to this coupling a rapid carrier transport from the QW to the QD excited states takes place. As a result, the QW photoluminescence (PL) completely quenches at low excitation intensities. The threshold intensities for the appearance of the QW PL strongly depend on the relative position of the QW excitonic energy with respect to the WL ground state and the QD ground state energies. These intensities increase by orders of magnitude as the energy of the QW increases to approach that of the WL due to the increased efficiency for carrier tunneling into the WL states as compared to the less dense QD states below the QW energy.

Tuesday, March 22, 2011 2:30PM - 5:30PM –

Session L33 DMP DCOMP: Focus Session: Dielectric, Ferroelectric, and Piezoelectric Oxides: Lattice Dynamics, Polarons, and Structure C143/149

2:30PM L33.00001 Ultrafast Polaron Dynamics in Multiferroic $LuFe_2O_4$* , R.P. PRASANKUMAR, J. LEE, D. TALBAYEV, A.J. TAYLOR, CINT, Los Alamos National Laboratory, C.L. ZHANG, S.-W. CHEONG, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, X.S. XU, Department of Chemistry, University of Tennessee — The multiferroic material $LuFe_2O_4$ has attracted much recent attention due to its strong magnetoelectric coupling. We used ultrafast optical spectroscopy to examine $LuFe_2O_4$ by employing a 1.55 eV probe pulse to examine the $Fe^{2+} - > Fe^{3+}$ polaronic excitation as a function of temperature and pump photon energy. After 1.55 eV excitation, the photoinduced reflectivity change $\Delta R/R$ decreases within $\sim$1 picosecond (ps), after which a $\sim$30 ps acoustic phonon oscillation is observed. The initial fast drop in $\Delta R/R$ can be explained by $Fe^{2+} - > Fe^{3+}$ polaron hopping, and the subsequent rapid recovery is due to polaron redressing; this is observed at all temperatures. Pumping the Fe^{2+} on-site excitation at 3.1 eV revealed different dynamics. Notably, coupling between the on-site and charge transfer excitations was strongly suppressed above the antiferromagnetic ordering temperature, demonstrating the strong influence of charge and spin order on polaron dynamics.

2:42PM L33.00002 Amplitude and phase gratings based on spatially modulated densities of optically generated polarons in thermally reduced $LiNbO_3$[1] , HAUKE BRUENING, MIRCO IMLAU, University of Osnabrueck, Germany — In thermally reduced, nominally pure $LiNbO_3$ a variety of small polarons can be observed, being responsible for the distinct photochromic properties of this material. In this contribution we use a spatially modulated excitation of polarons for the recording of holographic gratings. These gratings inherit some of the pronounced features of the polarons like a stretched-exponential relaxation behavior with a lifetime in the ms-range. Beside amplitude gratings we also find phase gratings leading to a high diffraction efficiency in some recording and readout geometries. The origin of these phase gratings can't be explained by the classic photorefractive effect due to Fe_{Li} or other photorefractive dopants. In contrast, our findings are discussed in the frame of a model taking into account a local change of the refractive index by the polaronic distortion of the crystal lattice. Measurements of activation energies also indicate that these gratings can be attributed to the small bound (Nb_{Li}^{4+})-polaron.

[1]Financial support by Deutsche Forschungsgemeinschaft (IM 37/5-1) is gratefully acknowledged.

2:54PM L33.00003 Hamiltonian approach to Feynman's path-integral polaron treatment[1] , J.T. DEVREESE, S.N. KLIMIN, Theorie van Quantum en Complexe Systemen (TQC), Universiteit Antwerpen, Antwerpen, Belgium — The Feynman path-integral based all-coupling variational approach for the Fröhlich-polaron is re-formulated and extended using the Hamiltonian formalism with time-ordered operator calculus. Special attention is devoted to the excited polaron states. The energy levels and the inverse lifetimes of the excited polaron states are, for the first time, explicitly calculated within this all-coupling approach. The resulting transition energies are compared with the peak positions of the polaron optical conductivity, as recently calculated numerically using diagrammatic quantum Monte Carlo.

[1]This work was supported by FWO-V projects G.0356.06, G.0370.09N, G.0180.09N, G.0365.08, and the WOG WO.035.04N (Belgium).

3:06PM L33.00004 Comparison of the Raman low frequency spectra of NBT and KLT[1] , DANIEL JACKSON, RADHA PATTNAIK, Physics Dept., Lehigh University, HAOSU LUO, Shanghai Institute of Ceramics, Chinese Academy of Sciences, DWIGHT VIEHLAND, Materials Science Dept., Virginia Tech, JEAN TOULOUSE, Physics Dept., Lehigh University — We present the results of a detailed comparative study of the low frequency central peak in sodium bismuth titanate ($Na_{0.5}Bi_{0.5}TiO_3$ or NBT) and potassium lithium tantalate (K_{1-x} Li_xTaO_3 or KLT) from 90 degree angle Raman scattering with a resolution of 1 cm^{-1}. The Raman spectra of NBT were obtained over a wide temperature range from 78 to 950 K, spanning the two transitions, from cubic to tetragonal at ∼820 K and tetragonal to rhombohedral in the range 480-600 K. In an effort to better understand the nature of these phase transitions in NBT, we performed a detailed analysis of the central peak and soft mode combined, using different models. In particular, we compare the model in which these two features are uncoupled with the model in which they are coupled with a strength parameter, δ^2. These models are also discussed in the more general context of A-site substituted ABO_3 perovskites. The effects of an external electric field and mechanical pressure on the transitions will also be discussed.

[1]The US work is funded by a NSF-MWN grant DMR-0806592.

3:18PM L33.00005 Phonon structures and IR intensities in strained BaTiO3 , ALDO RAELIARIJAONA, University of Arkansas, HUXIANG FU — While soft modes and structural instability in cubic ferroelectrics have been well studied, the vibration properties in structurally stable phases are relatively less understood, however. Here we have carried out first-principle calculations, using density-functional perturbation theory, to determine the phonon structures and IR intensities at gamma point for tetragonal Barium titanate under different in-plane strains, in which lattice parameter ranges from 3.93 Å to 3.80 Å. We find that some modes shift strongly with the inplane strain, while other modes show surprisingly little change. The response of IR intensity is also revealed to be mode-dependent. The microscopic insight for these behaviors is examined.

3:30PM L33.00006 Neutron Diffuse Scattering Measurements of PZT , D. PHELAN, P.M. GEHRING, J. RODRIGUEZ, C. STOCK, NIST Center for Neutron Research, X. LONG, Y. XIE, Z.-G. YE, Simon Fraser University — Neutron diffuse scattering measurements were performed on a single crystal of $PbZr_{0.675}Ti_{0.325}O_3$. The data is compared and contrasted with other Pb-based piezoelectrics, such as the relaxor $PbMg_{1/3}Nb_{2/3}O_3$, and is discussed within the context of random fields.

3:42PM L33.00007 A Neutron Study of the Structure and Lattice Dynamics of Single Crystal PZT , PETER GEHRING, National Institute of Standards and Technology — The outstanding piezoelectric properties of $PbZr_{1-x}Ti_xO_3$ (PZT) perovskite ceramics have long been exploited in numerous device applications, making PZT arguably the most technologically important ferroelectric material in use today. Efforts to understand the piezoelectric mechanism have inspired a plethora of structural studies spanning decades, but solving the PZT phase diagram has proven to be famously problematic because single crystals have not been available save for Zr- and Ti-rich compositions that lie very near the end members $PbZrO_3$ and $PbTiO_3$, where the piezoelectricity is weakest. Thus, whereas PZT has been the subject of thousands of powder and ceramic investigations, no consensus regarding the crystal structures of PZT exists. We report the first neutron diffraction study of single-crystal PZT with compositions x = 0.325 and 0.460 [1]. Our data refute the thesis that the ferroelectric phases of PZT within this composition range, all of which are highly piezoelectric, are purely monoclinic (Cc or Cm). The broadening of certain Bragg peaks can be interpreted in terms of coexisting rhombohedral and monoclinic domains, whereby monoclinic order is enhanced by Ti-doping. This is consistent with the theoretical proposal that the tendency to form macroscopic monoclinic phases facilitates the mechanism of polarization rotation by reducing the energy required to reorient the electric polarization. Dispersions of the lowest energy TO and TA phonon modes were measured on a single crystal of PZT with x = 0.325 in the paraelectric phase at 650 K [2]. The TO mode energy drops at small wave-vectors suggesting that it is a soft mode associated with the ferroelectric phase transition at 590 K. Evidence of a second soft-mode, corresponding to a phase transition at 370 K at the R-point, is provided based on the redistribution of spectral weight as a function of temperature.

[1] D. Phelan *et al.*, Phys. Rev. Lett. **105**, 207601 (2010).
[2] D. Phelan *et al.*, submitted.

4:18PM L33.00008 Correlations between tetragonality, polarization, and ionic displacement in lead titanate-derived ferroelectric perovskite solid solutions[1] , ANDREW RAPPE, TINGTING QI, ILYA GRINBERG, University of Pennsylvania — We use first-principles density functional theory calculations to investigate the dependence of tetragonality on local structure in a variety of ferroelectric solid solutions. We demonstrate that tetragonality is strongly coupled to the B-cation displacement and weakly coupled to the A-cation displacement. Examination of various $BiM^{3+}O_3$ additives to $PbTiO_3$ for different M^{3+} ionic sizes reveals that substitution of either small B-cations or low doping of large B-cations gives rise to large spontaneous polarization and tetragonality. Understanding how the phase transition temperature (T_c) and tetragonality are affected by Pb- and Bi-based perovskite additives provides a rational path for designing new high-temperature piezoelectric materials.

[1]We acknowledge support from ONR, DOE and DOD

4:30PM L33.00009 First principles prediction of a morphotropic phase boundary in the $Bi(Zn_{1/2}Ti_{1/2})O_3$-$(Bi_{1/2}Sr_{1/2})(Zn_{1/2}Nb_{1/2})O_3$ alloy[1] , VALENTINO R. COOPER, Oak Ridge National Laboratory, ASEGUN S. HENRY, Georgia Institute of Technology, SHIGEYUKI TAKAGI, University of Tennessee, DAVID J. SINGH, Oak Ridge National Laboratory — We present a density functional theory study on alloys of the tetragonally distorted $Bi(Zn_{1/2}Ti_{1/2})O_3$ (BZT) and the rhombohedrally oriented $(Bi_{1/2}Sr_{1/2})(Zn_{1/2}Nb_{1/2})O_3$ (BSZN). We find that compositions with $\geq$ 50% BZT are tetragonally distorted with the polarization pointing mainly along the [001] direction. Conversely, for low concentrations of BZT the polarization is rhombohedrally oriented. Based on these results we propose a phase diagram with a possible monoclinc phase between 25% and 50% BZT where this material may have a useful piezoelectric response.

[1]This work was supported by the Materials Sciences and Engineering Division, Office of Basic Energy Sciences, U.S. Department of Energy (V.R.C., D.J.S.), the Office of Naval Research (S.T., D.J.S.) and UNCF (A.S.H.).

4:42PM L33.00010 Probing Ferroelectricity in Thin-film Perovskite $SnTiO_3$ with First-principles Structural Instability Analysis[1] , WILLIAM PARKER, JAMES RONDINELLI, SERGE NAKHMANSON, Argonne National Laboratory — Perovskite $SnTiO_3$ has been recently identified in a number of computational studies as an attractive, environmentally-friendly material with potential to replace ferroelectric $PbTiO_3$. However, additional computational evidence suggests that bulk perovskite $SnTiO_3$ may be metastable. Using density-functional theory and phonon-band instability analysis, we investigate avenues for epitaxial stabilization of ferroelectric perovskite $SnTiO_3$ thin films with applied strains of up to ± 2%.

[1]The U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences supports this project under contract No. DE-AC02- 06CH11357.

4:54PM L33.00011 Room temperature metastable monoclinic phase in $BaTiO_3$ crystals , TOM LUMMEN, JIANJUN WANG, Pennsylvania State University, University Park, Pennsylvania 16802, USA, MARTIN HOLT, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, Illinois 60439, USA, AMIT KUMAR, EFTIHIA VLAHOS, SAVA DENEV, LONG-QING CHEN, VENKATRAMAN GOPALAN, Pennsylvania State University, University Park, Pennsylvania 16802, USA — Low-symmetry monoclinic phases in ferroelectric materials are of considerable interest, due to their associated enhanced electromechanical coupling. Such phases have been found in Pb-based perovskite solid solutions such as lead zirconate titanate (PZT), where they form structural bridges between the rhombohedral and tetragonal ground states in compositional space. In this work, we directly image such a monoclinic phase in $BaTiO_3$ crystals at room-temperature, using optical second harmonic generation, Raman, and X-ray microscopic imaging techniques. Phase-field modeling indicates that ferroelectric domain microstructures in $BaTiO_3$ induce local inhomogeneous stresses in the crystals, which can effectively trap the transient intermediate monoclinic structure that occurs across the thermal orthorhombic-tetragonal phase boundary. The induced metastable monoclinic domains are ferroelectrically soft, being easily moved by electric fields as low as 0.5 kV cm^{-1}. Stabilizing such intermediate low-symmetry phases could very well lead to Pb-free materials with enhanced piezoelectric properties.

5:06PM L33.00012 Infrared spectroscopy of KDP under high pressure[1] , ANA AKRAP, CHRISTOPHER C. HOMES, Condensed Matter Physics and Materials Science Dept., Brookhaven National Laboratory, Upton, New York, RICARDO P.S.M. LOBO, Laboratoire de Physique et d'Étude des Matèriaux, ESPCI-ParisTech, CNRS-UPMC, 10 rue Vauquelin, F-75231 Paris Cedex 5, France, PATRICK SIMON, CRMHT, CNRS UPR 4212, Université d'Orléans, 1D Av. de la Recherche Scientifique, 45071 Orléans Cedex 02, France — We have determined infrared reflectivity of potassium dihydrogen phosphate (KDP) in the paraelectric ($T > T_c$ =135 K) and ferroelectric phase ($T < T_c$), at pressures ranging from ambient up to 10 kbar, for polarizations parallel and perpendicular to the ferroelectric axis. As the T_c is lowered and the paraelectric phase is suppressed by pressure, we track the behavior of several relevant phonon modes. Under pressure there is a significant increase in the oscillator strength of the 150 cm^{-1} mode, accompanied by its shift to lower energies. The ferroelectric soft mode is critically damped below 6.5 kbar, but becomes underdamped at higher pressures.[2] The coupling of the ν_4 mode at 500 cm^{-1} to the ferroelectric soft mode is investigated.

[1]Supported by the DOE under Contract No. DE-AC02-98CH10886.
[2]P.S. Peercy, Phys. Rev. Lett. **31**, 379 (1973).

5:18PM L33.00013 Elastic Anizotropy and Domain Stability in Ferroelectric Thin Films and Problem of Critical Thickness for Memory , ALEXANDER BRATKOVSKY, Hewlett-Packard Laboratories, A.P. LEVANYUK, UA Madrid — The most important effect of the depolarizing field in thin ferroelectric (FE) capacitors is the emergence of domains in place of monodomain state desirable for memory applications, and it depends on the parameters of system Ferroelectric- Electrode. We have studied FE films of BaTiO3, PbTiO3, and Pb (Zr)0.5(Ti)0.5O3 with SrRuO3 electrodes on SrTiO3 (100) substrate. Due to lattice misfit, the FE film becomes tetragonal with the polar axis perpendicular to the film. We have studied rarely addressed topic of relation between the equilibrium domain structure and limits of absolute stability of the monodomain state. We have found that in films with thickness close to the minimal one compatible with FE the stripe domains form with domain walls along the cubic axes in BTO and PTO films, while in PZT it is at 45 degrees to the axes. The orientational dependence of their energy is actually very weak, less than 1% is all above systems. The threshold of absolute instability of the monodomain state is shifted by electrostriction most significantly in BTO and PTO, where it gets close to the (formal) "critical thickness" for FE in monodomain films. In PZT, on the other hand, electrostriction hardly affects it [1].
[1] A.M. Bratkovsky and A.P. Levanyuk, Phil. Mag. 90, 113 (2009); arXiv: 0801.1669; Phys. Rev. Lett. 100, 149701 (2008).

Tuesday, March 22, 2011 2:30PM - 5:30PM –
Session L34 DMP: Focus Session: Interfaces in Complex Oxides - Heterointerfaces C141

2:30PM L34.00001 Electronic instabilities at paraelectric and superconducting interface: A mean field approach[1] , J.T. HARALDSEN, A.V. BALATSKY, Theoretical Division, Los Alamos National Laboratory and Center for Integrated Nanotechnologies, Los Alamos, NM 87545 — We examine the modified electronic states at the interface between superconducting and ferro(para)-electric films. We find that the coupling of a classical fluctuating paraelectric P and superconducting ψ order parameters can significantly modify these orders at the interface. Using a Ginzburg-Landau formalism, we show that linear and quadratic terms of the electric polarization produce instabilities in ψ at the interface, where the linear interaction produces a modulation of the order parameters and create an interface-induced ferroelectric polarization within the paraelectric bulk state. We will discuss implications of this work for the experiments on the epitaxial oxide films.

[1]Work was carried out under the help and support of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396.

2:42PM L34.00002 Effect of Cu magnetism on superconductivity at $YBa_2Cu_3O_7$ / $La_{0.7}Ca_{0.3}MnO_3$ interfaces , J. TORNOS, C. VISANI[1], J. GARCIA-BARRIOCANAL[2], C. LEON, N.M. NEMES, J. SANTAMARIA, GFMC, Departamento de Física Aplicada III, Universidad Complutense de Madrid, 28040 Madrid, Spain, M. GARCIA-HERNANDEZ, Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC). 28049 Cantoblanco. Madrid, YAOHUA LIU, A. HOFFMANN, S.G.E. TE VELTHUIS, Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA, J. FREELAND, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA, M. VARELA, S.J. PENNYCOOK, Condensed Matter Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6031, USA — The induced magnetism at the Cu edge of cuprate manganites interfaces has been proposed to depend on interface termination. We have prepared $YBa_2Cu_3O_7$ / $La_{0.7}Ca_{0.3}MnO_3$trilayers showing Cu magnetism at both cuprate interfaces as evidenced from an XMCD experiment. This result results from the same termination occurring at both interfaces. The effect of Cu magnetism on superconductivity depression proposed by J. Salafrance and S. Okamoto is discussed.

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2:54PM L34.00003 Quantum Phase Transitions in Ultrathin YBCO/LCMO Superlattices[1] , BENJAMIN GRAY, M. KAREEV, E.J. MOON, J. LIU, Phys. Dep., Univ. Arkansas Fayetteville, I-C. TUNG, M.J. BEDZYK, Mat. Sci. Eng., Northwestern Univ., M. VEENENDAAL, J.W. FREELAND, APS, Argonne National Lab., J. CHAKHALIAN, Phys. Dep., Univ. of Arkansas Fayetteville — The rational design of complex oxide heterostructures enables the investigation of novel materials with antagonistic order parameters. Our previous work has provided insight into the role of orbital reconstruction and covalent bonding at the interface of such heterostructures. In this talk, we will further address the intriguing interfacial properties and possible coupling between layers in superlattices composed of alternating superconductive YBa2Cu3O7-x and ferromagnetic La2/3Ca1/3MnO3 layers upon approaching the ultra-thin limit.

[1]J.C. was supported by DOD-ARO under the Contract No. 0402-17291 and NSF Contract No. DMR-0747808.

3:06PM L34.00004 Unconventional proximity effect and inverse spin-switch behavior in a model manganite/cuprate/manganite trilayer system , JUAN SALAFRANCA, Universidad Complutense de Madrid, Spain., SATOSHI OKAMOTO, Oak Ridge National Laboratory — The proximity effect in a model manganite/cuprate system is investigated theoretically. We consider a situation in which spin-polarized electrons in manganite layers antiferromagnetically couple with electrons in cuprate layers as observed experimentally. The effect of the interfacial magnetic coupling is found to be much stronger than the injection of spin-polarized electrons into the cuprate region. As a result, the superconducting transition temperature depends on the thickness of cuprate layer significantly. Since the magnetic coupling creates *anti*-spin-polarization, an applied magnetic field and the *anti*-polarization compete resulting in the inverse spin-switch behavior where superconducting transition temperature is increased by applying a magnetic field. This work was supported by the NSF Grant DMR-0706020 (J.S.) and by the Materials Sciences and Engineering Division, Office of Basic Energy Sciences, the US DOE (S.O.).

3:18PM L34.00005 Magnetoelectric Coupling in P(VDF-TRFE)/LCMO Heterojunctions[1] , ANIL KUMAR, University of Nebraska-Lincoln, USA, EVGENY KIRIANOV, Lincoln South-West High School, NE, USA, VASILY MOSHNYAGA, I. Physikalisches Institut, Universität Göttingen, Germany, PANKAJ SHARMA, ALEXEI GRUVERMAN, ANDREI SOKOLOV, University of Nebraska-Lincoln, USA — Engineered magnetoelectric heterojunctions have recently attracted significant interest due to the possibility to control magnetic properties by external electric fields. Doped lanthanum manganites are attractive candidates to use as a part of such junctions because of their strong coupling between charge, spin and lattice effects. On the other side the use of a ferroelectric (FE) as a gate electrode has dual benefits: it offers the possibility to design a non-volatile data storage device and provide large charge density change at the interface. The ferroelectric polymer, polyvinylidene fluoride (PVDF), is an interesting candidate due to its outstanding electromechanical, dielectric, and mechanical properties. Here we present results of our transport studies of $La_{.67}Ca_{.33}MnO_3$ /P(VDF-TrFE) heterojunction. Manganite thin films were grown by MAD technique, followed by Langmuir-Blodgett deposition of ferroelectric polymer. Results are explained by electron accumulation induced metal-insulator transition in the LCMO layer.

[1]Supported by Nebraska NRI and NSF- MRSEC.

3:30PM L34.00006 ABSTRACT WITHDRAWN –

3:42PM L34.00007 Emergent phenomena at the heterointerface of multiferroic $BiFeO_3$ and ferromagnetic $La_{0.7}Sr_{0.3}MnO_3$[1] , PU YU, Department of Physics, University of California, Berkeley — Novel phenomena and functionalities at the heteroepitaxial complex oxide heterostructures have been attracting much scientific attention from the fundamental physics as well as the technological applications. Essentially, the charge and spin reconstruction at the interface could lead to exotic, totally unexpected state of matters at the interface, such as conductive interface between insulating materials and interfacial ferromagnetism at the proximity of antiferromagnet. In this talk, I will present a systematic study of the electronic (charge) and magnetic (spin) interactions in an all-oxide model heterostructure system consisting of the ferromagnet (FM) $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) and the multiferroic (ferroelectric (FE) and antiferromagnetic (AFM)) $BiFeO_3$(BFO). The study has demonstrated the existence of magnetic coupling at this interface, manifested in the form of an enhanced coercive field as well as an exchange bias. Using x-ray magnetic circular dichroism, the origin of the significant exchange bias has been attributed to a novel ferromagnetic state in the antiferromagnetic BFO sublattice at the interface with LSMO. Based on this finding, the electrical control of magnetic coupling has been explored in the field effect geometry. The magneto-transport measurement clearly demonstrates a reversible switch/control between two distinct exchange bias states by isothermally switching the FE polarization of BFO. This is an important step towards controlling magnetization with electric fields, which may enable a new class of electrically controllable spintronic devices and provide a new basis for producing electrically controllable spin polarized currents. Finally, at the end of the talk, a generic interpretation will be proposed for the understanding of magnetoelectric coupling in the current model system.

[1]The author thanks the support from the Semiconductor Research Corporation-Nanoelectronics Research Initiative-Western Institute of Nanoelectrics program as well as U.S. Department of Energy under contract No. DE-AC02-05CH11231.

4:18PM L34.00008 Modified Magnetotransport in Digital Manganite Superlattices[1] , BRITTANY NELSON-CHEESEMAN, Materials Science Division, Argonne National Laboratory, TIFFANY SANTOS, Center for Nanoscale Materials, Argonne National Laboratory, SAM BADER, ANAND BHATTACHARYA, Materials Science Division and Center for Nanoscale Materials, Argonne National Laboratory — We investigate how the series of manganite superlattices, $(LaMnO_3)_{2n}(SrMnO_3)_n$, responds to an out-of-plane magnetic field in order to better understand how the magnetism and magnetotransport are modified in a short period superlattice. The n=1 superlattice shows magnetotransport and magnetic hysteresis similar to the random alloy with positive low field magnetoresistance (MR) due to anisotropic magnetoresistance (AMR) and negative MR at high fields due to colossal magnetoresistance (CMR). However, the n=2 superlattice behaves differently with large negative MR at high fields, and no positive low field MR for T<100K. The lack of positive low field MR has also been seen in $La_{2/3}Sr_{1/3}MnO_3$ films with perpendicular magnetic anisotropy, suggesting that the n=2 sample moments contain an out-of-plane, canted or frustrated component at low fields. The reemergence of positive low field MR for the n=2 sample above 100K indicates that the driving force for the different moment orientation is strongly temperature dependent.

[1]US DOE, BES, MSE Division, Contract No. DE-AC02-06CH11357

4:30PM L34.00009 $La_{0.7}Sr_{0.3}MnO_3$ Epitaxial Films on $SrTiO_3$(001): Interface Effects & Electronic Distribution , J.-S. LEE, D.A. ARENA, National Synchrtron Light Source, Brookhaven National Lab, C.-C. KAO, Stanford Synchrotron Radiation Light Source, SLAC, P. YU, Dept. of Physics, UC-Berkeley, R. RAMESH, Dept. of Physics, UC-Berkeley and Mater. Sci. Div., LBNL — $La_{1-x}Sr_xMnO_3$ is an attractive material for incorporation into spin-dependent electronic devices and optimally doped $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) is among the most widely studied colossal magneto-resistance materials. Using a combination of soft x-ray absorption spectroscopy and hard x-ray reflectivity, we found that epitaxial films of LSMO grown on STO(001) substrates exhibit an inhomogeneous 3d electron-distribution along surface normal direction, divided between an intermediate layer (enriched in Mn^{3+}) and a nominal mixed-valence layer (Mn^{3+} & Mn^{4+}) of LSMO. This electronic redistribution near the interface is in turn correlated with an unusual remanent magnetic state.

4:42PM L34.00010 $La_{0.7}Sr_{0.3}MnO_3$ Epitaxial Films on $SrTiO_3$(001): Interface Effects & Magnetic Configuration , D.A. ARENA, J.-S. LEE, C.S. NELSON, National Synchrotron Light Source, Brookhaven National Lab, C.-C. KAO, Stanford Synchrotron Radiation Light Source, SLAC, P. YU, Dept. of Physics, UC-Berkeley, R. RAMESH, Dept. of Physics, UC-Berkeley and Mater. Sci. Div., LBNL, R. FAN, C.J. KINANE, S. LANGRIDGE, ISIS, Harwell Campus, STFC, UK — Mixed valence manganites, in which a delicate interaction between electronic, orbital, magnetic and structural degrees of freedom produces rich phase diagrams reflecting the competing, nearly-degenerate ground states, have been under intense investigation for decades. We present evidence for an unusual magnetic configuration in $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) epitaxial films grown on $SrTiO_3$(001) substrates. At low temperatures, the remanent state of the near-surface region in thick LSMO films is aligned anti-parallel to the the applied magnetic field. This unusual magnetic configuration is also correlated with an in-plane structural fluctuation, as measured by x-ray diffraction. We suggest that the unexpected magnetic ordering in these films may also be associated with an orbital reconstruction of the Mn e_g orbitals.

4:54PM L34.00011 Magnetoelectric coupling at the interface of $BiFeO_3/La_{0.7}Sr_{0.3}MnO_3$ multilayers , MARIA J. CALDERON, Inst. Ciencia de Materiales de Madrid-CSIC, R. YU, Rice University, S. LIANG, University of Tennessee, Oak Ridge National Lab, J. SALAFRANCA, Universidad Complutense de Madrid, S. DONG, Southeast University and Nanjing University, S. YUNOKI, RIKEN and Japan Science and Technology Agency, A. MOREO, E. DAGOTTO, University of Tennessee, Oak Ridge National Lab, L. BREY, Inst. Ciencia de Materiales de Madrid-CSIC — Magnetoelectric coupling has recently been demonstrated in a system composed of the ferromagnetic manganite $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) and the ferroelectric antiferromagnetic $BiFeO_3$ (BFO) [1,2]. Using a realistic microscopic model we study the effects of the charge redistribution and orbital reconstruction on the LSMO/BFO interface ground state. We find that the BFO interface (ferro)magnetism is affected by the charge density at the interface which, in turn, can be modified by the ferroelectric polarization on BFO. This interface induced magnetoelectric coupling leads to the recently observed electric field controlled exchange bias.

[1] S. M. Wu et al, Nature Materials 9, 756 (2010).
[2] P. Yu et al, Phys. Rev. Lett. 105, 027201 (2010).

5:06PM L34.00012 Modulation doping of double-exchange ferromagnetism in an antiferromagnetic manganite: Theory and Synthesis[1] , ANAND BHATTACHARYA, T.S. SANTOS, Argonne National Laboratory, B.J. KIRBY, NIST, Gaithersburg, SANJEEV KUMAR, IFW, Dresden, S.J. MAY, Argonne National Laboratory; Drexel University, J.A. BORCHERS, B.B. MARANVILLE, NIST, Gaithersburg., J. ZARESTKY, Oak Ridge National Laboratory, S.G.E. TE VELTHUIS, Argonne National Laboratory, JEROEN VAN DEN BRINK, IFW, Dresden — In this talk we shall discuss the concepts that underlie modulation doping in the context of manganites, particularly the high bandwidth $La_{1-x}Sr_xMnO_3$, and how modulation doped structures are realized using oxide-MBE based techniques. The transport and magnetic properties of modulation doped antiferromagnetic digital superlattices of $(LaMnO_3)_1/(SrMnO_3)_1$ will be discussed in the context of theoretical ideas about exchange interactions in these materials going back to the seminal work of de Gennes, and compared to similar structures in other parts of the $La_{1-x}Sr_xMnO_3$ phase diagram.

[1]U. S. Department of Energy, BES, Contract No. DE-AC02-06CH11357; NIST, U.S. Department of Commerce.

5:18PM L34.00013 Modulation doping of double-exchange ferromagnetism in an antiferromagnetic manganite: Magnetic Structure , T.S. SANTOS, A. BHATTACHARYA, S.G.E. TE VELTHUIS, Argonne National Lab, B.J. KIRBY, J.A. BORCHERS, B.B. MARANVILLE, NIST NCNR, S.J. MAY, Drexel U., S. KUMAR, J. VAN DEN BRINK, IFW Dresden, J. ZARESTKY, Ames Lab — In his pioneering work, de Gennes described a canted antiferromagnetic (AF) state that arises when mobile carriers are added to an insulating AF manganite. However, attempts to realize this canted AF state have been impeded by phase segregation into mixed F and AF phases for x=0.1-0.2. Using a digital synthesis technique to carry out modulation doping of charge carriers into an AF host near x=0.5, we exploit the competing double-exchange and superexchange interactions to realize the canted AF state predicted by de Gennes. We observed the canted AF state using polarized neutron reflectometry and neutron diffraction using polarized neutrons and polarization analysis. Theoretical consideration using the two-orbital model shows that these additional carriers cause a local enhancement of F double-exchange with respect to AF superexchange, resulting in local canting of the AF spins, where the canting angle depends on the doping level. We observe that the canting angle varies with the spreading of charge near the delta-doped layer. Funded by DOE-BES: Scientific User Facilities Div. & Div. of Materials Science & Engineering, and US Dept. of Commerce

Tuesday, March 22, 2011 2:30PM - 5:30PM –
Session L35 DCMP: Metals: Alloys and Impurities C140

2:30PM L35.00001 First Principles Stability and Coherency Strain in Mg3RE (RE=rare earth) D019 Metastable Precipitates in Mg , A. ISSA, J. SAAL, C. WOLVERTON, Northwestern University — As the need for strong yet lightweight materials intensifies, magnesium alloys have become increasingly important. Although lightweight, these alloys exhibit low strength, particularly in comparison to aluminum alloys. The potential to greatly strengthen magnesium alloys has driven current research, with a recent focus on strengthening precipitates, particularly involving rare earth (RE) dopants. The morphology of these precipitates dictates their effect on the strength of the alloy, and quantifying the coherency strain between the precipitates and the Mg matrix is key to determining the morphology of the precipitate. The large size of the potential composition space makes a systematic experimental study costly and time consuming. Therefore, we apply density functional theory (DFT) to systematically predict the formation energies and coherency strains of D019 precipitates in Mg-RE systems along several crystallographic directions. In particular, we look for D019 precipitates that favorably form plate-shaped morphologies along non-basal planes, as this morphology should be effective obstacles to plastic deformation. These Mg-RE systems also provide an interesting testing ground for the accuracy of DFT methods for intermetallic compounds containing f-electrons.

2:42PM L35.00002 Chemical Correlations in Atomic Size-Mismatch Disordered Alloys Predicted from KKR-DCA[1] , D.A. BIAVA, Dept. of Physics, University of Illinois, Urbana, IL 61801, D.D. JOHNSON, Ames Laboratory/US DoE and the Dept. of Materials Science & Engineering, Iowa State University, Ames, Iowa 50011 — The dynamical cluster approximation (DCA) has been implemented in a Korringa-Kohn-Rostoker (KKR) electronic-structure method to predict electronic and structural properties of disordered alloys, in particular, chemical short-range order (SRO). We adapted an optimal-basis method[2] to the KKR-DCA to account for variations in atomic size due to different configurations present in size-mismatch alloys. In comparison to experiment, we find excellent agreement for predicted lattice constants and SRO, with origins identified in the electronic structure and affecting mechanical properties at finite temperatures. We also show how coarse-grained symmetry of the DCA can be exploited to reduce memory and computation time, allowing us to perform for the first time self-consistent KKR-DCA calculations with 2^{16} or more configurations (and atoms) on a single compute node.

[1]Work supported by NSF DMR-0705089 and, in part, Ames Laboratory (DE-AC02-07CH11358) operated by Iowa State University.
[2]A. Alam and D.D. Johnson, Phys. Rev. B 80, 125123 (2009)

2:54PM L35.00003 Modified Embedded Atom Method potential for Fe-C system , LAALITHA LIYANAGE, Mississippi State University, JEFF HOUZE, SEONG-GON KIM, MARK TSCHOPP, SUNGHO KIM, Mississippi State University, MIKE BASKES, Los Alamos National Laboratory, MARK HORSTEMEYER, Mississippi State University — A Modified Embedded Atom Method potential for the Fe-C alloy system was developed. Pair parameters were constructed based on the structural and elastic properties of element pairs in the L12 reference structure from ab-initio simulations and then adjusted to reproduce heat of formation and elastic constants of cementite, and the interstitial energies for iron. The single element potential of carbon correctly predicts graphite and diamond as the two minimum energy structures.The potential parameters were optimized using an optimization method combining Latin hypercube sampling of the N-dimensional parameter space and multi-objective optimization. The potential was tested for stability of cementite by molecular dynamic simulation at room temperature.

3:06PM L35.00004 The unified mechanism of aging effects in both martensite and parent phase for shape-memory alloys: atomic-level simulations , J. DENG, X. DING, State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an 710049, China, T. SUZUKI, K. OTSUKA, Ferroic physics Group, National Institute for Materials Science, Tsukuba 305-0047, Ibaraki, Japan, T. LOOKMAN, A. SAXENA, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, J. SUN, State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an 710049, China, X. REN, Ferroic physics Group, National Institute for Materials Science, Tsukuba 305-0047, Ibaraki, Japan — Most shape-memory alloys (SMAs) subject to the aging effects not only in the martensite phase but also in the parent phase. These aging effects have been attracted much attention as they strongly affect the practical applications of SMAs. So far, the intrinsic mechanism of them has remained controversial due to the difficulty in visualization of what happens in atomic scale. In the present study, by using a combination of molecular dynamics method and Monte-Carlo method [1], we investigate the aging effects in both martensite and parent phase. We successfully reproduced the thermal behaviors of aging effects for SMAs, i.e., the A_f temperature increase with aging time in martensite and the M_s temperature decrease with aging time in parent phase, which keep good agreement with the experimental observations [2]. In addition, quantitative analysis of the atomic configurations during aging reveals that the aging effects are not associated with a change in the average structure.

3:18PM L35.00005 Enhanced High Temperature Mechanical Behavior of FeCo-Based Alloys , ROBERT CAMMARATA, Johns Hopkins University, DEZHI ZHANG, Chinese Academy of Sciences, CHIA-LING CHIEN, Johns Hopkins University — FeCo alloys have been used for a variety of soft magnetic material applications, including for use in high temperature engine applications. However, inferior mechanical properties, in particular relatively low creep resistance, can limit their use at elevated temperatures. We have investigated a variety of microstructural engineering approaches to improve the creep resistance without significantly degrading the magnetic properties. Two such approached will be discussed: oxide dispersion strengthening and annealing treatments leading to grain growth and precipitation hardening. We have shown that both of these methods allow for sensitive control of the resulting microstructural evolution. This control in turn allows for substantial improvement in both the room temperature yield strength as well as the high temperature creep resistance. Detailed microstructural characterization as well as tensile and testing results will be presented.

3:30PM L35.00006 Fermi surface of an important nano-sized metastable phase: Al_3Li , STEPHEN DUGDALE, University of Bristol, UK, JUDE LAVEROCK, Boston University, USA, ASHRAF ALAM, MINA ROUSSENOVA, University of Bristol, UK, JOANNE WENSLEY, University of Cambridge, UK, JADWIGA KWIATKOWSKA, Polish Academy of Sciences, NOBU SHIOTANI, KEK-PF, Japan — Nanoscale particles embedded in a metallic matrix are of considerable interest as a route towards identifying and tailoring material properties. In particular, Al-Li alloys, which form ordered nanoscale precipitates of $L1_2$ Al_3Li for a range of Li concentrations, have been deployed successfully in the aerospace industry owing principally to their superior strength-to-weight ratio. These precipitates, however, are metastable and only form within the surrounding Al matrix, meaning their electronic structure, thought to be important in contributing to the enhanced material properties through its Young's modulus, has so far been inaccessible through conventional techniques. Here, we take advantage of the strong positron affinity of Li to directly probe the Fermi surface of metastable Al_3Li nanoscale precipitates of Al-Li.

3:42PM L35.00007 Metastable states along the Bain path in AgZr with AFLOW[1] , MICHAEL MEHL, Naval Research Laboratory, GUS HART, Brigham Young University, MICHAL JAHNATEK, STEFANO CURTAROLO, Duke University — AgZr crystallizes in the B11 structure, which is bcc-like with stacking AABB along [001]. Using AFLOW[2] we find another low energy structure, "Z2" ,[3] an fcc-like variant of B11. The B11 to Z2 transition follows the Bain path, with c/a changing from 1.9 (B11) to 2.6 (Z2). This seems similar to results for elemental bcc solids,[4] where we find a secondary Bain path minimum which is elastically unstable. Here there is no simple path from the Z2 structure back to the B11 structure, and the Z2 structure is metastable. Using first- principles DFT we demonstrate the possibility of a pressure induced phase transition from B11 to Z2 at 35 GPa. We also examine the $L1_0$ structure, which is higher in energy than Z2 at zero pressure. We find that a transition from B11 to $L1_0$ at 32 GPa, so that $L1_0$ is the true high-pressure phase of AgZr. We discuss the stability of all three of these phases at both zero and high pressure, and the possibility of similar transitions in more useful materials.

[1]Partial support from US -ONR and US DoD HPC

[2]S. Curtarolo *et al.*, http://materials.duke.edu/aflow.html

[3]Z.W. Lu *et al.*, *Phys. Rev. B* **44**, 512 (1991)

[4]M. J. Mehl *et al.*, *Phys. Rev. B* **70**, 014105 (2004)

3:54PM L35.00008 Localized Rattling of Al atoms in $VAl_{10+\delta}$, DOUGLAS SAFARIK, Los Alamos National Laboratory, TOMASZ KLIMCZUK, Institute for Transuranium Elements, Karlsruhe, ANNA LLOBET, DARRIN BYLER, Los Alamos National Laboratory, EKHARD SALJE, Cambridge University — We have studied the localized rattling mode in the 'Einstein solid' $VAl_{10+\delta}$ using a suite of thermodynamic, transport, and neutron diffraction measurements. The rattling originates from Al atoms that occupy the large void within Z_{16} Friaf polyhedra, of which there are eight per unit cell in the $VAl_{10+\delta}$ structure. Our heat capacity, thermal expansion, and electrical resistivity data are all qualitatively consistent with a low-frequency harmonic vibration of the atom. However, our neutron diffraction data show that the rattling atom potential is better described as sixth-order, rather than harmonic. Using a single-site, sixth-order effective potential for the rattling atom, we can explain our thermodynamic, transport, and structural data, including the unusual temperature dependence of the elastic constants.

4:06PM L35.00009 High-energy diffraction measurements of deeply undercooled Co-Pd liquids using electrostatic levitation[1] , G.E. RUSTAN, Iowa State University, N.A. MAURO, J.C. BENDERT, K.F. KELTON, Washington University, A. KREYSSIG, A.I. GOLDMAN, Iowa State University — Co-Pd liquids in their deeply undercooled state have attracted a great deal of interest because of the potential for magnetically triggered nucleation of the solid phase. We report on the results of high-energy x-ray diffraction measurements, using 129 keV x-rays at the Advanced Photon source, on a series of liquid Co-Pd alloys in a containerless environment employing electrostatic levitation. Diffraction data were collected using a flat-plate two-dimensional detector during free cooling from temperatures well above the liquidus, to as much as 200 degrees C of undercooling for compositions ranging from 50:50 to 80:20 (Co:Pd). The composition dependence and temperature dependence of differences in structure will be discussed.

[1]This work was supported by the National Science Foundation under grant DMR-08-01757, DMR-06-06065, DMR-08-56199 and NASA under grants NNX07AK27G and NNX09AJ19H.

4:18PM L35.00010 Ab initio studies of the effect of nanoclusters on magnetostriction of Fe1-xGax alloys[1] , HUI WANG, YANNING ZHANG, University of California, Irvine, TENG YANG, Z.D. ZHANG, Institute of Metal Research and International Centre of Materials Physics, Chinese Academy of Sciences, LIZHI SUN, RUQIAN WU, University of California, Irvine — We investigated the effects of B2-like and D0-like nanoclusters on the magnetostriction of Fe-xGax alloys, through systematic density functional calculations. While the B2-like Fe-Ga clusters still undergo slightly tetragonal distortion, D03-like Fe-Ga clusters remain to be cubic in the Fe matrix. Moreover, we found that B2-like nanostructures produce negative magnetostriction whereas D03- like nanostructures give small positive magnetostriction in Fe-xGax alloys. The formation of nanoscale precipitates cannot be the reason for the extraordinary enhancement of magnetostriction of Fe1-xGax alloys.

[1]Work was supported by the NSF, ONR and CAS, and supercomputer centers of DOD and CAS.

4:30PM L35.00011 The lost heat capacity and entropy in the helical magnet MnSi , SERGEI STISHOV, ALLA PETROVA, Institute for High Pressure Physics of Russian Academy of Sciences, Troitsk, Moscow Region, Russia, ANATOLY SHIKOV, Russian Research Center Kurchatov Institute, Moscow 123182, Russia, THOMAS LOGRASSO, Ames Laboratory, Iowa State University, Ames, IA, EYVAZ ISAEV, Department of Physics, Chemistry and Biology, SE-581 83, Linkoping University, Sweden, BORIE JOHANSSON, Applied Materials Physics, Materials Science Department, The Royal Technological University, SE-100 44 Stockholm, Sweden, LUKE DAEMEN, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — We report results of measurements and analysis of the heat capacity of MnSi. The measurements included data collection at a magnetic field of 4T, which suppresses strongly the longitudinal spin fluctuations and the phase transition. To analyze the experimental data, calculations of the phonon spectrum and phonon density of states in MnSi were performed. Inelastic neutron scattering with a polycrystalline sample of MnSi was used to validate the computational results. The combination of the experimental and theoretical data turned out to be decisive in revealing some hidden features of the thermal excitations in MnSi. In particular, the analysis of the available data led conclusively to the existence of a negative contribution to the heat capacity and entropy in MnSi at $T > T_c$, implying that a specific spin ordering process did occur in the paramagnet phase of MnSi.

4:42PM L35.00012 A common magnetic origin for the Invar effects in fcc iron-based ferromagnets , CHRIS HOOLEY, University of St Andrews, U.K., FRANCOIS LIOT, Max Planck Institut fur Eisenforschung, Germany — Using first-principles calculations, in conjunction with Ising magnetism, we undertake a theoretical study to elucidate the origin of the experimentally observed Invar effects in disordered fcc iron-based ferromagnets. First, we show that our theory can account for the Invar effects in iron-nickel alloys, the anomalies being driven by the magnetic contributions to the average free energies. Second, we present evidence indicating that the relationship between thermal expansion and magnetism is essentially the same in all the studied alloys, including those which display the Invar effect and those which do not. Hence we propose that magnetism plays a crucial role in determining whether a system exhibits normal thermal expansion, the Invar effect, or something else. The crucial determining factor is the rate at which the relative orientation of the local magnetic moments of nearest-neighbor iron atoms fluctuates as the system is heated.

4:54PM L35.00013 Electronic Origin of Fast Sulfur Diffusion in 3d Transition Metals , DMITRI NOVIKOV, UTRC, United Technologies Corporation, 411 Silver Lane, 129-21 East Hartford, CT 06108, ALAN CETEL, MICHAEL MALONEY, KEVIN SCHLICHTING, BRAD COWLES, Pratt & Whitney, 400 Main Street, East Hartford, CT 06108, SERGEY OKATOV, ILIYA LOMAYEV, YURI GORNOSTYREV, CJSC Institute of Quantum Materials Science, Ekaterinburg, Russia, SEGEI BURLATSKY, United Technology Research Center — The microscopic origins of abnormally fast diffusion of sulfur in nickel have been investigated. Transition state theory of vacancy mediated diffusion of substitutional impurities with parameters calculated from first-principle density-functional theory (DFT) was used to determinate of the diffusion coefficients of S and Al impurities in fcc Ni. Sulfur diffusion coefficient was found to be two orders of magnitude higher than for aluminum in good agreement with experimental data. We found that sulfur has a very low barrier for jump toward vacancy and also significantly decreases migration barriers for neighboring nickel atoms. We discuss the microscopic factors contributing to the dramatic difference in S and Al diffusion coefficients and show that electronic structure and chemical bonding play crucial role in enhanced diffusion of S. We also found that S considerably increases Ni self-diffusion rate. The implications of S effect on the stability of thermally grown oxides in superalloys are discussed.

5:06PM L35.00014 Nitrogen Adsorption, Solubility and Transport within Group V Metals , PANITHITA ROCHANA, EKIN OZDOGAN, JENNIFER WILCOX, Department of Energy Resources Engineering, Stanford University — It is well known that Group V metals have strong-binding characteristics to diatomic molecule, e.g. N_2, O_2, H_2, and CO. Within this study, N_2 has been investigated to determine the mechanism of surface adsorption, dissociation and subsequent atomic diffusion into the bulk crystal structure of vanadium(V). Alloys of ruthenium(Ru)-V have been examined indicating that Ru can be used to tune the electronic structure of the bulk to enhance atomic diffusion. Electronic structure calculations based on density functional theory have been studied on the investigation of N_2 adsorption on 3 low-index surfaces, (110), (100) and (111). Preliminary investigations indicate that the V(111) surface binds N_2 the strongest at fcc site (E_{ads} = 1.4eV). To determine bulk solubility, binding energy calculations are carried out as a function of N concentration. N was found to be stable primarily at O-sites within the bulk V lattice. Bader charge and density of states analyses are analyzed to investigate the mechanism of bulk absorption and solubility phenomena. Results will be presented on the adsorption, bulk solubility, and transport of N in V and V-based alloys. The application to this study is toward the design of an N_2-selective dense membrane in which atomic N may be produced on the permeate side with hydrogen as a sweep gas for the ammonia synthesis process.

5:18PM L35.00015 The wake of H in V, Nb and Ta at elevated temperatures: Irreversibility and non-central forces revisited , FRANZ REIDINGER — At elevated temperatures U and Do of the Arrhenius equation for diffusion describe the amplitude and relaxation rate, respectively, of the stern wave wake of H in V, Nb and Ta. The key evidence for this hypothesis is the close correlation between the isotope dependence of U derived from the Gorsky measurements[1] and the shear distortion of the orthorhombic phases of NbH(D) and TaH(D). The isotope dependence of U can be expressed in closed form: U=a$\sqrt{M}$ + b$\sqrt{m}$ where M and m are the atomic numbers of the host metal and H isotope and a and b are 7.4 and 37 for Nb and Ta, and 0 and 55 for V, respectively, in units of meV. I explain this correlation in two steps: a) the cubic symmetry of the nearest neighbor strain field[2] of the interstitial H is the result of a dynamic superposition, possibly caused by a JT resonance[3], of the two orthorhombic variants of β-NbH0.75 and b) the successful characterization of the diffusion process as jump diffusion[4] eliminates the transition state from consideration. Instead it is the relaxation of the just emptied site from its residual orthorhombic distortion towards the cubic symmetry of the bcc metal which is being measured. 1)Z Qi, J Voelkl, R Laesser and H Wenzl: J. Phys. F 13, 2053 (1983) 2)G Bauer, E Seitz, W Schmatz and H Horner: Sol. State Comm. 17, 161 (1975) 3)G C Abell: J. Phys. F 12, 1143 (1982) 4) V Lottner, A Heim and T Springer: Z. Physik B 32, 157 (1979).

Tuesday, March 22, 2011 2:30PM - 5:18PM –

Session L36 DMP: Focus Session: Graphene Structure, Dopants and Defects: Adsorbates C142

2:30PM L36.00001 First-principles calculations of gated adatoms on graphene[1] , KEVIN T. CHAN, HOONKYUNG LEE[2], MARVIN L. COHEN, Dept. of Physics, University of California, Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — The two-dimensional surface of graphene is well-suited for adsorption of adatoms or molecules. The application of a gate voltage can be used to precisely control the electron concentration of the adsorbate-graphene system. Such control over electronic properties of adsorbates on graphene might have useful applications in areas such as catalysis and hydrogen storage. In this work, the gating of a variety of adatoms adsorbed on graphene is studied using first-principles calculations. We compute the projected density of states, local electrostatic potential, and charge density of the adatom-graphene system as a function of gate voltage. We demonstrate that adatoms on graphene can be ionized by gating, and that the ionization causes a sharp change in the electrostatic potential. Additional interesting features of our results are also discussed.

[1]This work was supported by NSF Grant No. DMR10-1006184 and DOE under Contract No. DE-AC02-05CH11231. Computational resources were provided by the IT Division at LBNL.

[2]Present address: Dept. of Mechanical Engineering and Materials Science, Dept. of Chemistry, and the Smalley Institute for Nanoscale Science and Technology, Rice University

2:42PM L36.00002 High-resolution measurement of SiO2 surface potential using scanning Kelvin-probe microscopy[1] , WILLIAM CULLEN, KRISTEN BURSON, MAHITO YAMAMOTO, MICHAEL FUHRER, University of Maryland — It is now widely recognized that the dominant contribution to disorder in SiO_2-supported graphene is due to scattering from charged impurities. These charged impurities give rise to a conductivity which is linear in carrier density, and create electron-hole puddles in graphene. The screened potential variation produced in graphene has been imaged using scanning tunneling microscopy/spectroscopy (STM/STS) by spatially mapping the variation in the Dirac point, revealing a length scale of 20 nm for the charge puddles. However, there is a substantial gap in resolution between the STM measurements and previous measurements with much greater potential sensitivity but limited spatial resolution. Here we attempt to bridge this gap using scanning Kelvin-probe microscopy (SKPM) of SiO_2 in ultrahigh vacuum. Our measurement takes advantage of the high spatial resolution allowed by UHV non-contact AFM while maintaining UHV control of the sample environment.

[1] Y. Zhang et al., Nature Physics 5, 722 (2009)
[2] J. Martin et al., Nature Physics 4, 144 (2008)

[1]Supported by UMD-NSF-MRSEC grant #DMR 0520471 and the Center for Nanophysics and Advanced Materials.

2:54PM L36.00003 Revealing the dominant scatterer in Graphene on SiO_2[1] , MASA ISHIGAMI, Department of Physics and Nanoscience Technology Center, University of Central Florida — Freely suspended graphene sheets display high-field effect mobility, reaching 2×10^5 cm^2 /V s. Yet, suspended graphene sheets are fragile and impractical for most experiments and applications. Graphene sheets on SiO_2 are easier to handle but possess low-carrier mobilities, which can even vary by an order of magnitude from sample to sample. Poor and unpredictable transport properties reduce the utility of SiO_2-bound graphene sheets for both fundamental and applied sciences. Therefore, understanding the impact of substrates is crucial for graphene science and technology. We [1] have measured the impact of atomic hydrogen adsorption on the electronic transport properties of graphene sheets as a function of hydrogen coverage and initial, pre-hydrogenation field-effect mobility. The saturation coverages of atomic hydrogen for different devices are found to be proportional to their initial mobility, indicating that the number of native scatterers is proportional to the saturation coverage of hydrogen. By extrapolating this proportionality, we show that the field-effect mobility can reach 1.5×10^4 cm^2 /V s in the absence of the hydrogen-adsorbing sites. The affinity to atomic hydrogen is the signature of the most dominant type of native scatterers in graphene-based field-effect transistors on SiO_2. The dominant scatterer is identified by comparing the reactivity of charge puddles, ripples and resonant scatterers to atomic hydrogen.

[1] J. Katoch, J.H. Chen, R. Tsuchikawa, C. W. Smith, E.R. Mucciolo, and M. Ishigami, Uncovering the dominant scatter in graphene sheets on SiO2, Physical review B. Rapid Communications, 82, 081417 (2010).

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

3:30PM L36.00004 Magnetic field effects on the local electronic structure near a single impurity in Graphene[1] , LING YANG, Department of Physics and Astronomy, University of California, Riverside, California, 92521, JIAN-XIN ZHU, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, SHAN-WEN TSAI, Department of Physics and Astronomy, University of California, Riverside, California 92521 — Impurities in graphene can have a significant effect on the local electronic structure of graphene when the Fermi level is near the Dirac point. We study the problem of an isolated impurity in a single layer graphene in the presence of a perpendicular magnetic field. We use a linearization approximation for the energy dispersion and employ a T-matrix formalism to calculate the Green's function. We investigate the effect of an external magnetic field on the Friedel oscillations and impurity-induced resonant states. Different types of impurities, such as vacancies, substitutional impurities, and adatoms, are also considered.

[1]LY and SWT acknowledge financial support from NSF(DMR-0847801)and from the UC Lab Fees Research Program.

3:42PM L36.00005 Tunable magnetoresistance behavior in suspended graphitic multilayers through ion implantation , CARLOS DIAZ-PINTO, XUEMEI WANG, SUNGBAE LEE, Department of Physics, Texas Center for Superconductivity, University of Houston, VIKTOR HADJIEV, Texas Center for Superconductivity, University of Houston, DEBTANU DE, WEI-KAN CHU, HAIBING PENG, Department of Physics, Texas Center for Superconductivity, University of Houston — A linear positive magnetoresistance (MR) is often observed in graphitic multilayers, yet its origin remains inconclusive. Recently, a non-Markovian transport theory predicts a strong positive MR in two dimensional systems under the influence of both short- and long-range disorders, while a negative MR is expected with only one type of disorder. Here, we address the role of disorders on the MR behavior of suspended graphitic multilayers through ion implantation. Boron implantation is found to drastically change the MR behavior: the linear positive MR transforms into a negative MR after the introduction of short-range disorders (boron), in consistence with the non-Markovian theory. This suggests that the origin of the unexplained linear positive MR in graphitic structures is the non-Markovian transport under the interplay between long-range disorders (charged surface adsorbents) and short-range disorders (defects inside the lattice). After ion implantation, short-range disorders dominate, leading to a distinct negative MR behavior.

3:54PM L36.00006 Raman spectroscopic study of chemically-doped few layer graphenes , PINGHENG TAN, WEIJIE ZHAO, JUN ZHANG, JIAN LIU — Graphene, the latest carbon allotrope discovered at 2004, has attracted intensively scientific interest owing to its distinctive properties. Chemical doping is expected to substantially increase the density of free charge carriers by charge transfer and to modify the Fermi level of doped materials. Here, we investigated charge transfer and optical phonon mixing in few layer graphenes in detail by utilizing sulfuric acid as an electron-acceptor dopant. Sulfuric acid molecules are found to be only physically adsorbed on the surface layers of graphenes and no intercalation happens. The top and bottom layers of bilayer graphenes can be intentionally doped differently by concentrated sulfuric acid. The difference of hole doping between the top and bottom layers results in phonon mixing of symmetric and antisymmetric modes in bilayer graphenes. The Raman frequency evolution with the doping level qualitatively agrees with recent ab initio theoretical calculations. Sulfuric acid molecules can be expected as a stable electron-acceptor dopant for graphenes to study the physical properties of few layer graphenes at different doping levels.

4:06PM L36.00007 The doping mechanism in graphene , RAZVAN A. NISTOR, DENNIS M. NEWNS, GLENN J. MARTYNA, IBM T. J. Watson Research Center — Doping graphene by adsorbing chemical species on its surface is one way to control the carrier concentration of this novel material. Using large-scale *ab initio* simulations and electronic structure calculations, we show the carbon layer acts as a metal catalyst facilitating the disproportionation reaction of adsorbed chemical species on its surface. This reaction leads to the formation of charge transfer complexes which thereby dope the graphene. We also investigate the charge transfer in graphene-silicon and defected graphene-silicon-oxide interfaces. Our microscopic understanding of the doping mechanism in graphene, which brings to light the catalytic power of the material, is important in the development of carbon-based electronics.

4:18PM L36.00008 Understanding Graphene Coatings: Characterization of Solvent Exfoliated Few-Layer Graphene by Raman Scattering , JORGE CAMACHO[1], LESTER LAMPERT, WILLSON ARIFIN, ROBBY FLAIG, TIMOTHY RUE, TYLER KRISKO, JAMES HAMILTON, University of Wisconsin-Platteville — Graphene has unique properties like its ballistic transport at room temperature combined with chemical and mechanical stability and these properties can be extended to few-layer of graphene. Potential large-area applications that include transparent conductive coatings and fuel cell electrodes require dispersing graphene in a fluid phase. Graphene nano-platelets can be synthesized by dispersion and exfoliation of graphite in organic solvents such N-methyl-pyrrolidine (NMP) and cyclohexylpyrrolidone (CHP). However, liquid-phase exfoliation produces graphene with defects that can disrupt the electronic properties. One of the remaining questions is whether the defects created during synthesis can be minimized. We report a Raman spectroscopic study showing that defects in few-layer graphene produced by liquid-phase exfoliation of graphite can be controlled by the type or mixture of solvents used.

[1]Nanotechnology Center for Collaborative Research & Development

4:30PM L36.00009 First Principles Study of Interactions between Dopant Atoms in Graphene[1] , NABIL AL-AQTASH, IGOR VASILIEV, New Mexico State University — We study the interactions between the boron (B) and nitrogen (N) dopant atoms in graphene. Our calculations are carried out using density functional theory combined with the generalized gradient approximation for the exchange-correlation functional. The total energies, equilibrium geometries, electronic charge distributions, and densities of states of doped graphene sheets are examined in cases of B-B, N-N, and B-N co-doped graphene. The interaction energy between the two dopant atoms is found to be inversely proportional to the square of the separation distance. We find the B-B and N-N interactions to be repulsive and the B-N interaction to be attractive. The changes in the density of states observed in B- and N-doped graphene are explained in terms of electronic charge transfer.

[1]Supported by DOE DE-FG36-08GO88008.

4:42PM L36.00010 Bonding and charge transfer induced by metal adatom adsorption on graphene , XIAOJIE LIU, C.Z. WANG, M. HUPALO, Y.X. YAO, M.C. TRINGIDES, Ames Laboratory - USDOE, Iowa State University, WEN-CAI LU, Institute of Theoretical Chemistry, Jilin University, Changchun, China, K.M. HO, Ames Laboratory - USDOE, Iowa State University — Structures and adsorption energies of alkali, simple, transition as well as rare earth metal adatoms on graphene were studied systematically by first-principles calculations. Bonding character and charge transfer between the metal adatoms and the graphene were also analyzed using the quasi-atomic minimal basis set orbitals (QUAMBOs) approach. We showed that the interaction between the alkali metal adatoms and graphene can be characterized as ionic with minimal effects on the lattice and electronic states of the graphene layer. On the other hand, transition metal adsorption exhibits strong covalent bonding and induces large distortion in the lattice and electronic states of the graphene. For trivalent simple metal adatom adsorption, mixed covalent and ionic bonding is observed. Interaction of rare earth adatoms with graphene can be either ionic or covalent depending on the specific elements. Charge redistributions upon the metal adsorptions also induce significant electric dipole moments and changes in the magnetic moments of the adatoms. These results are confirmed by STM studies of the nucleated island density in epitaxial growth experiments.

4:54PM L36.00011 Transport properties of metalo-organic functionalized graphene[1] , STEFAN C. BADESCU[2], VICTOR M. BERMUDEZ, THOMAS L. REINECKE, NRL, Washington, DC — Transition metal atoms can act as strong covalent anchors for organic molecules on graphene. The hybridization between the metallic d orbitals and the p orbitals of graphene provides a doping method without breaking C-C bonds. Using first-principle calculations for a range of adsorbed transition metals we identify the induced impurity levels and we reveal a dependence of the spin states on adsorbate coverage. We construct sets of maximally localized Wannier functions that interpolate accurately the calculated bandstructures. These sets are used then to describe the electronic transport from the dilute regime to finite coverages.

[1]This work was supported in part by ONR.
[2]Currently at AFRL, Dayton, Ohio

5:06PM L36.00012 The electronic structure and chemical bonding of graphene doped with Group IA and Group VIIA elements: A density functional theory study , YIMING MI, Graduate Department, Shanghai University of Engineering Science, SHUICHI IWATA, Graduate School of Frontier Sciences, The University of Tokyo — The ground state geometry and the electronic structure of graphene doped with group IA and VIIA elements were calculated with the first principles plane wave pseudopotential approaches within the density functional theory formalism in this paper. In terms of the generalized gradient approximation(GGA), GW approximation and optimizing atomic positions, a reliable geometry of the structure was acquired. The calculated formation energies for different configurations under ambient temperature implied that a new kind of material will produce. The results acquired here allow one to suggest new material with semiconductor or semimetallic behavior by adjusting the relative concentration of the doped atoms carefully.

Tuesday, March 22, 2011 2:30PM - 5:30PM –
Session L37 DMP: Focus Session: Graphene Structure, Dopants, and Defects: Magnetism C146

2:30PM L37.00001 Missing atom as a source of carbon magnetism , IVAN BRIHUEGA, Dept. Fisica de la Materia Condensada. Universidad Autonoma de Madrid — Introducing vacancies in graphene-like systems by irradiation has been shown to be an efficient method to vary its mechanical behavior, tune its electronic properties and even to induce magnetism in otherwise non-magnetic samples [1-2]. While the role played by these vacancies as single entities has been extensively addressed by theory [3-6], experimental data available refer to statistical properties of the whole heterogeneous collection of vacancies generated in the irradiation process. Here, by artificially generating isolated vacancies on a graphite surface and measuring their local density of states on the atomic scale, we have shown how single vacancies modify the electronic properties of this graphene-like system [7]. Our scanning tunneling microscopy experiments, complemented by tight binding calculations, reveal the presence of a sharp electronic resonance at the Fermi energy around each single graphite vacancy, which implies a dramatic reduction of the charge carriers' mobility and can be associated with the formation of local magnetic moments. Finally, we have extended our investigations to other graphene systems.

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[2] A. V. Krasheninnikov and F. Banhart, *Nature Materials* **6**, 723 (2007)
[3] V. M. Pereira, F. Guinea, J. M. Lopes dos Santos, N. M. R. Peres and A. H. Castro Neto, *Phys. Rev. Lett.* **96**, 036801 (2006)
[4] P. O. Lehtinen, A. S. Foster, Y. C. Ma, A. V. Krasheninnikov and R. M. Nieminen , *Phys. Rev. Lett.* **93**, 187202 (2004).
[5] J. J. Palacios, J. Fernández-Rossier and L. Brey, *Phys Rev. B* **77**, 195428 (2008)
[6]. O. V.Yazyev, *Phys. Rev. Lett.* **101**, 037203 (2008).
[7] M. M. Ugeda I. Brihuega, F. Guinea and J. M. Gómez Rodríguez, *Phys. Rev. Lett* **104**, 096804 (2010)

3:06PM L37.00002 Kondo quantum criticality in graphene , BRUNO UCHOA, University of Illinois at Urbana-Champaign, T.G. RAPPOPORT, Universidade Federal do Rio de Janeiro, A.H. CASTRO NETO, Boston University — Graphene fits in a large class of "pseudogap" materials which are allowed to exhibit quantum criticality as a result of the interplay of strong correlations and a vanishing density of states near the Fermi points. In the presence of magnetic impurities, we show there is a symmetry class of localized orbitals which, in combination with quantum interference effects inbuilt in the honeycomb lattice, can lead to a novel class of Kondo quantum criticality in graphene [1]. In this class, graphene effectively screens the local spin as a super-ohmic dissipative environment and the RKKY interaction decays spatially with a fast power-law $\sim 1/R^7$, rather than the standard $1/R^3$ decay expected for Dirac fermions. We also show that unlike metals, the exchange coupling between the localized and itinerant spins can be controlled across the quantum critical region with the application of an external gate voltage. This effect may permit the first experimental observation of quantum criticality in graphene at zero magnetic field, directly with scanning tunneling probes and gating.

[1] B. Uchoa et al., arXiv:1006.2512 (2010)

3:18PM L37.00003 Kondo effect in graphene in the presence of Rashba spin-orbit interaction , MAHDI ZAREA, Ohio/Northwestern University, NANCY SANDLER, SERGIO ULLOA, Ohio University — We present an exact solution for the Anderson model of a single-orbital magnetic impurity on graphene in the Kondo regime. Different positions for the impurity are considered: on top of a carbon atom, substitutional or interstitial (middle of the hexagon cell). We show that regardless of the impurity position, the effective exchange Hamiltonian always describes a single- channel Kondo problem. The inclusion of the Rashba spin-orbit interaction changes the linear energy dispersion to a quadratic one near the Dirac points with the corresponding change in the density of states. This in turn, modifies the value of the critical Kondo coupling as compared to the case where the spin-orbit is absent. Moreover, spin-orbit interactions, introduce a Dzyaloshinsky-Moriya (DM) term in the Kondo Hamiltonian away from particle-hole symmetry. Although still in the single channel region, the effective exchange coupling is augmented by the DM term and the Kondo temperature shows an exponential increase. Supported by NSF-PIRE and MWN/CIAM

3:30PM L37.00004 Transport in irradiated graphene: Kondo and charge fluctuation effects , VIVEK AJI, SUNG-PO CHAO, University of California at Riverside — Observation of an upturn in resistance at low temperatures in irradiated graphene has renewed the interest in the nature of the Kondo effect in systems with linear density of states. The vanishing density of states near the Dirac point leads to a much wider local moment regime but a cross over to the charge fluctuation at very low carrier densities indeed occurs. In this talk I will show how the Kondo scale and the resistance versus temperatures evolves from one regime to the other, and compare our results with experimental data. Our chief conclusion is that a good agreement with data can be achieved only if one posits that the energy of the impurity level varies linearly with the chemical potential.

3:42PM L37.00005 Spin and Transport Properties of Doped Graphene , KATHLEEN MCCREARY, WEI HAN, ROLAND KAWAKAMI, University of California, Riverside — Graphene is an ideal system to investigate the interplay of magnetic moments and conduction electrons. Electrostatic gates are able to tune the electron and holes concentrations substantially, and localized magnetic moments can form, in principle, through a variety of methods including vacancies, edges, and adsorbed impurities. Theory predicts a coupling of the localized moments and the conduction electrons, leading to gate tunable indirect coupling between moments which can be ferromagnetic or antiferromagnetic. In this study, we perform magnetotransport measurements on graphene devices where the graphene surface is modified inside an ultrahigh vacuum chamber through a variety of methods including hydrogen adsorption, Ar sputtering, and molecular beam deposition of transition metals [1]. Both /in situ/ and /ex situ/ magnetotransport measurements are performed, where the latter involves the air-free transfer to a low temperature (1.6 - 300 K), high field (7 T) cryostat. We will report results on the temperature-dependent, high-field magnetotransport characteristics of doped graphene.

[1] K. Pi, K. M. McCreary, W. Bao, W. Han, Y. F. Chiang, Y. Li, S.-W. Tsai, C. N. Lau, and R. K. Kawakami, Phys. Rev. B 80, 075406 (2009).

3:54PM L37.00006 ABSTRACT WITHDRAWN —

4:06PM L37.00007 Can Carbon Be Ferromagnetic? , HENDRIK OHLDAG, SLAC National Accelerator Center, PABLO ESQUINAZI, University Leipzig, ELKE ARENOHOLZ, Lawrence Berkeley National Laboratory, DANIEL SPEMANN, MARTIN ROTHERMEL, ANNETTE SETZER, TILMAN BUTZ, University Leipzig — The existence of long range magnetic order at room temperature in carbon based structures without magnetic elements is very unexpected. Theoretical results from different groups suggest that the existence of long range magnetic order in a graphite structure is possible, if one takes the effects of defects and/or the incorporation of hydrogen atoms into account. SQUID results provided first systematic hints for the existence of magnetic order at room temperature in virgin as well as irradiated highly oriented pyrolytic graphite (HOPG) samples. We present a x-ray dichroism study of graphite surfaces [1] that addresses the origin and magnitude of ferromagnetism in metal-free carbon. Using element specific x-ray microscopy we can show that metallic impurities do not play a role in the ferromagnetism of carbon and that carbon can be ferromagnetic without ferromagnetic impurities. A detailed spectroscopic study shows that in addition to carbon *pi*-states, also hydrogen-mediated electronic states exhibit a net magnetization with magnetic remanence at room temperature. The observed magnetism is restricted to the top $\sim$10 nm of the sample where the actual magnetization reaches a value similar to classic ferromagnetic materials like e.g. Nickel. [1] H. Ohldag et al., Phys. Rev. Lett. **98,** 187204 (2007) and submitted to NJP (2010)

4:18PM L37.00008 Extinction of ferromagnetism in HOPG by thermal annealing[1] , XIAOCHANG MIAO, ARTHUR HEBARD, Department of Physics, University of Florida, Gainesville, FL 32611, SEFAATTIN TONGAY, BILL APPLETON, Nanoscience Institute for Medical and Engineering Technologies, University of Florida, Gainesville, FL 32611 — Observations of ferromagnetism (FM) in highly ordered pyrolytic graphite (HOPG) have generated vigorous research activity to clarify its origin, especially when transition metals are known to be absent. We report that the ferromagnetism of pristine HOPG samples as measured by hysteretic magnetization loops can be diminished and eventually extinguished with sufficiently long high vacuum anneals at temperatures greater than 2000°C. Concomitant with the extinction of ferromagnetism, we observe an anneal-induced increase in grain size (accompanied by possible edge reconstruction) confirmed by XRD measurement and improved transport properties, including lower in-plane and out-of-plane resistance, higher electron and hole mobility and improved charge compensation. The implied anneal-induced reduction of defects and vacancies suggests that the FM of pristine HOPG is correlated with localized states located at zigzag edges, vacancies and related defects.

[1]Work supported ONR-00075094 and NSF-1005301

4:30PM L37.00009 Local Moment Formation of an Anderson Impurity on Graphene , CHUNHUA LI, Department of Physics and Texas Center for Superconductivity, University of Houston, Houston, Texas, 77204, USA, JIAN-XIN ZHU, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, C. S. TING, Department of Physics and Texas Center for Superconductivity, University of Houston, Houston, Texas, 77204, USA — We study the effect of a magnetic impurity on a single layer of graphene within an Anderson impurity model. Due to the vanishing local density of state at the Fermi level in graphene, the impurity spin cannot be effectively screened out. Treating the problem within the Gutzwiller approximation, we found a region in the parameter space of U-E^f where the impurity electron is in the local moment state, which is characterized by a zero effective hybridization between the bath electron and magnetic impurity. Here U is the onsite Coulomb repulsion of the impurity and E^f is its energy level with respect to the Fermi energy. The competition between U and E^f is also discussed. While larger U reduces double occupation and favors local moment formation, a deeper impurity level prefers double occupation and a nonzero hybridization and thus a Kondo screened state. For a fixed U, by continuously lowering the impurity level, the impurity first enters from a Kondo screened state to a local moment state and then departs from this state and re-enters into the Kondo screened state.

4:42PM L37.00010 Spin-dependent scattering from gated potential obstacles in graphene systems[1] , MAHMOUD ASMAR, SERGIO ULLOA, Ohio University — We study the scattering of Dirac fermions in a sheet of graphene from potential obstacles created by external gates in the presence of both intrinsic and extrinsic Spin-Orbit(SO) interactions [1]. Obtaining an analytical solution in real-space representation for the eigenvectors allows us to calculate the phase shifts generated by a finite-size obstacle in the presence of SO interactions [2]. These states take into account the total angular momentum of the Hamiltonian, which includes spin, pseudo-spin and orbital angular momentum. We find an interesting interplay of both SO interactions, which results in oscillations of the spin-flip cross sections with energy; this also generates a difference between both cross sections for different interaction ranges. These results may open a possibility of obtaining spin-polarized currents that are of importance in the field of spintronics.

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[1]Supported by NSF PIRE and MWN/CIAM.

4:54PM L37.00011 ABSTRACT WITHDRAWN –

5:06PM L37.00012 Ferromagnetically coupled local moments along an extended line defect in graphene[1] , CARTER T. WHITE, NRL, SMITHA VASUDEVAN, GWU, DANIEL GUNLYCKE, NRL — Recently an extended line defect was observed composed of octagonal and pentagonal carbon rings embedded in a graphene sheet [Nat. Nanotech. 5, 326 (2010)]. We report results of studies we have made of this defect using both first-principles and semi-empirical methods. Two types of boundary-localized states arising from the defect are identified. The first (second) type has eigenstates with wavefunctions that are anti- symmetric (symmetric) with respect to a mirror plane that is perpendicular to the graphene sheet and passes through the line defect center line. The boundary-localized anti-symmetric states are shown to be intimately connected to the zigzag edge states of semi-infinite graphene. They exhibit little dispersion along the defect line and lie close to the Fermi level giving rise to a spontaneous spin polarization along the defect once electron-electron interactions are included at the level of a mean field approximation to a Hubbard Model. Within this approach, symmetry requires that the principal moments couple ferromagnetically both along and across the line defect leading to approximately 2/3 more up than down spin electrons per defect repeat unit.

[1]This work was supported by ONR, directly and through NRL.

5:18PM L37.00013 Correlating Magnetotransport and Diamagnetism of sp2-Bonded Carbon Networks Through the Metal-Insulator Transition , P.M. VORA, J.M. KIKKAWA, Department of Physics and Astronomy, University of Pennsylvania, P. GOPU, M. ROSARIO-CANALES, J.J. SANTIAGO-AVILES, Department of Electrical Engineering, University of Pennsylvania, C.R. PEREZ, Y. GOGOTSI, Department of Materials Science and Engineering, Drexel University — Titanium carbide-derived carbons (TiC-CDCs) are porous sp2-bonded networks synthesized by exposing TiC to chlorine gas at an elevated temperature. The latter "chlorination temperature" adjusts the size of graphitic domains within this material. We perform magnetoresistance, temperature dependent resistance, and SQUID magnetization measurements on TiC-CDC samples prepared at different chlorination temperatures. Transport reveals a metal-insulator transition where high (low) chlorination temperature samples are on the metallic (insulating) side of the transition. Magnetoresistance measurements are consistent with electronic transport in the weak and strong localization regimes for metallic and insulating samples, respectively. The diamagnetic contribution to the total magnetization increases with chlorination temperature, suggesting that the metal-insulator transition is associated with the expansion of graphitic domains. We also discuss a magnetoresistance anomaly observed in insulating samples. This work supported by NSF DMR-0907266 and NSF MRSEC DMR-05-20020.

Tuesday, March 22, 2011 2:30PM - 4:42PM –

Session L38 DCP DBP: Focus Session: Quantum Coherence in Biology II A130/131

2:30PM L38.00001 The role of quantum coherence in excitonic energy transfer: quantum process tomography, molecular dynamics and efficiency measures[1] , ALAN ASPURU-GUZIK, Department of Chemistry and Chemical Biology, Harvard University — Long-lived electronic coherences in various photosynthetic complexes at cryogenic and room temperature have generated vigorous efforts both in theory and experiment to understand their origins and explore their potential role to biological function. The ultrafast signals resulting from the experiments that show evidence for these coherences result from many contributions to the molecular polarization. Quantum process tomography (QPT) is a technique whose goal is that of obtaining the time-evolution of all the density matrix elements based on a designed set of experiments with different preparation and measurements. The QPT procedure was conceived in the context of quantum information processing to characterize and understand general quantum evolution of controllable quantum systems, for example while carrying out quantum computational tasks. We introduce our QPT method for ultrafast experiments, and as an illustrative example, apply it to a simulation of a two-chromophore subsystem of the FMO photosynthetic complex, which was recently shown to have long-lived quantum coherences. Our FMO model is constructed using an atomistic approach to extract relevant parameters for the simulation of photosynthetic complexes that consists of a quantum mechanics/molecular mechanics approach combined with molecular dynamics and the use of state-of-the-art quantum master equation approaches. We provide a set of methods that allow for quantifying the role of quantum coherence, dephasing, relaxation and other elementary processes in energy transfer efficiency in photosynthetic complexes, based on the information obtained from the atomistic simulations, or, using QPT, directly from the experiment. The possible presence or absence of effects due to correlated protein motion is discussed. The role of non-Markovianity will be discussed. The ultimate goal of the combination of this diverse set of methodologies is to provide a reliable way of quantifying the role of long-lived quantum coherences and obtain atomistic insight of their causes.

[1]Supported by DARPA Quantum Effects in BIological Environments and MIT/Harvard/BNL DOE Center for Excitonics.

3:06PM L38.00002 Multidimensional electronic spectroscopy of phycobiliproteins from cryptophyte algae , DANIEL TURNER, University of Toronto — We describe new spectroscopic measurements which reveal additional information regarding the observed quantum coherences in proteins extracted from photosynthetic algae. The proteins we investigate are the phycobiliproteins phycoerythrin 545 and phycocyanin 645. Two new avenues have been explored. We describe how changes to the chemical and biological environment impact the quantum coherence present in the 2D electronic correlation spectrum. We also use new multidimensional spectroscopic techniques to reveal insights into the nature of the quantum coherence and the nature of the participating states.

3:42PM L38.00003 Simulation study of 2D spectrum of molecular aggregates coupled to correlated vibrations[1] , DARIUS ABRAMAVICIUS, VYTAUTAS BUTKUS, LEONAS VALKUNAS, Physics Dept. Vilnius University, SHAUL MUKAMEL, Chemistry Dept. University of California Irvine — Oscillatory dynamics of two-dimensional (2D) spectra of photosynthetic pigment-protein complexes raise the questions of how to disentangle various origins of these oscillations, which may include quantum beats, quantum transport, or molecular vibrations. We study the effects of correlated overdamped fluctuations and under-damped vibrations on the 2D spectra of Fenna-Matthews-Olson (FMO) aggregate, which has well-resolved exciton resonances, and a circular porphyrin aggregate (P6), whose absorption shows vibrational progression. We use a generic exciton Hamiltonian coupled to a bath, characterized by a spectral density. Fluctuations have smooth, while vibtations have δ-type spectral densities. We show how various scenarios of correlated molecular fluctuations lead to some highly oscillatory crosspeaks. Molecular vibrations cause progression of diagonal peaks in the 2D spectrum and make their corresponding cross-peaks highly oscillatory. We, thus, demonstrate that bath fluctuations and molecular vibrations of realistic molecular aggregates are highly entangled in 2D spectroscopy.

[1]DA acknowledges grant VP1-3.1-SMM-07-V, SM - the grants CHE0745892 (NSF), DRPA BAA-10-40 QUBE.

3:54PM L38.00004 Coherent Control of Single Molecules at Room Temp , NIEK VAN HULST, DAAN BRINKS, RICHARD HILDNER, ICFO - the Institute of Photonic Sciences (Barcelona) Spain — Electronic coherence plays a key role in natural processes like ultrafast energy transfer and charge separation. Coherent control has proven powerful, however in complex biosystems with different conformations and environments, the intrinsic inhomogeneity of the synchronized subset severely limits the achievable degree of control. The ultimate solution to overcome intrinsic inhomogeneities is the investigation of the behavior of one molecule at a time. Here we report the observation and manipulation of vibrational wave-packet interference and electronic coherence in *individual molecules* at ambient conditions. Adapting time and phase distribution of the optical excitation field to the dynamics of each molecule we achieve a superior degree of control. The time-phase maps show distinct diversity between different, yet chemically identical, molecules. We induce Rabi-oscillations and control the coherent superposition state in a single molecule. Broadly distributed coherence decay times are found for different individual molecules giving direct insight into the structural heterogeneity of the local surroundings. Our approach allows single-molecule coherent control in a variety of complex inhomogeneous systems and thus to study the role of coherence in energy transfer of single biocomplexes under natural conditions. D.Brinks *et al. Nature* **465**, 905 (2010); R.Hildner *et al. Nat.Physics* doi:10.1038/nphys1858 (2010).

4:06PM L38.00005 Shaped ultrafast pulses for coherent control of energy flow in light harvesting complexes[1] , MOHAN SAROVAR, K. BIRGITTA WHALEY, University of California, Berkeley — We report on preliminary investigations of the use of evolutionary algorithms for the design of shaped femtosecond laser pulses to control energy flow in the Fenna-Matthews-Olson (FMO) light harvesting complex. We shape the experimentally accessible phase degrees of freedom of pulses of various duration and assess the ability to control (i) the exciton population on distinct chromophores, and (ii) the purity of the FMO complex state at short times. We assess the experimental feasibility of the designed pulses and sketch directions for future improvement of the pulse design technique.

[1]We acknowledge support from DARPA under the QuEST program

4:18PM L38.00006 Towards experimental verifications of the transport mechanisms in light-harvesting dynamics[1] , F. CARUSO, S. MONTANGERO, T. CALARCO, S.F. HUELGA, M.B. PLENIO, Ulm Univ. — Recently, we identified the key mechanisms explaining the very- high efficiency and robustness of excitation energy transfer in bacterial photosynthesis, finding that dephasing noise may remarkably enhance the capability of transmitting energy (classical/quantum information) in light-harvesting systems (in communication complex networks [Caruso et al., PRL 2010]), by opening up additional transport pathways and suppressing the ineffective ones. To verify the relevance of such mechanisms in the actual bio-molecular systems, we propose how to gain control over the light-harvesting dynamics by using quantum optimal control tools. In this way, by means of optimally shaped and 'robust' laser pulses, we can: i) faithfully prepare the photosystem in some specific initial state (local site or coherent superposition, e.g. quasi-dark and -bright states), and ii) probe efficiently the dynamics, under realistic experimental conditions, i.e. sample of randomly oriented light-harvesting complexes and extra laser constraints related to an experiment in progress. These results could allow us to more easily discriminate the different transport pathways, to characterize the environmental properties, and so enhance our comprehension of coherent processes in biological complexes.

[1]EU Marie-Curie Fellowship

4:30PM L38.00007 Photobiomodulation (PBM) Applications in Ophthalmology , ROBERT DOTSON, Private Medical Practice — In a very real sense, we are all creatures of light. This fact is just now beginning to impact medicine, as quantum theory begins to spread outside the confines of physics and into the life sciences. No longer can living organisms simply be viewed as retorts for biochemical reactions. They also demonstrate an energy component that will prove to be the unifying force of life in all its varied forms. With the advent of this shift in the life sciences, light is becoming an increasingly important diagnostic and therapeutic tool within medicine. Ophthalmologists have long been concerned with light and its application and, consequently, have an interest in the coming scientific revolution, photomedicine. A brief history of the use of low energy light for healing, a review of known mechanisms by which photons interact with living cells, and a review of some of the established cellular effects will be presented. Finally, brief clinical studies will be presented illustrating the benefits of PBM - specifically regarding: corneal healing, glaucoma, and dry age-related macular degeneration. The purpose of this talk is to introduce the emerging field of PBM to the physics community at large.

Tuesday, March 22, 2011 2:30PM - 5:18PM –

Session L39 DBP DPOLY DCP: Focus Session: Single Molecule Biophysics III: Novel Single Molecule Approaches to Biology A124/127

2:30PM L39.00001 High-resolution laser-based detection for magnetic tweezers , KEIR NEUMAN, National Institutes of Health — Magnetic tweezers are a versatile and powerful single-molecule manipulation technique capable of applying force and torque on single bio-molecules. They afford several unique advantages over other single-molecule manipulation techniques such as optical tweezers or atomic force microscopy. The hallmark of magnetic tweezers is the ability to twist bio-molecules without the need for complex optical instrumentation. Perhaps less known but of equal significance, magnetic tweezers rely on a slowly decaying magnetic field gradient (1 mm) to impose force so they are intrinsically configured in a passive force clamp mode. These features make magnetic tweezers particularly well suited for the study of nucleic acid structure, DNA topology, and protein-nucleic acid interactions. The one downside to most magnetic tweezers to date is that they rely on video tracking methods to determine the position of the particle. Despite recent progress, the spatial and temporal resolution and accuracy are fundamentally limited by image tracking techniques. I will describe recent improvements utilizing laser-based detection to overcome these limitations. We implemented back-scattered laser-based detection combined with video image tracking to achieve high-resolution, high-bandwidth, three-dimensional position tracking.

3:06PM L39.00002 Massively Parallel Single-Molecule Manipulation Using Centrifugal Force , WESLEY WONG, KEN HALVORSEN, Harvard University — Precise manipulation of single molecules has led to remarkable insights in physics, chemistry, biology, and medicine. However, two issues that have impeded the widespread adoption of these techniques are equipment cost and the laborious nature of making measurements one molecule at a time. To meet these challenges, we have developed an approach that enables massively parallel single- molecule force measurements using centrifugal force [1]. This approach is realized in the centrifuge force microscope, an instrument in which objects in an orbiting sample are subjected to a calibration-free, macroscopically uniform force- field while their micro-to-nanoscopic motions are observed. We demonstrate high- throughput single-molecule force spectroscopy with this technique by performing thousands of rupture experiments in parallel, characterizing force-dependent unbinding kinetics of an antibody-antigen pair in minutes rather than days. Currently, we are taking steps to integrate high-resolution detection, fluorescence, temperature control and a greater dynamic range in force. With significant benefits in efficiency, cost, simplicity, and versatility, single-molecule centrifugation has the potential to expand single-molecule experimentation to a wider range of researchers and experimental systems.

[1] K. Halvorsen, W.P. Wong, Biophysical Journal - Letters 98 (11), (2010).

3:18PM L39.00003 Horizontal Magnetic Tweezers for Micromanipulation of Single DNA-Protein Complexes , C. MCANDREW, Catholic University, A. SARKAR, P. MEHL, CUA — We report on the development of a new magnetic force transducer or "tweezer" that can apply pico-Newton forces on single DNA molecules in the focus plane. Since the changes in DNA's end-to-end extension are coplanar with the pulling force, there is no need to continually refocus. The DNA constructs (λ-DNA end labeled with a 3μm polystyrene bead and a 2.8μm paramagnetic sphere) and appropriate buffer are introduced to a custom built 400μL to 650μL closed cell. This closed cell isolates our sample and produces low-noise force and extension measurements. This chamber rests on a stage fixed to a three axis micromanipulator. Entering the flat chamber are two micropipettes, a 2.5μm id pipette for aspirating the polystyrene bead and a 20μm id pipette for injecting proteins of interest. The suction and the injection pipettes are rigidly mounted to a hydraulic, three-axis micromanipulator. DNA-bead constructs, once introduced to the chamber, can be located by moving the stage over the objective. We have shown that we can easily and reputably find, capture, and manipulate single molecules of DNA within a force range of 0.1pN to 100pN.

3:30PM L39.00004 Modeling the effects of internal and external fluctuations on lifetimes of proteins measured by an AFM , ERIC CORWIN, University of Oregon, MAXIME CLUSEL, Institut Laue-Langevin & CNRS Montpellier — Measurements of the distribution of the time to unfold a single- molecule of a given protein under an externally applied force have emerged as an important tool with which to study the mechanical stability and energy landscape of a protein. In such an experiment the protein is potentially subject both to internal fluctuations in structure as well as external fluctuations in temperature and applied force. We report on a theoretical exploration of the effects that each kind of fluctuation may have on the measured lifetime distribution. We show that it is extremely difficult to distinguish internal fluctuations from external fluctuations in the lifetime distribution. We find that the rate distribution has higher sensitivity to the origins of fluctuations. Therefore, we propose an experimental protocol to estimate the approximate magnitude of internal fluctuations by intentionally adding increasing amounts of external fluctuations and measuring the skewness of the resulting rate distribution.

3:42PM L39.00005 Onset of excluded volume in poly(ethylene oxide) elasticity measurements , ANDREW DITTMORE, Materials Dept., UCSB, DUSTIN B. MCINTOSH, Physics, UCSB, OMAR A. SALEH, Materials Dept., UCSB — We use magnetic tweezers to control tension in an 80 kDa poly(ethylene oxide) (PEG) chain. In good solvent, force effectively transforms the swollen coil into a series of smaller polymers ("tension blobs") and progressively diminishes self-avoidance interactions between distant parts of the chain. Excluded volume effects dominate the low-strain elasticity, where the extension follows a 2/3 power law in force in accordance with scaling predictions. These effects disappear as the polymer first enters a linear power-law regime, and then a high-force asymptotic regime well described by the Marko-Siggia wormlike chain model. All told, we observe two transitions between three elastic regimes. We show that the transition forces can be used to determine the polymer's Kuhn length, excluded volume, and thermal blob size, and find that PEG requires roughly 30 Kuhn lengths before self-avoidance becomes significant. Thus, we show that single-molecule elasticity can quantify the onset of a polymer's excluded volume, a problem that has eluded bulk measurement techniques.

3:54PM L39.00006 Peptide Nucleic Acids as Tools for Single-Molecule Sequence Detection and Manipulation , HAGAR ZOHAR, CRAIG HETHERINGTON, CARLOS BUSTAMANTE, SUSAN MULLER, University of California, Berkeley — The ability to strongly and sequence-specifically attach modifications such as fluorophores and haptens to individual double-stranded (ds) DNA molecules is critical to a variety of single-molecule experiments. We propose using modified peptide nucleic acids (PNAs) for this purpose and implement them in two model single-molecule experiments where individual DNA molecules are manipulated via microfluidic flow and optical tweezers, respectively. We demonstrate that PNAs are versatile and robust sequence-specific tethers.

4:06PM L39.00007 Resolving Single Molecule Lysozyme Dynamics with a Carbon Nanotube Electronic Circuit , YONGKI CHOI, ISSA S. MOODY, ISRAEL PEREZ, TATYANA SHEPS, GREGORY A. WEISS, PHILIP G. COLLINS, Depts. of Physics and Astronomy, Chemistry, and Molecular Biology, Univ. of California at Irvine, Irvine, CA 92697 — High resolution, real-time monitoring of a single lysozyme molecule is demonstrated by fabricating nanoscale electronic devices based on single-walled carbon nanotubes (SWCNT). In this sensor platform, a biomolecule of interest is attached to a single SWCNT device. The electrical conductance transduces chemical events with single molecule sensitivity and 10 microsecond resolution. In this work, enzymatic turnover by lysozyme is investigated, because the mechanistic details for its processivity and dynamics remain incompletely understood. Stochastically distributed binding events between a lysozyme and its binding substrate, peptidoglycan, are monitored via the sensor conductance. Furthermore, the magnitude and repetition rate of these events varies with pH and the presence of inhibitors or denaturation agents. Changes in the conductance signal are analyzed in terms of lysozyme's internal hinge motion, binding events, and enzymatic processing.

4:18PM L39.00008 Mechanical properties of NRR domain from human Notch 1 studied by single molecule AFM force spectroscopy , ROBERT SZOSZKIEWICZ, ASHIM DEY, Dept. of Physics, Kansas State University — For proteins in living cells, forces are present from macroscopic to single molecule levels. Single molecule atomic force microscopy in force extension (FX-AFM) mode measures forces at which proteins undergo major conformational transitions with $\sim$10 pN force sensitivity (FX-AFM). Here, we present the results of the FX-AFM experiments on a construct comprising the NRR domain from human Notch 1. It is believed that understanding the mechanical properties of Notch at the single molecule level can help to understand its role in triggering some breast cancers. The experimental results on the Notch construct and further analysis revealed several conformational transitions of this molecule under force. These results opened a path for further investigations of Notch constructs at various physiologically relevant conditions.

4:30PM L39.00009 Non-Perturbative Tracking of Processive DNA Synthesis with Single-Molecule Fluorescence , EVERETT LIPMAN, CHARLES WICKERSHAM[1], Department of Physics, University of California, Santa Barbara — We have demonstrated recently that double-stranded DNA labeled with a periodic series of fluorescent dyes can be used to track a single helicase. Here we describe how this technique can be modified to follow DNA synthesis. By means of a stepwise loss of fluorescence during strand displacement, we monitor processive motion of a single $\phi 29$ DNA polymerase without labeling or altering the enzyme or the template strand, and without applying any force. We observe a wide range of speeds, with the highest exceeding by several times that observed in other single-molecule experiments. Because this method enables repeated observations of the same polymerase traversing identical segments of DNA, it should prove useful for studying sequence-specific effects in DNA replication and transcription.

[1]Present address: California Institute for Quantitative Biomedical Research, UC Berkeley

4:42PM L39.00010 Single molecule studies reveal new mechanisms for microtubule severing[1] , JENNIFER ROSS, JUAN DANIEL DIAZ-VALENCIA, MARGARET MORELLI, UMass Amherst, DONG ZHANG, DAVID SHARP, AECOM — Microtubule-severing enzymes are hexameric complexes made from monomeric enzyme subunits that remove tubulin dimers from the microtubule lattice. Severing proteins are known to remodel the cytoskeleton during interphase and mitosis, and are required in proper axon morphology and mammalian bone and cartilage development. We have performed the first single molecule imaging to determine where and how severing enzymes act to cut microtubules. We have focused on the original member of the group, katanin, and the newest member, fidgetin to compare their biophysical activities in vitro. We find that, as expected, severing proteins localize to areas of activity. Interestingly, the association is very brief: they do not stay bound nor do they bind cooperatively at active sites. The association duration changes with the nucleotide content, implying that the state in the catalytic cycle dictates binding affinity with the microtubule. We also discovered that, at lower concentrations, both katanin and fidgetin can depolymerize taxol-stabilized microtubules by removing terminal dimers. These studies reveal the physical regulation schemes to control severing activity in cells, and ultimately regulate cytoskeletal architecture.

[1]This work is supported by the March of Dimes Grant #5-FY09-46.

4:54PM L39.00011 Polymer Nanocomposites as a Facile Method for Engineering Acto-Myosin Networks at the Interface , MATTHEW CAPORIZZO, University of Pennsylvania Department of Materials Science and Engineering, YUJIE SUN, YALE GOLDMAN, University of Pennsylvania Department of Physiology, RUSSELL COMPOSTO, University of Pennsylvania Department of Materials Science and Engineering, NANO-BIO INTERFACE CENTER COLLABORATION — Filamentous actin acts as the rails for the molecular motor myosin in muscle contraction and intercellular mass transport. Consequently, understanding the process by which actin organizes, polymerizes, and binds is fundamental for the design of myosin based actuators capable of responding to external stimuli. Starting with atomically smooth, freshly cleaved mica optically coupled to glass slides, a random copolymer nanoparticle composite is engineered for *in situ* single molecule TIRF/AFM studies with controlled roughness, electrostatic binding strength, and binding site density. Four distinct regimes of actin binding are observed; no attachment, end-on attachment, weak side-on attachment, and side-on immobilization. Transitions between regimes are likely to mark competition between the affinity to charged nanoparticles and the inherent resistance of the semi-rigid filaments to bending. Surface conditions optimal for actin immobilization are identified, and Myosin V stepping kinetics are studied on the artificially immobilized filaments, confirming filament support of motility. Supported by NSF grant DMR-0425780.

5:06PM L39.00012 Electrostatic Effects on the Elasticity of Single ssDNA Molecules , DUSTIN B. MCINTOSH, OMAR A. SALEH, University of California Santa Barbara — Nucleic acids are highly-charged polyelectrolytes whose structure and function strongly depend on the concentration and type of salt ions in solution. We have created a simple experimental system for studying nucleic acid/ ion interactions, based on magnetic-tweezer measurements of the elasticity of single denatured ssDNA molecules in solutions with a known salt concentration. Using this system, we were able to reconcile single-molecule force-extension data with scaling theories of self-avoiding polymers, and we found that the Kuhn length of ssDNA scales with the Debye length in NaCl solutions. (Saleh et al., PRL 102, 068301 (2009)). Here, we use the system to investigate interactions of ssDNA with multivalent salts. We find that, in divalent salt, ssDNA elasticity is qualitatively similar to that in monovalent salt, but with significant quantitative differences. Notably, at low ionic strength, ssDNA in divalent salt maintains the same low-force scaling behavior ("Pincus blob" regime) as seen in monovalent salts. However, there are differences in the elastic behavior at high forces ($>$ a few pN). In addition, analysis of the low-force scaling behavior indicates it requires $\sim$100 fold smaller concentrations of divalent salt to condense ssDNA. We discuss the data in the context of electrostatic theories, including Debye-Huckel, as well as bulk experiments on similar systems.

Tuesday, March 22, 2011 2:30PM - 5:18PM –

Session L40 DBP: Focus Session: Noisy Dynamics as Survival Strategies and Nanopores A122/123

2:30PM L40.00001 TBA , MATTHEW R. BENNETT, Rice University — This abstract not available.

3:06PM L40.00002 Evolution and Biophysics of the *Escherichia coli lac* Operon , J. CHRISTIAN RAY, The University of Texas M. D. Anderson Cancer Center, OLEG IGOSHIN, Rice University, SELWYN QUAN, RUSSELL MONDS, Stanford University, TIM COOPER, The University of Houston, GÁBOR BALÁZSI, The University of Texas M. D. Anderson Cancer Center — To understand, predict, and control the evolution of living organisms, we consider biophysical effects and molecular network architectures. The lactose utilization system of *E. coli* is among the most well-studied molecular networks in biology, making it an ideal candidate for such studies. Simulations show how the genetic architecture of the wild-type operon attenuates large metabolic intermediate fluctuations that are predicted to occur in an equivalent system with the component genes on separate operons. Quantification of gene expression in the *lac* operon evolved in growth conditions containing constant lactose, alternating with glucose, or constant glucose, shows characteristic gene expression patterns depending on conditions. We are simulating these conditions to show context-dependent biophysical sources and costs of different lac operon architectures.

3:18PM L40.00003 The effects of nongenetic memory on population level sensitivity to stress[1] , RHYS ADAMS, DMITRY NEVOZHAY, The University of Texas MD Anderson Cancer Center, ELIZABETH VAN ITALLIE, MATTHEW BENNETT, Rice University, GABOR BALAZSI, The University of Texas MD Anderson Cancer Center — While gene expression is often thought of as a unidirectional determinant of cellular fitness, recent studies have shown how growth retardation due to protein expression can affect gene expression levels in single cells. We developed two yeast strains carrying a drug resistance protein under the control of different synthetic gene constructs, one of which was monostable, while the other was bistable. The gene expression of these cell populations was tuned using a molecular inducer so that their respective means and noises were identical, while their nongenetic memory properties were different. We tested the sensitivity of these two cell population distributions to the antibiotic zeocin. We found that the gene expression distributions of bistable cell populations were sensitive to stressful environments, while the gene expression distribution of monostable cells were nearly unchanged by stress. We conclude that cell populations with high nongenetic memory are more adaptable to their environment.

[1]This work was funded by the National Institutes of Health through the NIH Director's New Innovator Award Program, 1-DP2- OD006481-01.

3:30PM L40.00004 Interplay of Noisy Gene Expression and Dynamics Explains Patterns of Bacterial Operon Organization[1] , OLEG IGOSHIN, Rice University — Bacterial chromosomes are organized into operons – sets of genes co-transcribed into polycistronic messenger RNA. Hypotheses explaining the emergence and maintenance of operons include proportional co-regulation, horizontal transfer of intact "selfish" operons, emergence via gene duplication, and co-production of physically interacting proteins to speed their association. We hypothesized an alternative: operons can reduce or increase intrinsic gene expression noise in a manner dependent on the post-translational interactions, thereby resulting in selection for or against operons in depending on the network architecture. We devised five classes of two-gene network modules and show that the effects of operons on intrinsic noise depend on class membership. Two classes exhibit decreased noise with co-transcription, two others reveal increased noise, and the remaining one does not show a significant difference. To test our modeling predictions we employed bioinformatic analysis to determine the relationship gene expression noise and operon organization. The results confirm the overrepresentation of noise-minimizing operon architectures and provide evidence against other hypotheses. Our results thereby suggest a central role for gene expression noise in selecting for or maintaining operons in bacterial chromosomes. This demonstrates how post-translational network dynamics may provide selective pressure for organizing bacterial chromosomes, and has practical consequences for designing synthetic gene networks.

[1]This work is supported by National Institutes of Health grant 1R01GM096189-01.

4:06PM L40.00005 Population-level control of gene expression[1] , DMITRY NEVOZHAY, RHYS ADAMS, Department of Systems Biology, UT M. D. Anderson Cancer Center, ELIZABETH VAN ITALLIE, MATTHEW BENNETT, Department of Biochemistry and Cell Biology and Institute of Biosciences and Bioengineering, Rice University, GABOR BALAZSI, Department of Systems Biology, UT M. D. Anderson Cancer Center — Gene expression is the process that translates genetic information into proteins, that determine the way cells live, function and even die. It was demonstrated that cells with identical genomes exposed to the same environment can differ in their protein composition and therefore phenotypes. Protein levels can vary between cells due to the stochastic nature of intracellular biochemical events, indicating that the genotype-phenotype connection is not deterministic at the cellular level. We asked whether genomes could encode isogenic cell populations more reliably than single cells. To address this question, we built two gene circuits to control three cell population-level characteristics: gene expression mean, coefficient of variation and non-genetic memory of previous expression states. Indeed, we found that these population-level characteristics were more predictable than the gene expression of single cells in a well-controlled environment.

[1]This research was supported by the NIH Director's New Innovator Award 1DP2 OD006481-01 and Welch Foundation Grant C-1729.

4:18PM L40.00006 Functional Differentiation in EVS modeling , IRINA TROFIMOVA, CI Laboratory, WILLIAM SULIS, McMaster University — Ensembles with Variable Structures (EVS) were introduced in mid-1990s as stochastic milti-agent models in which agents possessed either formal diversity (described in a multi-dimensional vector space of abstract characteristics) or resource-oriented diversity (Trofimova, 2000). The process of functional differentiation (i.e. appearance of functional roles) is modelled as constraints on the flow of resources which pass through agents of the model. These constraints are: 1) the maximum amount of resource that an individual can accept from outside, 2) the maximum amount of resource that an individual can give back to the population or other environment, 3) distribution of the exchange of the resource over time (frequency and amount of the resource per step), and 4) the maximum amount of contacts that an individual can hold with such environment (sociability). Sociability appears to have a major impact on clustering dynamics within the population and to be an order parameter in phase transition in clustering behaviour, therefore it interfered with functional differentiation. Two patterns of functional differentiation were observed, before and after the phase transition in clustering, corresponding to sociability values below and after the critical points.

4:30PM L40.00007 Fitness in fluctuating environments , SORIN TANASE NICOLA, ILYA NEMENMAN, Emory University — Often environments change faster than the time needed to evolve optimal phenotypes through cycles of mutation and selection. We focus on this case, but assume that environmental oscillations are slower than an individual's lifetime. This is relevant, for example, for bacterial populations confronted with daily environmental changes. We analyze a resource-limited competition between a mutant phenotype and the ancestor. Environmental dynamics is represented by periodically varying, off-phase parameters of the corresponding Lotka-Volterra model. For the very slow dynamics (but still faster than the fixation time scale) the strength and the sign of selection are functions of the birth/death rates averaged over all of the environmental states and independent of the period of the fluctuations. For faster fluctuations, selection depends on the particular sequence of the successive environmental states. In particular, a time reversal of the environmental dynamics can change the sign of the selection. We conclude that the fittest phenotype in a changing environment can be very different from both the optimal phenotype in the average environment, and the phenotype with the largest average fitness.

4:42PM L40.00008 Development of an electrical nanopore device towards the control of the translocation of DNA with single base resolution[1] , HONGBO PENG, BINQUAN LUAN, STANISLAV POLONSKY, STEPHEN ROSSNAGEL, GUSTAVO STOLOVITZKY, IBM Research at Thomas J. Watson Research Center — Recently, application of nanopores to low-cost DNA sequencing has attracted great interest as there is great need to reduce the cost of sequencing a whole human genome to $1000. A key issue in the field of nanopore DNA sequencing is to control the DNA translocation. Here we will report the development of what we call a "DNA transistor": a nanopore-based electrical device for controlling the translocation of DNA with single base resolution. The key part of this device is a free standing membrane, within which multiple layers of electrically addressable metal electrodes separated by dielectric layers are embedded. A 1-5 nanometer size pore is made through the membrane. We demonstrated that such a device is electrically viable for the electrode layer or the spacing dielectric layer as thin as 3 nm in 1 mM KCl solution. Induced electrical signals on the nano-electrodes by the translocating DNA, as well as the modulation of DNA translocation speed by the voltage bias applied on the nanoelectrodes are also observed. Our ongoing experiments test if the modulated electrical field can trap or translocate DNA at a single base resolution.

[1]This work is supported by NHGRI under grant number R01HG005110.

4:54PM L40.00009 ABSTRACT WITHDRAWN –

5:06PM L40.00010 Polymerization of nanopores for controlled surface charges[1] , WASEEM ASGHAR, AZHAR ILYAS, RICHARD TIMMONS, SAMIR IQBAL, The University of Texas at Arlington — The solid-state nanopores have emerged as a novel candidate for DNA sequencing and protein analysis. Traditional approaches for nanopore diameter shrinking use electron microscopy induced shrinking and deposition processes. These approaches are limited due to less control on surface composition of the deposited film, slow deposition rate and initial membrane thickness dependant shrinking processes. We report a novel approach of pulsed plasma polymer deposition which addresses all of the above described issues. The surface chemical composition and geometry of solid-state nanopores are controlled by plasma deposition of highly conformal thin polymeric films. Surface energy and pore-wall surface charges are controlled using appropriate monomer during plasma deposition process.

[1]This work was supported by National Science Foundation Career Grant (ECCS 0845669).

Tuesday, March 22, 2011 2:30PM - 5:30PM –

Session L41 DCP: Condensed Phase Dynamics and Structure A115/117

2:30PM L41.00001 Temperature and Lengthscale Dependence of Solvophobic Solvation in a Water-like Liquid , JOHN DOWDLE, PETER ROSSKY, University of Texas at Austin — Temperature and lengthscale dependence of the solvation of cavity solutes is investigated along the saturation curve of the Jagla liquid, a simple liquid consisting of particles that interact via a spherically symmetric potential combining hard and soft core interactions. The results are compared with an identical calculation for a model of a typical atomic liquid, the Lennard-Jones potential, and with predictions for cavity solubilities in water made by the recently developed cavity equation of state. We find that the Jagla liquid captures the qualitative thermodynamic behavior of hydrophobic hydration as a function of temperature for both small and large lengthscale solutes. The results suggest that a competition between two lengthscales that favors low- density, open structures as temperature is decreased is an essential interaction of a liquid that models hydrophobic hydration.

2:42PM L41.00002 Effects of Physical Confinement on the Hysteresis between Melting and Freezing Temperatures of Decanol[1] , SAMUEL AMANUEL, JARGALSAIKHAN DULMAA, AMER KHRAISAT, Department of Physics and Astronomy, Union College, Schenectady, NY 12308 — There is substantial evidence that physical confinement alters melting and freezing temperatures of materials. These have been qualitatively explained using free energy considerations. However, it is not clear how physical confinement influences melting and freezing when the bulk material itself exhibits substantial supercooling. Bulk 2-decanol, for instance, exhibits substantial hysteresis between its melting (approximately -23°C) and freezing (-3°C) temperatures. Evidently, both its melting and freezing temperatures are influenced by physical size. However, the hysteresis between the freezing and melting temperatures seems less sensitive to physical size. This may be the result of differences in homogeneous versus heterogeneous nucleation in physically confined 2-decanol.

[1]This work has been supported by Faculty Research Fund, Union College.

2:54PM L41.00003 Evaluating the Liquid Liquid Phase Transition Hypothesis of Supercoooled Water , DAVID LIMMER, DAVID CHANDLER, University of California, Berkeley — To explain the anomalous behavior of supercooled water it has been conjectured that buried within an experimentally inaccessible region of liquid water's phase diagram there exists a second critical point, which is the terminus of a first order transition line between two distinct liquid phases. The so-called liquid-liquid phase transition (LLPT) has since generated much study, though to date there is no consensus on its existence. In this talk, we will discuss our efforts to systematically study the metastable phase diagram of supercooled water through computer simulation. By employing importance-sampling techniques, we have calculated free energies as a function of the density and long-range order to determine unambiguously if two distinct liquid phases exist. We will argue that, contrary to the LLPT hypothesis, the observed phenomenology can be understood as a consequence of the limit of stability of the liquid far away from coexistence. Our results suggest that homogeneous nucleation is the cause of the increased fluctuations present upon supercooling. Further we will show how this understanding can be extended to explain experimental observations of hysteresis in confined supercooled water systems.

3:06PM L41.00004 Anomalous lattice parameter isotope-shift in hexagonal ice Ih from first principle calculations[1] , BETÜL PAMUK, MARIVI FERNANDEZ-SERRA, PHILIP ALLEN, Stony Brook University — The lattice parameters of light (H_2O) and heavy (D_2O) Ih ice differ by 0.09% [1]. The larger lattice constant is that of the heavier isotope, contrary to normal expectations. This isotope shift of the lattice constant is linked to the zero point energy of phonons in ice. In particular, it can be linked to the anti-correlation of the O-H stretch frequency and the O-O distance in H-bonded materials. In order to determine which phonons give the anomaly, we calculate Grüneisen parameters of H_2O and D_2O ice using first principles density functional theory, within the frozen phonon approximation. Our results show a strong dependence on the density functional chosen. We analyze these differences and make connections to experiment. These results indicate that not only H-bond effects but also van der Waals interactions are necessary to reproduce the correct lattice constant zero-point shifts in ice.

[1] B. K. Röttger et. al., Acta Cryst. B **50**, 644-648 (1994).

[1]This work is supported by DOE award numbers DE-FG02-08ER46550 and DE-SC0003871.

3:18PM L41.00005 Local effects in the X-ray absorption spectrum of salt water , ERIC SCHWEGLER, Lawrence Livermore National Laboratory, HEATHER KULIK, Stanford University, NICOLA MARZARI, University of Oxford, ALFREDO CORREA, Lawrence Livermore National Laboratory, DAVID PRENDERGAST, Lawrence Berkeley National Laboratory, GIULIA GALLI, UC Davis — We have used first principles molecular dynamics and theoretical X-ray absorption spectroscopy (XAS) to investigate the aqueous solvation of cations in $MgCl_2$, $CaCl_2$, and NaCl solutions. We focus our discussion on the species-specific effects that Mg^{2+}, Ca^{2+}, and Na^+ have on the X-ray absorption spectrum of the respective solutions. For the divalent cations, we find that the water molecules that form a rigid first solvation shell around Mg^{2+} and a more flexible solvation shell around Ca^{2+} also exhibit differing hydrogen bonding characteristics. Acceptor hydrogen bonds present in the water surrounding Ca^{2+} enhance a post-edge peak near 540 eV in the XAS spectrum, while the absence of such hydrogen bonding features for the first shell surrounding Mg^{2+} corresponds to a diminished intensity at the post-edge peak. For Na^+, we find that a broad tilt angle distribution results in broadened post-edge features, despite donor-and-acceptor populations comparable to Ca^{2+}. We present re-averaged spectra of the $MgCl_2$, $CaCl_2$, and NaCl solutions that provide an explanation of concentration-dependent features that have been found in corresponding experimental measurements.

3:30PM L41.00006 Nuclear momentum distribution and potential energy surface in hexagonal ice[1] , LIN LIN, Princeton University, JOSEPH MORRONE, Columbia University, ROBERTO CAR, Princeton University, MICHELE PARRINELLO, ETH Zurich — The proton momentum distribution in ice Ih has been recently measured by deep inelastic neutron scattering and calculated from open path integral Car-Parrinello simulation. Here we report a detailed investigation of the relation between momentum distribution and potential energy surface based on both experiment and simulation results. The potential experienced by the proton is largely harmonic and characterized by 3 principal frequencies, which can be associated to weighted averages of phonon frequencies via lattice dynamics calculations. This approach also allows us to examine the importance of quantum effects on the dynamics of the oxygen nuclei close to the melting temperature. Finally we quantify the anharmonicity that is present in the potential acting on the protons.

[1]This work is supported by NSF and by DOE.

3:42PM L41.00007 The quantum nature of the hydrogen bond: insight from path-integral molecular dynamics , BRENT WALKER, XIN-ZHENG LI, ANGELOS MICHAELIDES, London Centre for Nanotechnology and Department of Chemistry, University College London, London WC1E 6BT, U.K — Hydrogen (H) bonds are weak, generally intermolecular bonds, that hold together much of soft matter, the condensed phases of water, network liquids, and many ferroelectric crystals. The small mass of H means H-bonds are inherently quantum mechanical; effects such as zero point motion and tunneling should be considered, although often are not. In particular, a consistent picture of quantum nuclear effects on the strength of H-bonds and consequently the structure of H-bonded systems is still absent. Here, we report *ab initio* path-integral molecular dynamics studies on the quantum nature of the H-bond. Systematic examination of a range of H-bonded systems shows that quantum nuclei weaken weak H-bonds but strengthen relatively strong ones. This correlation arises from a competition between anharmonic intermolecular bond bending and intramolecular bond stretching. A simple rule of thumb enables predictions to be made for H-bonded bonded materials in general with merely classical knowledge (e.g. H-bond strength or H-bond length). Our work rationalizes the contrasting influence of quantum nuclear dynamics on a wide variety of materials, including liquid water and HF, and highlights the need for flexible molecules in force-field based studies of quantum nuclear dynamics.

3:54PM L41.00008 Hydration phase diagram for BaO terminated $BaTiO_3$[1] , JOHN MARK MARTIREZ, Department of Chemistry, University of Pennsylvania, WISSAM AL-SAIDI, Department of Chemical and Petroleum Engineering, University of Pittsburgh, ANDREW RAPPE, Department of Chemistry, University of Pennsylvania — This study reveals geometries H_2O adopts upon adsorption on BaO terminated $BaTiO_3$(BTO) at low to high saturation. A hydration phase diagram for the aforementioned termination is presented, for moderate temperatures, and moderate to ultra high vacuum H_2O pressures. Calculations suggest a very stable H_2O adsorption for wide range of pressures, including high vacuum conditions (p_{H_2O} 10^{-12} bar). This opens venues for mechanistic studies and hopefully will serve as a guide to condition that might suppress H_2O adsorption on BTO for applications where it is undesired.

[1]The authors acknowledge support from the AFOSR under Grant FA9550-07-1-0397, from the DOE under Grant DE-FG02-07ER15920, and computational support from the HPCMO.

4:06PM L41.00009 ABSTRACT WITHDRAWN –

4:18PM L41.00010 Topological reaction coordinates to explore the structure of atomic clusters and organic molecule isomers from first principles , FABIO PIETRUCCI, CECAM EPF Lausanne (CH), WANDA ANDREONI, CECAM and Institut de Théorie des Phénomènes Physique EPF Lausanne (CH) — We introduce a simple reaction coordinate based on spectral graph theory which describes the topology of the network of chemical bonds around a given atom. We employ the reaction coordinate in combination with DFT-based first-principles metadynamics to systematically explore the possible structures of silicon and carbon clusters (including fullerene-like cages) for sizes of tens of atoms. From our extensive exploration we are able to estimate the fractal dimension of the configuration space, which both for silicon and carbon clusters turns out to be quite low. Using the same approach we simulate the interconversion among a large number of chemically relevant organic molecules which are isomers of the C_4H_5N formula unit, and we demonstrate the possibility of automatically exploring isomerisation, association, and decomposition reactions without prior knowledge of the products involved.

4:30PM L41.00011 Transport through a quantum dot with excitonic dot-lead coupling[1] , FLORIAN ELSTE, DAVID R. REICHMAN, ANDREW J. MILLIS, Columbia University — We study the effect of a Coulombic dot-lead interaction on transport through a quantum dot hybridized to two Luttinger-liquid leads.[2] A bosonization approach is applied to treat the interaction between charge fluctuations on the dot and the dynamically generated image charge in the leads.[3] The nonequilibrium distribution function of the dot and the tunneling current are computed within a master-equation approach. Particular attention is paid to two situations: (i) a quantum dot placed between two leads such that it cuts the Luttinger liquid into two semi-infinite quantum wires; (ii) a quantum dot side-hybridized to two parallel infinite quantum wires. The presence of the excitonic dot-lead coupling is found to enhance transport in the vicinity of the Coulomb-blockade threshold. This behavior is in contrast to the usual power-law suppression of electronic tunneling which is found if this interaction is ignored.

[1]AJM acknowledges support from NSF-DMR-0705847 and FE from the Deutsche Forschungsgemeinschaft.
[2]F. Elste, D. R. Reichman, and A. J. Millis, arXiv:1010.2251
[3]F. Elste, D. R. Reichman, and A. J. Millis, Phys. Rev. B **81**, 205413 (2010)

4:42PM L41.00012 Spectroscopic and Theoretical Investigations of the Potential Energy Surfaces of Molecules with Intramolecular π-type Hydrogen Bonding[1] , ESTHER OCOLA, HEE-WON SHIN, ABDULAZIZ AL-SAADI, JAAN LAANE, Texas A&M University — Spectroscopic methods and theoretical calculations have been utilized to investigate the conformations of several cyclic organic molecules. The laser induced fluorescence (LIF) spectra of 2-indanol show the presence of four conformations. The one with intramolecular hydrogen bonding between the –OH group and the benzene ring is of lowest energy. The potential energy surface (PES) in terms of the ring puckering and internal rotational vibrations, which govern the conformational changes, was determined. 3-Cyclopenten-1-ol possesses a similar PES as established from its infrared and Raman spectra and theoretical calculations. This PES also shows the presence of four conformations. The π-bonding conformer lies at lowest energy. LIF has been used to study the conformational energies of 2-hydroxytetralin, and 2-cyclohexenol has been investigated by infrared and Raman techniques. The analyses of the hydrogen bonding in these molecules as well as in a dozen others were supported by both *ab initio* and DFT calculations.

[1]Supported by R.A. Welch grant A-0396.

4:54PM L41.00013 Raman Spectra and the Potential Energy Function for the Internal Rotation of 1,3-Butadiene and its Isotopomers[1] , JAAN LAANE, PRAVEENKUMAR BOOPALACHANDRAN, Texas A&M University, NORMAN CRAIG, Oberlin College — The gas-phase Raman spectra of 1,3-butadiene-d_0, 2,3-d_2, 1,1,4,4-d_4, and –d_6 have been collected with CCD detection with numerous scans of ten hours or more. For each isotopomer eight Raman transitions in the 240-330 cm^{-1} region corresponding to double quantum jumps of the A_u internal rotation (ν_{13}) were observed for the *trans* conformer. Weaker bands in the 170-260 cm^{-1} region were assigned to the *gauche* conformation, which lies at higher electronic energy. A periodic potential function for the internal rotation, which fits the data for all the isotopomers, was determined. This function shows the *gauche* form to be 966 cm^{-1} higher in energy and the barrier between the *trans* and *gauche* structures to be 2055 cm^{-1}. The *cis* structure has an energy 408 cm^{-1} higher than the *gauche*. Fourteen combination band or hot band series involving ν_{13} for the *trans* conformer were also observed, and these allow the internal rotation levels in various excited vibrational states to be determined.

[1]Supported by R.A. Welch grant A-0396.

5:06PM L41.00014 Transition and Excited States of 1,1'-azo-bis-1,2,3-triazole , VLADIMIR GONCHAROV, Vanderbilt University, OLGA GONCHAROVA, Vertex Pharmaceuticals Inc., KALMAN VARGA, Vanderbilt University — A novel photochromic molecule has been recently synthesized[1]. The photo-isomerization of this nitrogen-rich small molecule is efficiently controlled by a xenon flash lamp suggesting a potential in photonic and molecular mechanics applications. We perform a synergistic quantum molecular dynamics (QMD), real-time time dependent density functional theory (TDDFT) and TDDFT- perturbation theory study to capture and elucidate the transition state, excitation energies and optical properties of the molecule. We also use it to test performance of recently developed real-time TDDFT method[2] to calculate hyperpolarizabilities and compare results with the Sternheimer method.

[1]Yu-Chuan Li et al. *J. Am. Chem. Soc.*, 2010, 132, 12172
[2]V. Goncharov, K. Varga, *Phys. Rev. B* 2010, submitted.

5:18PM L41.00015 Importance of Electronic Relaxation for Inter-Coulombic Decay in Aqueous Systems[1] , DAVID PRENDERGAST, Molecular Foundry, Lawrence Berkeley National Laboratory (LBNL), CRAIG P. SCHWARTZ, RICHARD J. SAYKALLY, Chemistry Dept., University of California, Berkeley and Chemical Sciences, LBNL, SHERVIN FATEHI, Kenneth S. Pitzer Center for Theoretical Chemistry, University of California, KEITH V. LAWLER, Chemical Sciences, LBNL, C. WILLIAM MCCURDY, Chemical Sciences, LBNL and Departments of Applied Science and Chemistry, University of California, Davis — Inspired by recent photoelectron spectroscopy experiments on hydroxide solutions, we have examined the conditions necessary for enhanced (and, in the case of solutions, detectable) intermolecular Coulombic decay (ICD) – Auger emission from an atomic site other than that originally excited. We present general guidelines, based on energetic and spatial overlap of molecular orbitals, for this enhancement of ICD-based energy transfer in solutions. These guidelines indicate that this decay process should be exhibited by broad classes of biomolecules and suggest a design criterion for targeted radiooncology protocols. Our findings indicate that ICD processes in hydroxide solutions are not dependent on hydroxide hydrogen bond donation.

[1]Supported by DOE BES Contract No. DE-AC02-05CH11231.

Tuesday, March 22, 2011 2:30PM - 5:30PM –
Session L42 DPOLY: Dillon Medal Symposium A302/303

2:30PM L42.00001 John H. Dillon Medal Talk: Protein Fibrils, Polymer Physics: Encounter at the Nanoscale , RAFFAELE MEZZENGA, ETH - Zurich — Aggregation of proteins is central to many aspects of daily life, ranging from blood coagulation, to eye cataract formation disease, food processing, or neurodegenerative infections. In particular, the physical mechanisms responsible for amyloidosis, the irreversible fibril formation of various proteins implicated in protein misfolding disorders such as Alzheimer, Creutzfeldt-Jakob or Huntington's diseases, have not yet been fully elucidated. In this talk I will discuss how polymer physics and colloidal science concepts can be used to reveal very useful information on the formation, structure and properties of amyloid protein fibrils. I will discuss their physical properties at various length scales, from their collective liquid crystalline behavior in solution to their structural features at the single molecule length scale and show how polymer science notions can shed a new light on these interesting systems. 1) "Understanding amyloid aggregation by statistical analysis of atomic force microscopy images" J. Adamcik, J.-M. Jung, J. Flakowski, P. De Los Rios, G. Dietler and R. Mezzenga, Nature nanotechnology, 5, 423 (2010)

3:06PM L42.00002 Interdiffusion in bilayers of PCBM fullerene and poly(3-hexyl thiophene) P3HT , EDWARD J. KRAMER, NEAL D. TREAT, MICHAEL A. BRADY, UCSB, MICHAEL F. TONEY, SSRL, MICHAEL L. CHABINYC, CRAIG J. HAWKER, UCSB — Bulk heterojunction (BHJ) photovoltaic materials, typified by blends of PCBM and P3HT, are often regarded as immiscible in the absence of casting solvent. We use dynamic secondary ion mass spectrometry and grazing incidence wide angle X-ray scattering to probe the interdiffusion of bilayers of P3HT and deuterated dPCBM. We find that the as cast P3HT film is semicrystalline, while the dPCBM film is amorphous, and that there is complete interdiffusion between dPCBM and P3HT after annealing for 300 s at T = 150°C, a typical treatment to improve device efficiency. This interdiffusion occurs without disrupting the ordered lamellar stacking in the P3HT crystallites, showing that PCBM is miscible with amorphous P3HT at this temperature (the size and/or perfection of the P3HT crystallites actually increases during the annealing). At T < 150°C rapid diffusion of dPCBM into P3HT still occurs but the dPCBM concentration reaches an apparent solubility limit after long anneals, a limit that decreases with decreasing temperature. This result suggests that dPCBM will phase separate from amorphous P3HT in the BHJ on cooling from 150°C to room temperature.

3:18PM L42.00003 , GEROGES HADZIIOANNOU, —

3:30PM L42.00004 Coarse grained polystyrene simulations: Static and dynamic properties[1] , KURT KREMER, Max Planck Institute for Polymer Research, Mainz, Germany — By combining input from short simulation runs of rather small systems with all atomistic details together with properly adapted coarse grained models we are able quantitatively predict static and especially dynamical properties of both pure polymer melts of long entangled chains but also of systems with low molecular weight additives. Comparisons to rather different experiments such as diffusion constant measurements, NMR relaxation experiments and dielectric spectroscopy show a remarkable quantitative agreement without any adjustable parameter. The model is also able to distinguish different tacticities and to study the consequences for static and dynamic properties. Reintroduction of chemical details into the coarse grained trajectories allows the study of long time trajectories in all atomistic detail providing the opportunity for rather different means of data analysis.

[1]Work done in collaboration with D. Fritz, V. Harmandaris and N. van der Vegt.

3:42PM L42.00005 Effects of Side Chains on the Self-Assembly and Photovoltaic Properties of Conjugated Polymer Semiconductors , SAMSON JENEKHE, University of Washington — Conjugated polymer semiconductors are of growing interest in electronics and optoelectronics. Although it is now well established that the electronic band structure, charge transport, and electronic properties of conjugated polymers can be varied over a wide range through manipulation of the molecular backbone structure, little is known about the effects of alkyl side chains on the solid state morphology and properties of these materials. We have investigated homologous series of conjugated homopolymers, block copolymers, and random copolymers with controlled variation of their alkyl sides towards understanding the effects the size and typology of the side chains on self-assembly, morphology, and photovoltaic properties. We found that diblock copoly(3-alkylthiophenes) exhibit highly crystalline and phase-separated nanostructures in blend films with fullerene derivatives, resulting in superior photovoltaic properties compared to the corresponding homopolymers. The solid state morphology and photovoltaic efficiency of a series of donor-acceptor copolymer semiconductors that have the same optical band gap but different alkyl side chains were found to vary dramatically. Self-assembled block copolymer nanowires with widths of 10-30 nm and aspect ratios of up to 900 have been found to be promising building blocks for constructing efficient bulk heterojunction solar cells.

3:54PM L42.00006 Nacre-Mimetic Composites via Single-Step Self-Assemblies of Polymer-Coated Colloids , OLLI IKKALA, Helsinki University of Technology/Aalto University School of Science and Technology, MOLECULAR MATERIALS TEAM — We demonstrate a scalable single-step self-assembly of polymer-modified plate-like colloidal platelets for nacre-mimetic materials, which overcomes the problem of sequential deposition to prepare hard and soft nacre-mimetic assemblies, which is inherently slow and not scalable. The materials have low density and show good mechanical properties, i.e., modulus of 45 GPa and strength 250 MPa, i.e. partly surpassing those of nacre (Walther et al, Nano Letters 2010, Angew Chem 2010). We expect that the concepts open a route for biomimetic materials from the lab to technology.

4:06PM L42.00007 On the Crystallinity and Chain Conformation in PEO / Layered Silicate Nanocomposites , SPIROS H. ANASTASIADIS[1], K. CHRISSOPOULOU, S. BOLLAS, Foundation for Research and Technology - Hellas, Heraklion Crete, Greece, K. ANDRIKOPOULOS, S. FOTIADOU, D. CHRISTOFILOS, Aristotle University of Thessaloniki, Thessaloniki, Greece, G.A. VOYIATZIS, Institute of Chemical Engineering and High Temperature Chemical Processes, Patras, Greece — The structure of nanohybrid materials as well as the chain conformation under confinement is investigated in hydrophilic polymer / layered silicate nanocomposites. A series of PEO / sodium montmorilonite hybrids was synthesized utilizing melt intercalation with compositions covering the whole range from pure polymer to pure clay. Intercalated nanocomposites with mono- and bi-layers of PEO chains are obtained in all cases. The intercalated chains as well as the ones adsorbed on the outer surface of the clay particles remain purely amorphous; nevertheless, their conformations exhibit different characteristics from those of the amorphous bulk material with the intercalated PEO chains adopting preferably gauche conformations. It is only for compositions where a large amount of excess polymer exists outside the completely full galleries that the polymer crystallinity is recovered. Sponsored by NATO's Scientific Affairs Division, by the Greek GSRT and by the EU.

[1]Also at University of Crete, Heraklion Crete, Greece

4:18PM L42.00008 Formation and application of functional coatings on synthetic fibers , KIRAN GOLI, ALI OZCAM, KRISTEN ROSKOV, RICHARD SPONTAK, ORLANDO ROJAS, JAN GENZER, NC State University — We present two simple methods for modifying synthetic fibers made of polypropylene (PP) and poly(ethylene terephthalate) (PET). Specifically, we alter the inert PP fiber mats by physisorbing denatured proteins, and cross-linking the protein layers using glutaraldehyde. The amino- and hydroxyl-functionalities present in the protein coatings serve as attachment points for polymerization initiators. In addition, PET fibers are modified chemically by amidation with 3-aminopropyltriethoxysilane (APTES), followed by hydrolysis, which yields silanol groups that permit surface attachment of the initiator molecules. "Grafting from" polymerization from such modified PP and PET surfaces is employed following the atom transfer radical polymerization protocol to form functional and responsive polymer coatings. These include arrays of poly(2-hydroxyethyl methacrylate) (PHEMA) as well as chemically-modified PHEMA layers. Selected applications of these functional fibers will be outlined briefly, including, capture of metals or other contaminants from waters, prevention of protein adsorption, and attachment of metallic nanoparticles.

4:30PM L42.00009 Peptide assembly for nanoscale control of materials , DARRIN POCHAN, University of Delaware — Self-assembly of molecules is an attractive materials construction strategy due to its simplicity in application. By considering peptidic, charged synthetic molecules in the bottom-up materials self-assembly design process, one can take advantage of inherently biomolecular attributes; intramolecular folding events, secondary structure, and electrostatic interactions; in addition to more traditional self-assembling molecular attributes such as amphiphilicty, to define hierarchical material structure and consequent properties. Design strategies for materials self-assembly based on small (less than 24 amino acids) beta-hairpin peptides will be discussed. Self-assembly of the peptides is predicated on an intramolecular folding event caused by desired solution properties. Importantly, kinetics of self-assembly can be tuned in order to control gelation time. The final gel behaves as a shear thinning, but immediately rehealing, solid that is potentially useful for cell injection therapies. The morphological, and viscoelastic properties of these peptide hydrogels will be discussed. In addition, slight changes in peptide primary sequence can have drastic effects on the self-assembled morphology. Additional sequences will be discussed that do not form hydrogels but rather form nanoscale templates for inorganic material assembly.

4:42PM L42.00010 Food Materials - a natural playground for soft matter physics , ADAM BURBIDGE, Nestec SA — Traditional food science has its origins in chemistry, and has therefore tended to focus on trying to link molecular formulation and functional performance. Nevertheless, foods are almost always complex hierarchically structured materials of biological origin, far from thermodynamic equilibrium. These kinds of systems provide a challenge of relating structure to function, which is a natural playground for many ideas and concepts of soft matter physics. In this talk I will briefly outline the incredibly rich structural complexity of food products and highlight some areas which are appear to be amenable to physically based reasoning. Despite some notable contributions, food materials physics is a field very much in it's infancy, and I will highlight some outstanding (in both senses of the word) problems!

4:54PM L42.00011 Assembly of conjugated-polymer-based nanostructures driven by solution-state crystallization , RYAN HAYWARD, FELICIA BOKEL, EUNJI LEE, BRENT HAMMER, P.K. SUDEEP, EMILY PENTZER, TODD EMRICK, University of Massachusetts Amherst — Conjugated polymers such as regioregular poly(3-alkyl thiophenes), are well known to crystallize into extended one-dimensional nanowires or fibrils. This behavior is not only important for the efficiency of charge transport in device layers, but can also provide a driving force to assemble different optoelectronic components into well- defined nanostructures. We have investigated the assembly of two systems that rely on solution-state crystallization of poly(3-hexyl thiophene) (P3HT). In the first case, co- crystallization of freely dissolved and particle-bound P3HT provides hybrid fibrils of polymers flanked with n-type inorganic nanoparticles. In the second case, crystallization of P3HT-poly(3-triethylene glycol thiophene) diblock copolymers yields fibrils that can form supramolecular helical assemblies in the presence of salt. We seek to elucidate the mechanisms of self-assembly and the optoelectronic properties of the resulting nanostructures.

5:06PM L42.00012 Temperature responsive hydrogel nanofibers and nanoparticles , JANNE RUOKO-LAINEN, Aalto University/Department of Applied Physics — Poly(N-isopropylacrylamide) (PNIPAM) is one of the most extensively investigated synthetic temperature-responsive polymers. In this work temperature-responsive PNIPAM based triblock copolymer hydrogels, their self-assembly and phase behavior in bulk, are described. Additionally, recent results from responsive hydrogel nanofibers and hydrogel nanoparticles are shown. It is known that block copolymers form well-organized nano structures in bulk or thin films when annealed thermally or in solvent vapours. However, in the case of nanofibers or nanoparticles, the annealing leads in most cases to aggregation and particle sintering. This work utilizes aerosol-based gas phase method where the preparation and annealing of hydrogel nanoparticles with well-organized, hierarchical inner structures are performed without any particle coagulation or sintering. In the method, the block copolymers assemble within aerosol nanoparticles to form, for instance, lamellar onion-like or gyroid inner structures.

5:18PM L42.00013 Orientation and Order in High-Efficiency Polymer Solar Cell Active Layers , M.R. HAMMOND, R.J. KLINE, L.J. RICHTER, C.L. SOLES, D.M. DELONGCHAMP, NIST, T. XU, L. YU, Univ. Chicago, M.F. TONEY, SSRL — Using a combination of scattering and spectroscopy techniques, we have characterized molecular orientation and order in bulk heterojunction (BHJ) organic photovoltaic cells based upon thieno[3,4-*b*]thiophene-*alt*-benzodithiophene copolymers (PTB) and fullerene derivatives. The various techniques probe complimentary aspects of the full distribution of (e.g.) polymer chain orientations, so analysis of the data in tandem allows us to evaluate the relative likelihood of several model distributions. Specifically, X-ray diffraction data yielded a full orientation distribution for the polymer pi-stacking direction within well-ordered regions, with the nominal result of a strong preference for pi-stacking in the vertical direction. This structural characteristic may enhance vertical charge mobility and thus be one factor leading to the outstanding performance of PTB based devices. However, the most plausible model distribution would suggest that those ordered (diffracting) regions of the PTB BHJ films comprise only a small percentage of the total polymer volume within the film.

Tuesday, March 22, 2011 2:30PM - 5:18PM –

Session L43 DMP DPOLY GERA: Focus Session: Polymers for Energy Storage and Conversion – Emerging Applications A306/307

2:30PM L43.00001 Dillon Medal Break –

3:06PM L43.00002 Block copolymers exhibiting simultaneous electronic and ionic conduction for use in lithium battery electrodes , ANNA JAVIER, Lawrence Berkeley National Laboratory, SHRAYESH PATEL, University of California, Berkeley, DANIEL HALLINAN, Lawrence Berkeley National Laboratory, NITASH BALSARA, University of California, Berkeley — A block copolymer system that can demonstrate both electronic and ionic conductivity is analyzed for its performance in rechargeable lithium batteries. Here, the electrically active polymer is poly(3-hexylthiophene), while poly(ethylene oxide) is used as the lithium ion conductor. This block copolymer is then mixed with $LiFePO_4$ and used as the cathode material. Other components in the battery include a lithium metal anode and poly(styrene)-*block*-poly(ethylene oxide) (SEO) as the solid electrolyte. Lithium bis(trifluoromethane)sulfonimide (LiTFSI) is utilized to facilitate ionic conductivity in both the electrolyte and the cathode. The synthesis of the block copolymer and its device performance in rechargeable lithium metal batteries will be presented.

3:18PM L43.00003 All Solid State Rechargeable Lithium Batteries using Block Copolymers , DANIEL HALLINAN, NITASH BALSARA, U.C. Berkeley — The growing need for alternative energy and increased demand for mobile technology require higher density energy storage. Existing battery technologies, such as lithium ion, are limited by theoretical energy density as well as safety issues. Other battery chemistries are promising options for dramatically increasing energy density. Safety can be improved by replacing the flammable, reactive liquids used in existing lithium-ion battery electrolytes with polymer electrolytes. Block copolymers are uniquely suited for this task because ionic conductivity and mechanical strength, both important properties in battery formulation, can be independently controlled. In this study, lithium batteries were assembled using lithium metal as negative electrode, polystyrene-b-poly(ethylene oxide) copolymer with lithium salt as electrolyte, and a positive electrode. The positive electrode consisted of polymer electrolyte for ion conduction, carbon for electron conduction, and an active material. Batteries were charged and discharged over many cycles. The battery cycling results were compared to a conventional battery chemistry.

3:30PM L43.00004 Solubility of Lithium Polysulfides in a Block Copolymer Electrolyte for Lithium/Sulfur Batteries , ALEXANDER TERAN, NITASH BALSARA, University of California, Berkeley and Lawrence Berkeley National Laboratory — The primary challenges to commercialization of the high-energy-density lithium sulfur battery are dendrite growth of the lithium metal at the anode and capacity fade due to loss of active mass through dissolution at the cathode. Nanostructured solid polymer electrolytes offer one potential solution to reduce the amount of capacity fade seen in lithium metal/sulfur batteries by keeping the active material localized at the cathode and to prevent the growth of dendrites at the anode due to their high shear moduli. The block copolymer electrolyte poly(styrene)-*block*-poly(ethylene oxide) (SEO) has shown acceptable ionic conductivity and sufficient shear modulus to retard lithium dendrite growth. The solubility of the lithium polysulfide reaction intermediates Li_2S_x, where $1 \leq x \leq 8$, was studied in SEO copolymers with a range of molecular weights and salt concentrations using small angle X-ray scattering, X-ray diffraction, and differential scanning calorimetery.

3:42PM L43.00005 Solution Processable Hybrid Polymer-Inorganic Thermoelectric Materials , SHANNON YEE, University of California, Berkeley, NELSON COATES, KEVIN SEE, JEFFREY URBAN, Lawrence Berkeley National Laboratory, RACHEL SEGALMAN, University of California, Berkeley — In the last decade thermoelectric material improvements have largely been attributed to a reduction in thermal conductivity due to nanostructuring. An alternative approach is to decouple and optimize the power factor using the unique properties of organic-inorganic interfaces. One method to do this could rely on the electrical properties of a conducting polymer in combination with the thermoelectrical proprieties of an inorganic semiconductors. It is expected that the thermal conductivity of this hybrid material would be low due to the inherent phonon mismatch between polymers and inorganics. Recently we have developed a method for producing a solution processable bulk thermoelectric material ($ZT>0.1$) using a hybrid polymer-inorganic systems consisting of crystalline tellurium nanowires coated in a thin layer of PEDOT:PSS. The interface properties of these materials scale and bulk films demonstrate enhanced transport properties beyond those of either component. Here, we present our methodology, theoretical explanation, and experimental transport properties of this new class of materials where the thermal conductivity, electrical conductivity, and thermopower predictably vary as a function of polymer loading in the hybrid composite.

3:54PM L43.00006 Microscopic mechanism of energy storage in PVDF-CTFE from ab-initio calculations , V. RANJAN, NC State University, Raleigh, NC, MARCO BUONGIORNO NARDELLI, J. BERNHOLC, NC State University, Raleigh, NC and CSMD, ORNL, TN — Polypropelene is most used capacitor dielectric for high energy density storage. However, exotic materials such as copolymerized Polyvinylidene fluoride (PVDF) could potentially lead to an order of magnitude increase in the stored energy density [1,2]. In contrast to linear dielectric properties of polypropelene, several polymers in the PVDF family display nonlinear dielectric properties under electric field. The nonlinearity was postulated to be due to a phase transition from non-polar to a polar structure, whose energy is lowered by an electric field [2]. Our calculations map out the atomistic details of phase transformations for both pure PVDF and PVDF-CTFE. Interestingly, admixture of a small amount of copolymer lowers both the polarization and the energy barriers for the transformation. The barrier lowering facilitates the transformation and may result in reduced loss in the charge-discharge cycle, enabling tuning of material properties for energy storage applications.

[1] B. Chun et al, Science **313**, 334 (2006).
[2] V. Ranjan et al, Phys. Rev. Lett. **99**, 047801 (2007).

4:06PM L43.00007 Nanotube Forests for Electrochemical Energy Storage from Electrostatic Assembly[1] , LIN SHAO, WOO-SIK JANG, Yale University, JODIE LUTKENHAUS, Texas A&M University — With increasing global energy consumption, efficient energy storage sytems are urgently needed. Currently, lithium-ion batteries are prevalent in many of these applications because of their established reliability and superior performance relative to older technologies; however, Li-ion batteries can be limited by mass transfer and safety concerns. Here, we present nanostructured polymer-based electrodes that potentially address these limitations. We apply layer-by-layer (LbL) assembly and nanotemplating to realize LbL-nanotube cathode arrays containing vanadium pentoxide and polyaniline. Both polyaniline and V2O5 store charge via doping/undoping and intercalation/deintercalation, respectively. The aim is to create high surface area electrodes that minimize the diffusion resistance of reactants, which could boost power density. The (LbL) growth profile was monitored using UV-Vis spectroscopy and profilometery. Electrochemical properties were characterized using cyclic voltammetery. Scanning electron microscopy images confirm that large areas of LbL nanotubes can be made. Future work will assess how nanostructured cathodes will behave electrochemically as nanotube aspect ratio is varied.

[1]NSF-CBET 0938842

4:18PM L43.00008 Block-Copolymer Lithium Battery Electrolytes , HANY EITOUNI, Seeo, Inc — With high energy density at low cost, Li ion has become the most prevalent portable rechargeable battery chemistry in the world. As demand for smaller and lighter batteries grows, the energy density limitation of Li ion batteries presents a significant hurdle. Pushing the existing Li ion platform to higher energy densities compromises lifetime and safety, and these have emerged as the most pressing challenges in today's industry. The weakest link in terms of safety and stability of Li ion batteries is the organic liquid electrolyte that facilitates ionic transport between the electrodes. The continuous electrochemical degradation of the electrolyte at the electrodes causes poor cycle life of the batteries, and in some cases, runaway reactions that lead to explosions. Dry polymer electrolytes coupled to Li metal anodes had been considered a high energy alternative to liquid-based systems, as the solid-solid interface promised to alleviate the stability problems of the liquid electrolyte. However, repeated cycling of Li metal anodes leads to dendrite formation, reducing battery life and compromising safety. Recent theoretical work indicates that dendrite growth can be stopped if the shear modulus of current polymer electrolytes can be increased by three orders of magnitude without a significant decrease in ionic conductivity. Thus, the mechanical properties of polymer electrolytes are particularly important in rechargeable solid-state lithium batteries. Because ion transport in polymers is coupled to the motion of the molecules that are solvating the ions, the presence of mobile molecules is essential to allow for a conductive medium. However, the same mobility of molecules is detrimental to the polymer's structural integrity. There is, thus, a clear need to develop methodologies for decoupling the conductive and mechanical properties of polymer electrolytes. Electrolytes comprised of self-assembled block-copolymer nanostructures overcome this principal constraint.

4:54PM L43.00009 Effect of Nanoscale Morphology on Selective Ethanol Transport through Block Copolymer Membranes , ASHISH JHA, NITASH BALSARA, UC Berkeley — We have examined the possibility of using A-B block copolymers for selective separation of alcohols from aqueous mixtures. The A block is not soluble in the liquids of interest and serves as the structural block while B serves as the transporting block. The size of the transporting channels has been controlled by varying the molecular weight, and the geometry has been controlled by varying the composition of the copolymer. Experimental results that reveal the dependence of membrane transport on the size and geometry of the transporting domains will be presented.

5:06PM L43.00010 Simulation study of charge distribution near an ionomer-electrode interface[1] , ELSHAD ALLAHYAROV[2], PHILIP TAYLOR, Physics Department, Case Western Reserve University, Cleveland OH, USA — Molecular dynamics simulations have been used to investigate the nature of the electrostatic field and of the proton density distribution in a Nafion-like ionomer in contact with an electrode. We compare our results for a heterogeneous ionomer, in which a partial phase separation has resulted in separate nanoscopic regions of hydrophobic and hydrophilic material, with those predicted by one-dimensional theoretical models in which Poisson-Boltzmann techniques are used to derive self-consistent potentials and concentration distributions. We further examine the effects of the strong inhomogeneous electrostatic fields in changing the morphology of the ionomer in the vicinity of the electrode from its original form in the bulk material.

[1]Work supported by DOE Grant DE-FG02-05ER46244
[2]also at OIVTRAN Moscow, Russia, and HHU Düsseldorf, Germany

Tuesday, March 22, 2011 2:30PM - 5:30PM –
Session L44 DPOLY: Surfaces, Interfaces, and Polymer Thin Films II A309

2:30PM L44.00001 Dillon Medal Break –

3:06PM L44.00002 Confinement and elastic modulus in polymer nanofibers , EYAL ZUSSMAN, MICHAEL BURMAN, ARKADII ARINSTEIN, Technion — Size-dependant behavior is considered in electrospun polymer nanofibers. Experimental results unambiguously show that the abrupt increase in the elastic modulus of polymer nanofibers, below a cross-over diameter, relative to the bulk could not be attributed to surface energy effect. Polyamide (*Nylon-6.6*) nanofibers were tested by using either bending or tensile deformation modes (the surface energy affects the effective modulus only in the case of bending, and has no effect in the case of tensile deformation). It turns out that the obtained experimental data cannot be explained by the influence of surface energy upon the elastic modulus either qualitatively or quantitatively. This fact supports the explanation which is based on the geometrical confinement of the supermolecular structures of nano-objects.

3:18PM L44.00003 Size-dependent behavior of electrospun polymer nanofibers under small deformation , ARKADII ARINSTEIN, EYAL ZUSSMAN, Technion — A model describing a mechanism resulting in size-dependent behavior of electrospun polymer nanofibers under small deformation is proposed. According this model, the polymer matrix of the nanofibers consists of correlated groups of chains/subchains, partially orientated along the fiber. These supermolecular structures which were formed during electrospinning are confined by the fiber boundary. Thus, when the fiber elongates under external force the relative rotations of these correlated regions are hindered. As a result the elastic modulus depends on the diameter of the deformed fiber. In case of small fiber diameters this restriction is dominant while this effect decreases with increase of fiber diameter, and tends to zero for large fiber diameters according to square-law which was verified by experimental observations.

3:30PM L44.00004 ABSTRACT WITHDRAWN –

3:42PM L44.00005 Ionic conduction at liquid-liquid interfaces[1] , FRANCISCO SOLIS, Arizona State University, MONICA OLVERA DE LA CRUZ, Northwestern University — In coexisting liquid phases with different dielectric constants, ionic species do not have, in general, uniform concentrations. Salt ions accumulate predominately in the liquid with higher dielectric constant. Furthermore, excess accumulation and depletion of ions appears at the interface between the liquids, In this presentation we explore the effects of these non-uniform ionic distributions in the AC conductivity of the liquid mixture. We describe in detail the frequency dependence of of the conductivity for each of the ionic components.

[1]We acknowledge the support of the NERC, which is a EFRC funded DOE Office of Science under Award DE-SC0000989

3:54PM L44.00006 Vapor-Phase Free Radical Polymerization in the Presence of Ionic Liquids , MALANCHA GUPTA — Ionic liquids (ILs) have recently attracted significant interest as an environmentally-friendly alternative to traditional volatile organic solvents because ILs are non-volatile, non-flammable, and can be easily recycled. ILs can be exploited in many ways to improve the selectivity and kinetics of chemical reactions, including polymer synthesis. Ionic liquids have negligible vapor pressure and are therefore stable under vacuum. A few studies have investigated ILs as substrates in inorganic vacuum deposition processes, but to our knowledge ILs have not been used in vapor phase polymerization systems. We have recently introduced ionic liquids into the initiated chemical vapor deposition (iCVD) process for the first time. The iCVD polymerization process occurs via a free-radical mechanism, and the deposited polymeric films are compositionally analogous to solution-phase polymers. Despite the wide range of polymers that have been synthesized using iCVD, it has proven difficult to polymerize monomers with low surface concentrations such as styrene and low propagation rates such as methyl methacrylate and it is difficult to produce block copolymers. In this talk, we will show that our novel ILiCVD system can address some of these shortcomings. We will explain the effects of deposition time, temperature, and monomer solubility on the morphology of the polymer and the molecular weight of the polymer chains.

4:06PM L44.00007 Molecular orientation and photo-degradation of PTCDA films on TiO_2(110) , ORHAN KIZILKAYA, EIZI MORIKAWA, CAMD, Louisiana State University, PHILLIP SPRUNGER, Louisiana State University — The molecular orientation and photo-degradation process of 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) films on TiO_2(110) were investigated by near edge X-ray absorption spectroscopy (NEXAFS). As the incidence angle of p-polarized synchrotron light with respect to the substrate surface normal increases, the intensity of the σ* resonances diminishes and the π* resonances is greatly enhanced. This finding indicates that the molecular orientation of the PTCDA film is flat on the TiO_2(110) surface. NEXAFS results of pristine and photo-degraded PTCDA films exposed to synchrotron white light at the VLSPGM beamline of CAMD revealed the photo-degradation mechanism. We found that the intensity of σ* states diminishes and the intensity of π* states of increases upon the PTCDA film exposed to white light for 30 minutes.

4:18PM L44.00008 Functionalization dependence of the electron beam sensitivity of bridged calix[6]arenes[1] , GREGORY SPENCER, Texas State University-San Marcos, DANIEL RALLS, ANUP BANDYOPADHYAY, MICHAEL BLANDA, Texas State University-San Marcos — Calixarenes have long been studied as a class of high resolution, negative electron beam resists. Previous work has shown the sensitivity can be improved by adding functional groups to the monomer's molecular rim to allow for a more efficient cross-linking mechanism. However, all previous studies dealt with either unfunctionalized resists or monomers that were fully functionalized. In this study, the number of attached functional groups was deliberately varied to directly observe its effect on sensitivity. A bridged calix[6]arene monomer was used as the basic structure. The number of these attached allyl groups ranged from 0 to 8 in steps of 2 per separate synthesis. The bridging units were xylenyl groups which produced both a cone conformer and a 1-2-3-alternate conformer. Resists were formed using all nine different calix[6]arenes and each was subjected to testing. Contrast curves for the cone and alternate conformers were measured by AFM. Resist sensitivities were found as a function of the number of attached groups. The sensitivity was found to be a strong function of the number of attached groups. These results will be discussed.

[1]Supported in part by NSF grant MRI 0414202 and IGERT 0549487.

4:30PM L44.00009 Surface Segregation of Small Macrocyclic , SHIH-FAN WANG, The University of Akron, Department of Polymer Science, XIAOPENG LI, The University of Akron, Department of Chemistry, RENFENG HU, Colorado School of Mines, Department of Chemical Engineering, BULENT AKGUN, National Institute of Standards and Technology, REBECCA AGAPOV, CHRYS WESDEMIOTIS, The University of Akron, Department of Polymer Science, DAVID T. WU, Colorado School of Mines, Department of Chemical Engineering, MARK D. FOSTER, The University of Akron, Department of Polymer Science — Surface segregation of the thin film blends containing 20wt% 2k macrocyclic polystyrene were studied using surface MALDI-ToF mass spectrometry (MS), time of flight secondary ion mass spectrometry (ToF-SIMS), and neutron reflectometry (NR). To provide contrast between the species for these techniques, the linear polymer in the blend was deuterated. MALDI-ToF MS results show that the 2k macrocyclic chains are depleted from the surface after a film of an isotopic macrocylic/linear blend (h-CPS2K/ d-LPS2K) is annealed at 125°C for 12hrs. The surface concentration of CPS is less than 1wt%, while the surface concentration of the hydrogenous component in an analogous h-LPS2K/ d-LPS2K film is 20wt% after annealing. The isotopic effect is not significant for the 2k blends and the architecture effect determines the surface segregation. ToF-SIMS and NR results corroborate this view.

4:42PM L44.00010 Structure Formation and Transition Mechanism in Two-Dimensional Molecular Chiral Phases[1] , YE-LIANG WANG, BING YANG, NAN JIANG, HUAN-YAO CUN, SHI-XUAN DU, Institute of Physics, Chinese Academy of Sciences, Beijing100190, China, YUE WANG, Jilin University, Changchun 130023, China, KARL-HEINZ ENRST, Empa, CH-8600 Dubendorf, Switzerland, HONG-JUN GAO, Institute of Physics, Chinese Academy of Sciences, Beijing100190, China — The self-assemble behavior of prochiral species, QA16C molecules, on a Au(111) surface and the induced chirality by 2D confinement on solid surfaces as well as its chiral transferring process will be presented in this presentation. Initial stages of a chiral phase transition in the monolayer of QA16C molecules on the Au(111) surface were investigated by scanning tunneling microscopy (STM) at submolecular resolution. The prochiral molecules form a homochiral lamella phase at low coverages upon adsorption. A transition to a racemate lattice is observed with increasing coverage. Enantiomers of a homochiral lamella line become specifically substituted by opposite enantiomers such that a heterochiral structure evolves. To explain this phenomenon, we propose a "chiral replacement" model: enantiomers replace QA molecules in enantiopure phase, leading to racemic one. Our findings are significant for the understanding and control of chiral phase transitions in related molecular systems like liquid crystals.

[1]NSFC,CAS

4:54PM L44.00011 Formation and Collapse of Biodegradable Polymer Monolayers at the Air-Water Interface , HAE-WOONG PARK, KIMBERLY OHN, YOU-YEON WON, Purdue University — Poly(lactide-*ran*-glycolide) (PLGA) is widely used as an excipient in formulations of aerosol drugs. It has recently been reported that the surface pressure-area isotherm of PLGA at the air-water interface shows a plateau at intermediate compression levels and a sharp rise in pressure upon further compression. In order to investigate the molecular origin of this behavior, we have conducted an extensive set of surface pressure and AFM imaging measurements with PLGA materials having a range of different molecular weights. The results suggest that (1) the plateau occurs due to the formation (and collapse) of a continuous water-free monolayer of the polymer under continuous compression, and (2) the monolayer becomes significantly resistant to compression at high compression because at that condition the collapsed domains become large enough to become glassy. We will also demonstrate that this property of PLGA allows the polymer to be used as an anchoring block to form a smooth biodegradable monolayer of block copolymers at the air-water interface.

5:06PM L44.00012 8CB-Langmuir Layer at air/water interface: Line Tension vs. Dipolar Repulsion , PRITAM MANDAL, Department of Physics, Kent State University, ANDREW BERNOFF, Dept. of Mathematics, Harvey Mudd College, Claremont, CA 91711, ADIN MANN, Dept.of Chemical Engineering, Case Western Reserve University, Cleveland, OH 44106, JAMES ALEXANDER, Dept. of Mathematics, Case Western Reserve University, Cleveland, OH 44106, ELIZABETH MANN, Department of Physics, Kent State University, ANDREW BERNOFF COLLABORATION, ADIN MANN AND JAMES ALEXANDER COLLABORATION — Langmuir ¯lms of 8CB, a smectic liquid crystal at room temperature, exhibits coexistence of phases with di®erent thicknesses. With decompression of a 8CB-liquid-monolayer gaseous holes appear in liquid monolayer. Molecular interactions controlling the phase separation include short-range van der Waals attraction and long range dipolar repulsion. At small distances where attraction dominates gaseous domains return to energy-minimizing circular shapes. But with size of the holes increasing beyond a critical value, dipolar repulsion becomes strong enough to deform the domains; forming even labyrinth patterns. We use Brewster angle microscopy to study the ¯lm. Our objective is to obtain a critical diameter of the domains beyond which they are non-circular. Experimental value will be compared with that from theory.

5:18PM L44.00013 Origins of the Failure of Classical Nucleation Theory for Nanocellular Polymer Foams[1] , RUSSELL THOMPSON, YEONGYOON KIM, University of Waterloo — The behavior of nanocellular polymer foams, in which nanometer-sized bubbles of fluid are dispersed in a polymer matrix, is dominated by its internal surfaces. In particular, nucleation of a nanocellular foam can involve fundamentally different physics from microcellular or regular foams due to properties of the surfaces. Nucleation rates for nano-bubbles in polymer have been calculated using both classical nucleation theory and self-consistent field theory. An identical model is used for both calculations showing that classical nucleation theory predictions are off by many orders of magnitude. The cause of the failure of classical nucleation theory can be traced primarily to its representation of a bubble surface as an infinite planar interface. For nanoscopic bubbles, the curvature of the bubble surface is comparable to the size of the polymer molecules. Polymers on the outside of a curved bubble surface can explore more conformations than can polymers next to a flat interface. This results in a lower free energy for the curved interface system with respect to a flat interface system, which gives a significantly smaller barrier energy to nucleation and thus a much higher nucleation rate.

[1]Funding: NSERC Strategic Projects Grant, NSERC Discovery Grant

Tuesday, March 22, 2011 2:30PM - 5:30PM –

Session L45 DAMOP: Strongly Correlated Physics with Atoms and Molecules A310

2:30PM L45.00001 Quantum phase transitions in a polarized gas of dipolar molecules forming flexible chain[1] , BARBARA CAPOGROSSO-SANSONE, ITAMP, Harvard-Smithsonian center for Astrophysics, Cambridge, MA, 02138, ANATOLY KUKLOV, Department of Engineering Science and Physics, CSI, CUNY, Staten Island, NY 10314, USA — We numerically demonstrate the formation of quantum flexible chains in a gas of polar molecules confined into a stack of N 1d or 2d optical lattice layers, and with dipole moment aligned perpendicularly to the layers. Molecules interact via dipole-dipole interaction. Ab initio simulations of a single chain pinned at one end reveal quantum roughening transition. Multi-chain ensemble is studied in the J-current model approximation and chain superfluidity (CSF) is found. Increasing density of the chains leads to quantum phase transition from CSF to N-layered molecular superfluid (N-SF). We discuss the nature of this transition and its dependence on density, and the conditions for experimental realization and detection of the chain soup.

[1]We acknowledge support by NSF, grant PHY0653135, and by ITAMP.

2:42PM L45.00002 The Hyperfine Molecular Hubbard Hamiltonian[1] , LINCOLN D. CARR, MICHAEL L. WALL, Colorado School of Mines — An ultracold gas of heteronuclear alkali-metal dimer molecules with hyperfine structure loaded into a one-dimensional optical lattice is investigated. The hyperfine molecular Hubbard Hamiltonian (HMHH), an effective low-energy lattice Hamiltonian, is derived from first principles [1]. The large permanent electric dipole moment of these molecules gives rise to long-range dipole-dipole forces in a dc electric field and allows for transitions between rotational states in an ac microwave field. Additionally, a strong magnetic field can be used to control the hyperfine degrees of freedom independently of the rotational degrees of freedom. By tuning the angle between the dc electric and magnetic fields and the strength of the ac field, it is possible to control the number of internal states involved in the dynamics as well as the degree of correlation between the spatial and internal degrees of freedom. The HMHH's unique features have direct experimental consequences such as quantum dephasing, tunable complexity, and the dependence of the phase diagram on the molecular state.

[1] M. L. Wall and L. D. Carr, Phys. Rev. A **82**, 013611 (2010).

[1]Funded by NSF

2:54PM L45.00003 The Prediction of a Gapless Topological "Haldane Liquid" Phase in a One-Dimensional Cold Polar Molecular Lattice[1] , JASON KESTNER, BIN WANG, JAY SAU, SANKAR DAS SARMA, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, MD — We show that ultracold two-component fermionic dipolar gases in an optical lattice with strong two-body on-site loss can be used to realize a tunable effective spin-one model. Fermion number conservation provides an unusual constraint that $\sum_i \left(S_i^z\right)^2$ is conserved, leading to a novel topological liquid phase in one dimension which can be thought of as the gapless analog of the Haldane gapped phase of a spin- one Heisenberg chain. The properties of this phase are calculated numerically via the infinite time-evolving block decimation method and analytically via a mapping to a one-mode Luttinger liquid with hidden spin information.

[1]Work supported by AFOSR-MURI, DARPA-QUEST, ARO-DARPA-OLE, and CNAM.

3:06PM L45.00004 Density wave patterns for fermionic dipolar molecules on a square optical lattice: mean field theory analysis , KARLIS MIKELSONS, JIM FREERICKS, Georgetown University — We model a system of ultra cold fermionic dipolar molecules on a two dimensional square lattice. Assuming that the molecules are in their nondegenerate hyperfine ground state, and that the dipole moment is polarized perpendicular to the planes, we approximate these molecules as spinless fermions with long range repulsive dipolar interactions. We use mean field theory to obtain the phase diagram as a function of the filling, the strength of interaction and the temperature. We find a number of ordered density wave phases in the system, as well as phase separation between these phases.

3:18PM L45.00005 Quantum Phases of Atom-Molecule Mixtures of Fermionic Atoms , NICOLAS LOPEZ, UCR — Nicolas Lopez (University of California, Riverside, USA) Chi-Yong Lin (National Dong Hwa University, Taiwan) Shan-Wen Tsai (University of California, Riverside, USA) Cold atom experiments have realized a variety of multicomponent quantum mixtures, including Bose-Fermi atomic mixtures. Mixtures of fermionic atoms and diatomic molecules, which are boson, have also been obtained by tuning of the interactions with external fields [1]. We study many-body correlations in such a system where the molecules are weakly bound and therefore pairs of fermionic atoms easily convert into and dissociate from the bound molecule state and this exchange mediates a long-range interaction between the fermions. We consider a simple many-body Hamiltonian that includes the destruction of fermionic atom pairs to form single bosonic molecules and vice versa [2]. We employ a functional renomalization-group approach and calculate the renormalized frequency-dependent interaction vertices and fermion self-energies. We find an instability from the disordered quantum liquid phase to a BCS phase and calculate the energy scale for the transition. The unusual frequency-dependence of this mediated interaction leads to strong renormalization of the self-energy, and also affects the couplings in the BCS channel. [1] M. Greiner, C. A. Regal, J. T. Stewart, and D. S. Jin, Phys. Rev. Lett. **94**, 110401 (2005) [2] E. Timmermans, K. Furuya, P. W. Milonni, and A. K. Kerman, Phys. Lett. A **285**, 228 (2001)

3:30PM L45.00006 Stability and Properties of the Polaron Condensate in a Strongly Interacting Boson-Fermion Mixture , ZENG-QIANG YU, SHIZHONG ZHANG, HUI ZHAI, Institute for Advanced Study, Tsinghua University, China — In this work we study dilute bosons embedded in a single component Fermi sea across a boson-fermion wide Feshbach resonance using a single channel model. The ground state is a condensation of bosonic polarons, and its stability requires that the interaction strength between bosons exceeds a critical value, which is a universal number at boson-fermion resonance and exhibits a maximum in unitary regime. We calculate the condensate fraction and sound velocity across resonance. The transition from polaron condensate to molecular Fermi gas is also discussed.

3:42PM L45.00007 Colliding clouds of strongly interacting fermions and out-of-phase spin modes[1] , EDWARD TAYLOR, WILLIAM SCHNEIDER, SHIZHONG ZHANG, MOHIT RANDERIA, The Ohio State University — Motivated by recent experiments at MIT, we consider the problem of what happens when two Fermi clouds prepared in different hyperfine states collide with each other at low velocities close to a Feshbach scattering resonance. Upon coming into contact with each other, we show that the two clouds evolve preferentially into a metastable upper branch (with amplitude given by the coherent quasiparticle residue Z) where interactions are repulsive, and not the ground state lower branch. As a result, even though the underlying interaction between the fermions is attractive, for sufficiently strong interactions in the unitary region, the clouds will "bounce" off each other. Using Boltzmann, sum rule and hydrodynamic approaches, we make predictions for the frequency of the bounce mode on the BEC side of resonance, including unitarity, where the scattering length is positive.

[1]Supported by NSF-DMR 0706203, NSF-DMR 0907366, and ARO W911NF-08-1-0338

3:54PM L45.00008 Ferromagnetic ordering in two-component Fermi gas: four particle problem , SHENGQUAN ZHOU, DAVID CEPERLEY, University of Illinois at Urbana-Champaign, SHIWEI ZHANG, College of William and Mary — To interpret the experiment of Jo et al. on implementing the Stoner model of itinerant ferromagnetism, we investigate the energy spectrum of a system of four interacting spin-half fermions using exact diagonalization on a finite grid. The formation of molecular bound states and the ferromagnetic transition of the excited scattering states are examined systematically as a function of the interaction coupling constant. If the interaction is modeled by an effective positive scattering length, the transition density to ferromagnetism changes significantly.

4:06PM L45.00009 Atom-dimer and dimer-dimer scattering in fermionic mixtures near a narrow Feshbach resonance , JESPER LEVINSEN, University of Cambridge, DMITRY PETROV, LPTMS, Universite Paris-Sud XI, France — We develop a diagrammatic approach for solving few-body problems in heteronuclear fermionic mixtures near a narrow interspecies Feshbach resonance. We calculate s-, p-, and d-wave phaseshifts for the scattering of an atom by a weakly-bound dimer. The fermionic statistics of atoms and the composite nature of the dimer lead to a strong angular momentum dependence of the atom-dimer interaction, which manifests itself in a peculiar interference of the scattered s- and p-waves. This effect strengthens with the mass ratio and is remarkably pronounced in 40K-(40K-6Li) atom-dimer collisions. We discuss the collisional relaxation of the dimers to deeply bound states and evaluate the corresponding rate constant as a function of the detuning and collision energy. Finally, we calculate the scattering length for two dimers formed near a narrow interspecies resonance.

4:18PM L45.00010 Phases of the attractive Hubbard model in a trap , ELIAS ASSMANN, TU Graz, GEORGE BATROUNI, Institut Non-Lineaire de Nice, SIMONE CHIESA, UT knoxville, HANS GERD EVERTZ, TU graz, RICHARD SCALETTAR, UC Davis — We present a quantum Monte Carlo study of the fermion attractive Hubbard model in a quadratic trap. A rather dramatic failure of the local density approximation occurs in the half-filled region where coupling to nearby superfluid domains induces a strong suppression of charge fluctuations. By monitoring the behavior of the equal-time pairing correlations, we show the existence of a low temperature phase consistent with quasi-long-range order.

4:30PM L45.00011 Thermodynamics of the 3D Hubbard model on approach to the Neel transition , LODE POLLET, ETH Zurich, SEBASTIAN FUCHS, University of Goettingen, EMANUEL GULL, Columbia University, EVGENY BUROVKSI, Lancaster University, EVGENY KOZIK, ETH Zurich, THOMAS PRUSCHKE, University of Goettingen, MATTHIAS TROYER, ETH Zurich — We study the thermodynamic properties of the 3D Hubbard model for temperatures down to the Néel temperature using cluster dynamical mean-field theory. In particular we calculate the energy, entropy, density, double occupancy and nearest-neighbor spin correlations as a function of chemical potential, temperature and repulsion strength. To make contact with cold-gas experiments, we also compute properties of the system subject to an external trap in the local density approximation. We find that an entropy per particle $S/N \approx 0.65(6)$ at $U/t = 8$ is sufficient to achieve a Néel state in the center of the trap, substantially higher than the entropy required in a homogeneous system. Precursors to antiferromagnetism can clearly be observed in nearest-neighbor spin correlators.

4:42PM L45.00012 Superconductivity in strongly repulsive fermions: the role of kinetic-energy frustration[1] , LEONID ISAEV, GERARDO ORTIZ, Indiana University Bloomington, CRISTIAN BATISTA, T-4, LANL — We discuss a physical mechanism of a non-BCS nature which can stabilize a superconducting state in a *strongly repulsive* electronic system. By considering the 2D Hubbard model with spatially modulated electron hoppings, we demonstrate how kinetic-energy frustration can lead to robust d-wave superconductivity at *arbitrarily* large on-site repulsion. This phenomenon should be observable in experiments using fermionic atoms, e.g. ^{40}K, in specially prepared optical lattices.

[1]PRL 105, 187002 (2010)

4:54PM L45.00013 Non-perturbative predictions for cold atom Bose gases with tunable interactions , BOGDAN MIHAILA, Los Alamos National Laboratory, FRED COOPER, Santa Fe Institute, CHIH-CHUN CHIEN, Los Alamos National Laboratory, JOHN F. DAWSON, University of New Hampshire, EDDY TIMMERMANS, Los Alamos National Laboratory — We discuss a theoretical description for dilute Bose gases as a loop expansion in terms of composite-field propagators by rewriting the Lagrangian in terms of auxiliary fields related to the normal and anomalous densities. We demonstrate that already in leading order this non-perturbative approach describes a large interval of coupling-constant values, satisfies Goldstone's theorem, yields a Bose-Einstein transition that is second-order, and is consistent with the critical temperature predicted in the weak-coupling limit by the next-to-leading order large-N expansion.

5:06PM L45.00014 Density functional theory for fermionic atom gases , MATTHIAS TROYER, PING NANG MA, SEBASTIANO PILATI, ETH Zurich, XI DAI, Chinese Academy of Sciences — We will show how Kohn-Sham density-functional theory (DFT), which forms the basis of most electronic structure calculations in material science, can be applied to ultracold atomic gases in optical lattices. We present the derivation of an exchange correlation functional for atomic gases and show first applications within a local spin density approximation. In particular we will show that the local density approximation in DFT is much more accurate than what is commonly referred to as "local density approximation" in the atomic gases community. As an outlook we will discuss how the development of DFT for ultracold atomic gases can form a strong link between materials science and atomic physics.

5:18PM L45.00015 Using off-diagonal confinement as a cooling method[1] , VALERY ROUSSEAU, Louisiana State University, KALANI HETTIARACHCHILAGE, JUANA MORENO, MARK JARRELL, DAN SHEEHY — We show that the recently proposed "off-diagonal confining" (ODC) method (Phys. Rev. Lett. 104, 167201 (2010)) can lead to temperatures that are smaller than with the conventional "diagonal confining" (DC) method, depending on the control parameters of the system. We determine these parameters using exact diagonalizations for the hard-core case, then we extend our results to the soft-core case by performing quantum Monte Carlo simulations for both DC and ODC systems at fixed temperatures, and analysing the corresponding entropies.

[1]This work was supported by NSF OISE-0952300.

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P1 DCMP: Magnetism and Localization in f Electron Systems Ballroom A1

8:00AM P1.00001 Ce115's and beyond[1] , J. D. THOMPSON, Los Alamos National Laboratory — Recent studies of members of the Ce115 ($CeMIn_5$ (M=Co, Rh)) family of heavy-fermion materials have allowed a new perspective on the relationship between magnetism and unconventional superconductivity in strongly correlated electron systems. The antiferromagnet $CeRhIn_5$ under pressure, superconducting $CeCoIn_5$in a magnetic field, and Cd-doped $CeCoIn_{5-x}Cd_x$ reveal a phase of long-range antiferromagnetic order that coexists microscopically with bulk, nodal superconductivity. Though the detailed relationship between these orders differs in each, evidence suggests that the order parameters are coupled irrespective of these differences and that similar conclusions may hold in structurally related $CePt_2In_7$ and the recently discovered 5f-electron compound $PuCoIn_5$. Characteristics of magnetism and superconductivity in theses 4f- and 5f-electron systems bear similarities to those in cuprate and iron-pnictide superconductors.

[1]In collaboration with E. D. Bauer, A. Bianchi, Z. Fisk, M. Kenzelmann, H. O. Lee, R. Movshovich, M. Nicklas, T. Park, F. Ronning, V. A. Sidorov and O. Stockert. Work at Los Alamos was performed under the auspices of the US DOE, OBES.

8:36AM P1.00002 How spins become pairs: Composite pairing and magnetism in the 115 heavy fermion superconductors , REBECCA FLINT, Massachusetts Institute of Technology — The highest temperature heavy fermion superconductors are found in the 115 family: $CeMIn_5$ (M=Co,Ir,Rh) and $PuMGa_5$ (M=Co,Rh) [1], where the heavy quasiparticles are only partially formed by the time they pair. The internal structure of the pair is thus just as important as the forces holding it together. We show that the heavy fermion condensate necessarily contains two d-wave components condensed in tandem: pairs of heavy quasiparticles on neighboring sites and composite pairs consisting of two electrons bound to a single local moment. These two components draw upon the antiferromagnetic and two-channel Kondo interactions, respectively, to cooperatively enhance the superconducting transition temperature, as we demonstrate within a symplectic-N solution [2,3] of the two-channel Kondo-Heisenberg model [4]. Additionally, the tandem condensate is electrostatically active, which we predict will result in a superconducting shift in the electronic quadrupolar frequency, as measured in Mossbauer spectroscopy.

[1] J. L. Sarrao and J.D. Thompson, J. Phys. Soc. Jap. 76, 051013(2007).
[2] R. Flint, M. Dzero and P. Coleman, Nat. Phys. 4, 643 (2008).
[3] R. Flint and P. Coleman, Phys. Rev. B 79, 014424(2009).
[4] R. Flint and P. Coleman, arXiv:0912.2339 (2009).

9:12AM P1.00003 Imaging the "Hidden Order" Transition in URu_2Si_2 , ANDREW SCHMIDT, University of California, Berkeley — In URu_2Si_2, bulk measurements indicating the formation of heavy bands begin at temperatures around 55 K but are interrupted by an unidentified electronic phase transition, the "hidden order," at $T_o = 17.5$ K. Heavy bands in a Kondo lattice are expected to form due to strong hybridization between electrons localized in real space on magnetic ions and those delocalized in momentum space. Why the "hidden order" appears has been an outstanding question in heavy fermion physics. We use spectroscopic imaging scanning tunneling microscopy (SI-STM) to image the electronic structure of URu_2Si_2 though T_o. Above T_o we find the Fano spectra expected for Kondo screening of a magnetic lattice, while below T_o a partial energy gap opens. Heavy-quasiparticle interference imaging shows that the gap forms due to a light momentum-space band splitting below T_o into two heavy fermion bands. Our observations of the "hidden order" transition are thus consistent with a sudden alteration in both the hybridization at each U atom and the associated heavy bands.

9:48AM P1.00004 Scanning Tunneling Microscopy and Spectroscopy of the Heavy Fermion Compounds URu_2Si_2 and $CeCoIn_5$[1] , PEGOR AYNAJIAN, Princeton University — Heavy electronic states originating from the f atomic orbitals underlie a rich variety of quantum phases of matter. We use atomic scale imaging and spectroscopy with the scanning tunneling microscope (STM) to examine the novel electronic states that emerge from the uranium f states in URu_2Si_2 [1]. We find that as the temperature is lowered, partial screening of the f electrons' spins gives rise to a spatially modulated Kondo-Fano resonance that is maximal between the surface U atoms. At T=17.5 K, URu_2Si_2 is known to undergo a 2^{nd} order phase transition from the Kondo lattice state into a phase with a hidden order parameter. From tunneling spectroscopy, we identify a spatially modulated, bias-asymmetric energy gap with a mean-field temperature dependence that develops in the hidden order state. Spectroscopic imaging further reveals a spatial correlation between the hidden order gap and the Kondo resonance, suggesting that the two phenomena involve the same electronic states. We further study the behavior of the Kondo lattice in a model heavy fermion compound $CeCoIn_5$ as a function of temperature and establish a direct comparison between the two heavy fermion compounds.

[1] P. Aynajian, *et al. Proc. Natl. Acad. Sci. USA* 107, 10383 (2010).

This work is funded by a DOE-BES grant. Infrastructure at the Princeton Nanoscale Microscopy Laboratory are also supported by grants from NSF-DMR, Keck Foundation, and NSF-MRSEC. PA also acknowledges support of a fellowship through the PCCM funded by NSF MERSEC.

[1]Work done in collaboration with Eduardo H. da Silva Neto, Colin V. Parker, Yingkai Huang, Abhay Pasupathy, John Mydosh, Eric Bauer, Paul Tobash, and Ali Yazdani.

10:24AM P1.00005 "Hidden order," heavy electron ferromagnetism, and non-Fermi liquid behavior in the pseudoternary system $URu_{2-x}Re_xSi_2$[1] , M. BRIAN MAPLE, Univeristy of California, San Diego — The identity of the ordered phase that occurs at temperatures below $T_o = 17$ K in the heavy fermion compound URu_2Si_2 has eluded researchers for two and a half decades. Features in various physical properties associated with this so-called "hidden order" (HO) phase are reminiscent of a charge or spin density wave that forms a gap over about 40% of the Fermi surface below T_o, while the remainder of the Fermi surface is gapped by the superconductivity below $T_c = 1.5$ K. In order to attain a better understanding of these phenomena, the physical properties of URu_2Si_2 have been studied as a function of applied pressure, chemical substitution, and magnetic field. Whereas the application of pressure suppresses the superconductivity and induces a phase transition from the HO phase to an antiferromagnetic phase, the substitution of Re for Ru results in the suppression of the superconductivity and the HO transition, the nearby emergence of ferromagnetic (FM) order, and unique critical behavior associated with the FM phase. Magnetization measurements on the $URu_{2-x}Re_xSi_2$ pseudoternary system as a function of x reveal the onset of ferromagnetism at a concentration $x_{cr} \approx 0.15$, which apparently represents a FM quantum critical point. Non-Fermi liquid (NFL) behavior in the physical properties such as the electrical resistivity and specific heat at low temperatures is found to extend deep into the FM region of the T - x phase diagram. Experiments conducted on $URu_{2-x}Re_xSi_2$ single crystals to investigate the superconducting, HO, and FM phases, characterize the NFL behavior, and establish the T - x phase diagram are described. The experimental results are compared to theoretical models for ferromagnetism in a Kondo lattice. Research performed in collaboration with N. P. Butch, J. R. Jeffries, B. T. Yukich, and D. A. Zocco

[1]Research supported by the U.S. Department of Energy under Grant Nos. DE-FG02-04ER46105 (crystal growth) and DE-FG52-06NA26205 (high pressure measurements) and the National Science Foundation under Grant No. 0802478 (low temperature measurements).

Wednesday, March 23, 2011 8:00AM - 11:00AM –
Session P2 DCMP: The Kondo Ground State in Graphene Ballroom A2

8:00AM P2.00001 Topological Kondo Ground State in Graphene[1] , HARI C. MANOHARAN, Stanford University — Dirac electrons in graphene comprise two-component wavefunctions and quantum symmetries intertwining pseudospin, chirality, and Berry's phase, all ultimately stemming from a node or topological degeneracy in the spectrum known as the Dirac point. Graphene represents one prototype example of a larger class of nodal metals in which a relativistic spectrum causes the density of states to vanish linearly. Based on the unique electronic structure of such systems, a large body of theoretical work has highlighted the propensity for Dirac electrons to condense in strongly correlated ground states when additionally coupled to the real spin degree of freedom. We report the observation of one of these elusive ground states, realized in graphene via unconventional Kondo screening of individual atomic spins by massless Dirac fermions. Low-temperature scanning tunneling microscopy reveals the emergence of a new energy scale and a striking bimodal Kondo resonance localized around magnetic atoms placed on a clean graphene monolayer. Quasiparticle interference maps and concomitant spectroscopy in a high magnetic field demonstrate the spin origin of the associated ground states, and their direct link to local conservation or breaking of effective time-reversal symmetry in the underlying Dirac Hamiltonian. We find these novel spin states to be topologically controlled by Berry phase interference; in the most exotic manifestation, we show experimental evidence for two electron flavors—decoupled in momentum space by a π Berry phase shift cancellation—participating in a chiral two-channel Kondo effect. We link these results to a new platform we have developed for the study of topological phases, artificial graphene assembled by atomic manipulation.

[1]This work performed in collaboration with L. S. Mattos, C. R. Moon, M. W. Sprinkle, C. Berger, K. Sengupta, A. V. Balatsky, W. A. de Heer, K. K. Gomes, W. Ko, W. Mar. We acknowledge support from DOE and NSF.

8:36AM P2.00002 Orbitally controlled Kondo effect in graphene[1] , TIM WEHLING, University of Hamburg — Graphene differs from usual metals or semiconductors in being a truly two-dimensional material with the charge carriers resembling massless Dirac fermions and the chemical potential being highly tunable by gate voltages. Recently, scanning tunneling spectroscopy experiments opened the exciting possibility to address the interaction of graphene with magnetic adatoms and to investigate the Kondo effect in a material that is simple, of immediate technological importance and offers unprecedented high tunability. Here, we develop a realistic description of the interaction of magnetic adatoms with graphene and explain the role of orbital symmetries: General symmetry arguments show that the Kondo effect in graphene is controlled not only by the spin but also by the orbital degree of freedom and spin-orbit coupling. For the example of Co adatoms, commonly used in experiments, we identify possible scenarios for the Kondo effect based on ab initio calculations. For a Co atom absorbed on top of a carbon atom, the Kondo effect is quenched by spin-orbit coupling below an energy scale of 15K. For Co with spin S=1/2 located in the center of a hexagon, a crossover from SU(4) Kondo physics at higher energies to an SU(2) Kondo effect on the scale of the Co spin-orbit coupling strength is encountered. The interplay of the orbital adatom physics and the peculiar band structure of graphene is directly accessible in Fourier transform tunneling spectroscopy or in the gate-voltage dependence of the Kondo temperature which is predicted to display a very strong, characteristic particle-hole asymmetry. The particular high symmetry situation provided by adatoms on graphene can pave the way for a deeper understanding of Kondo screening in general nanomagnetic structures.

[1]Support from SFB 668 and SPP 1459 are acknowledged.

9:12AM P2.00003 Kondo effect and STM spectroscopy of Dirac electrons in graphene[1] , KRISHNENDU SENGUPTA[2], Indian Association for the Cultivation of Science — We show that graphene, whose low-energy quasiparticles display Dirac like behavior, may exhibit a two-channel Kondo effect in the presence of magnetic impurities. We present a large Nanalysis for a generic spin Slocal moment coupled to Dirac electrons in graphene and demonstrate that the corresponding Kondo temperature can be tuned by an experimentally controllable applied gate voltage. We also study the STM spectra of these Dirac electrons in the presence of such impurities and demonstrate that such spectra depend qualitatively on the position of the impurity atom in the graphene matrix. More specifically, for impurity atoms atop the hexagon center, the zero-bias tunneling conductance, as measured by a STM, shows a peak; for those atop a graphene site, it shows a dip. We provide a qualitative theoretical explanation of this phenomenon and show that this unconventional behavior is a consequence of conservation/breaking of pseudospin symmetry of the Dirac quasiparticles by the impurity. We also predict that tuning the Fermi energy to zero by a gate voltage would not lead to qualitative change in the shape of the conductance spectra when the impurity is atop the hexagon center. A similar tuning of the Fermi energy for the impurity atop a site, however, would lead to a change in the tunneling conductance from a dip to a peak via an antiresonance. We discuss some recent experiments on a doped graphene sample that seem to have qualitative agreement with our theory and suggest further experiments to test our predictions.

[1]DST, India,
[2]Other authors: G. Baskaran, I. Paul and K. Saha

9:48AM P2.00004 Quantum critical Kondo screening in graphene , MATTHIAS VOJTA, Technische Universitaet Dresden — Magnetic impurities in neutral graphene provide a realization of the pseudogap Kondo model, which displays a quantum phase transition between phases with screened and unscreened impurity moment. In this talk, I discuss the physics of the pseudogap Kondo model with finite chemical potential μ. While carrier doping restores conventional Kondo screening at lowest energies, properties of the quantum critical fixed point turn out to influence the behavior over a large parameter range. Most importantly, the Kondo temperature T_K shows an extreme asymmetry between electron and hole doping. At criticality, depending on the sign of μ, T_K follows either the scaling prediction $T_K \propto |\mu|$ with a universal prefactor, or $T_K \propto |\mu|^x$ with $x \approx 2.6$. This asymmetry between electron and hole doping extends well outside the quantum critical regime and also implies a qualitative difference in the shape of the tunneling spectra for both signs of μ. Finally, the considerations are extended to the two-channel Kondo model where non-Fermi liquid behavior emerges at lowest energies.

10:24AM P2.00005 Gate-Controlled Ionization and Screening of Cobalt Adatoms on a Graphene Surface , VICTOR BRAR, U.C. Berkeley — Graphene impurities provide both a source of mobility-limiting disorder as well as a means to alter the graphene electronic structure in a desirable way. While these effects have thus far been primarily studied with spatially averaged techniques, understanding the microscopic physics of such behaviour requires local-probe exploration of the subnanometre-scale electronic and structural properties of impurities on graphene. In this talk I will describe scanning tunnelling microscopy and spectroscopy measurements made on individual Co atoms deposited onto back-gated graphene devices. We observe features in the tunneling local density of states (LDOS) of the Co adatoms related to both atomic resonances and phonon excitations. We also find that the electronic structure of Co adatoms can be tuned by application of the device gate voltage, and that the Co atoms can be reversibly ionized. Large screening clouds are observed to form around Co adatoms ionized in this way, and we observe that some intrinsic graphene defects also show charging behaviour. Our results provide new insight into charged-impurity scattering in graphene, as well as the possibility of using graphene devices as chemical sensors. The relationship between our measurements and recent transport experiments will also be discussed.

Wednesday, March 23, 2011 8:00AM - 10:24AM –

Session P3 DCMP FIAP DMP: FIAP/DCMP/DMP Prize Session: Pake, Adler, IAP Ballroom A3

8:00AM P3.00001 George E. Pake Prize Talk: Silicon:Germanium's Road to Market; A Sceptic's Guide From Surface Science to WiFi , BERNARD MEYERSON[1], IBM — There is an adage that goes, "Believe none of what you hear and only half of what you see." Though this overstates matters just a bit, it is nonetheless a valuable insight, as much of the success in developing and commercializing silicon;germanium(Si:Ge) technology was derived from the suspension of core scientific "truths" in favor of rigorous examination of their origins. In this talk I will review a series of foundational discoveries regarding the inception of growth for Si:Ge alloys that ultimately led to the pervasive deployment of this technology. Inextricably linked to the success of this work was a diverse team of extraordinarily talented individuals who each contributed remarkable insights at critical junctures, a valuable reminder of the potential of collaborative innovation to produce seminal discontinuities in science and technology. I will trace the evolution of collaborative innovation from this nucleus to a foundational business model by which much of current silicon technology is derived.

[1]Invited Pake Prize presentation

8:36AM P3.00002 David Adler Lectureship Award in the Field of Materials Physics Talk: Novel Nitride and Oxide Electronics[1] , STEPHEN PEARTON, University of Florida — Recent progress in development of GaN-based transistors for gas and bio-sensing applications and amorphous IGZO layers for use thin film transistors (TFTs)on flexible substrates, including paper,will be presented. For the detection of gases such as hydrogen, the gateless GaN transistors are typically coated with a catalyst metal such as Pd or Pt to increase the detection sensitivity at room temperature. Functionalizing the surface with oxides, polymers and nitrides is also useful in enhancing the detection sensitivity for gases and ionic solutions.The use of enzymes or adsorbed antibody layers on the semiconductor surface leads to highly specific detection of a broad range of antigens of interest in the medical and security fields. We give examples of recent work showing sensitive detection of glucose, lactic acid, prostate cancer and breast cancer markers and the integration of the sensors with wireless data transmission systems to achieve robust, portable sensors. The amorphous transparent conducting oxide InZnGaO4 (IGZO) is attracting attention because of its high electron mobility (10-50 cm2.V-1.sec-1), high transparency in the visible region of the spectrum and its ability to be deposited with a wide range of conductivities.This raises the possibility of making low-cost electronics on a very wide range of arbitrary surfaces, including paper and plastics. N-type oxides such as zinc oxide, zinc tin oxide, indium gallium oxide, and indium gallium zinc tin oxide (IGZO) exhibit surprisingly high carrier mobilities even for amorphous films deposited at 300K. This has been explained by the fact that the conduction in these materials is predominantly through non-directional s orbitals which are less affected by disorder than the directional sp3 orbitals which control electron transport in Si. Examples of progress and discussion of remaining obstacles to use of IGZO TFTs will be presented

[1]Work performed in collaboration with Fan Ren.

9:12AM P3.00003 Prize for Industrial Applications of Physics Talk: Low energy spread Ion source for focused ion beam systems-Search for the holy grail , BILL WARD — In this talk I will cover my personal experiences as a serial entrepreneur and founder of a succession of focused ion beam companies (1). Ion Beam Technology, which developed a 200kv (FIB) direct ion implanter (2). Micrion, where the FIB found a market in circuit edit and mask repair, which eventually merged with FEI corporation. and (3). ALIS Corporation which develop the Orion system, the first commercially successful sub-nanometer helium ion microscope, that was ultimately acquired by Carl Zeiss corporation. I will share this adventure beginning with my experiences in the early days of ion beam implantation and e-beam lithography which lead up to the final breakthrough understanding of the mechanisms that govern the successful creation and operation of a single atom ion source.

9:48AM P3.00004 Prize for Industrial Applications of Physics Talk: Start-up Company (Ad)Ventures – the Highs & Lows , NICHOLAS ECONOMOU, PointSpectrum,LLC — Each start-up company is a unique enterprise, with its own strengths, weaknesses, challenges and eventual outcome. However, there are many aspects common to all new technology companies, including the need for: 1. An innovative technology edge. 2. A solid product idea. 3. A team with experienced people in at least some of the key jobs. 4. Adequate initial funding to achieve some significant milestones. 5. Patient investors who can persevere through the inevitable hard times. 6. A liquidity/exit strategy clearly articulated from day one. The case studies of how other companies were started and developed can provide useful insights into what may lie ahead for the founders of a new company. Several examples from my own experience will be discussed. While they are all clearly different, there are common threads running through all of these stories. Some thoughts on what went right or wrong, and what could have been done better will be presented.

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P4 DPOLY: Kinetic Pathways to Assembly of Polymers, Particles and Biomolecules Ballroom A4

8:00AM P4.00001 Equilibration and metastability in block copolymer micelles , TIMOTHY LODGE, University of Minnesota — The strong incompatibility between a solvophobic block and the surrounding medium leads naturally to extremely slow chain exchange kinetics between micelles. The steric barrier between well-solvated coronas similarly inhibits micelle fusion/fission processes. Consequently, equilibration of block copolymer micelles is typically prohibitively slow. As a result, it is possible for one system to adopt quite different micellar shapes and sizes, depending on preparation method. However, by using low volatility solvents such as ionic liquids or paraffinic oils, combined with weakly solvophobic blocks, it is possible to design model systems with accessible critical micelle temperatures. This enables the study of both the mechanisms of chain exchange, by time-resolved small-angle neutron scattering, and the evolution of non-equilibrium structures, by dynamic light scattering. Examples of both approaches will be discussed.

8:36AM P4.00002 Uncovering the Biological Identity at the NanoScale; Fundamantal principles governing interactions between nanoparticles and living organisms , KENNETH DAWSON, University College Dublin — This abstract not available.

9:12AM P4.00003 Nanoparticle formation by block copolymer directed rapid precipitations—Flash NanoPrecipitaiton , ROBERT PRUD'HOMME, Princeton University — With widespread interest in the generic "nano" attention has been focused on strategies of making small particles. High-value applications that drive new process innovation include very hydrophobic pharmaceutical actives, dyes and pigments for ink jet printing, or the dispersal of highly toxic insecticides on carriers. While it is relatively easy to make inorganic nano-particles, for example CdS particles, it is much more challenging to make nanoparticles from low surface energy organic solids. Strategies for forming nano particles vary from supercritical spraying, supercritical freezing, milling, solvent exchange precipitation, and imbibing into polymeric micelles. The solute and process combine to give differences in crystalline/amorphous products, individual particles/agglomerates, and uniformity/polydispersity of sizes. We will give an overview of the techniques and the classes of products that each addresses. We have developed a new technology that has two components: (1) rapid and tailored micromxing in an impinging jet, and (2) novel block copolymer stabilizers. The impinging jet process allows the production of nano-particles by: 1) elimination of mass transfer limitations and compositional gradients within 10 ms as determined by independent measurements with competitive-parallel reactions, 2) production of high supersaturations and solute concentrations so that high production rates can be obtained, and 3) control of particle size by stabilization of the particle using block copolymer self-assembly. The process depends critically on control of three time scales: particle nucleation and growth, block copolymer micellization, and polymer adsorption on the particle to produce steric stabilization. We present data on characterization of the mixing times using competitive reactions, data on polymer micellization kinetics, and results on the successful production of β-carotene and taxol particles with control of the particle size between 40 nm to 600 nm. A range of block copolymers have been used : PS-b_PEO, PBA-b-PAA, and PCL-b-PEO. Homogeneous rapid nucleation and growth produces particle size distributions that are much narrower than those obtained by alternate size-reduction or precipitation routes, and results in a decreased tendency to Ostwalt ripen.

9:48AM P4.00004 ABSTRACT WITHDRAWN –

10:24AM P4.00005 Soft matter self-assembly driven by specific and nonspecific attractions: dynamic pathways and the Ostwald rule of stages[1] , STEPHEN WHITELAM, Lawrence Berkeley National Lab — Ostwald's rule of stages is one of the few rules-of-thumb we possess that suggests the dynamical pathway a material will take when crystallizing. It states that bulk phases intermediate in free energy between the parent phase and the stable solid will emerge before establishment of the stable solid. Although widely applicable, this rule is frequently seen to break down in experiments and computer simulations, showing it to be without theoretical foundation. A first step in going beyond this rule is to understand why it breaks down. Here we test Ostwald's rule of stages in a statistical mechanical model of crystallization. Our model describes particles that are prototypical of a class of materials (such as proteins and patchy nanoparticles) able to form solid phases stabilized by directional attractions, as well as sparse and dense fluidlike phases. We find that the rule holds in certain regimes of parameter space and breaks down in others. Importantly, its breakdown can be anticipated using simple arguments. We show that the qualitative crystallization pathway of the model depends in general on both the thermodynamic landscape prescribed by inter-particle interactions and on the relative rate of particle rotations and translations. This observation emphasizes that any general rule of crystallization must account for both thermodynamic and dynamic factors.

[1]This work was performed at the Molecular Foundry, Lawrence Berkeley National Laboratory, and was supported by the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02–05CH11231

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P5 FEd FPS: Broader Impact: Partnerships and Resources to Achieve Successful Public and K-12 Outreach and Engagement Ballroom C1

8:00AM P5.00001 Science Museum Resources and Partnerships for Public and K-12 Outreach and Engagement , LARRY BELL, Museum of Science, Boston — Science museums engage in a wide range of activities not apparent to exhibit hall visitors. Many of them can support research outreach to public and K-12 teachers and students. In addition to exhibits in science centers, and demonstrations on topics like electricity or cryogenics, science museums offer courses for children and adults, out-of-school programs for students, teacher professional development; some do K-12 curriculum development and some run science magnet schools. In recent years science museums have increased their capacity to communicate with the public about current research. The Museum of Science, for instance, created a Current Science and Technology Center in 2001 dedicated to science in the news and current research developments. Through this Center, the Museum partnered with Harvard University to provide a wide range of public engagement activities as part of Harvard's Nanoscale Science and Engineering Center focused on the Science of Nanoscale Systems and their Device Applications. In the past five years a number of new collaborations among science museums have developed, many in partnership with researchers and research centers. Perhaps the largest or these, the Nanoscale Informal Science Education Network (NISE Net) was launched in 2005 with funding from the National Science Foundation. The NISE Net links informal science education organizations together and to university research centers to raise the capacity of all the participant organizations to increase public awareness, understanding, and engagement with nanoscale science, engineering, and technology. Nearly 300 informal educational organizations in every state nationwide make use of NISE Net's educational materials, professional development, national and regional meetings, and online resources. NISE Net is an open source network with all of its materials freely available to everyone.

8:36AM P5.00002 Professional Society Resources and Partnerships for Public and K-12 Outreach and Engagement[1] , PHILIP W. HAMMER, American Institute of Physics — Outreach and public engagement lower the barriers that inhibit broader public appreciation of and participation in physics, and are important for inspiring the next generation of scientists and science-literate citizens. The APS and many other professional societies have made significant and sustained investments in public engagement because of the importance of these activities - APS, for example, has an entire department dedicated to outreach. In addition, professional societies have responded to members who desire resources for enabling and enhancing their own outreach efforts. A key question is always, "What works?" Professional societies can help provide the answers. In this talk, I will explore the critical interface played by professional societies as a bridge to the public, as a resource to members, and as a broker of partnerships. I will also feature numerous examples of creative and compelling ways to engage the public, including physicscentral.org, LaserFest, NISE Net, Comic Con, SOCKs, citizen science, and many more. A more important question is, "Is it fun?" I will show that the answer is an unqualified, "Yes!"

[1]The author gratefully acknowledges Rebecca Thompson, Head of APS Public Outreach, for her contributions to this work.

9:12AM P5.00003 National Laboratory Resources and Partnerships for Public and K-12 Outreach and Engagement , ADITI RISBUD, Lawrence Berkeley National Laboratory — Nanoscale science and engineering draws upon aspects of chemistry, physics, biology and engineering to address scientific problems in energy, healthcare, security and technology. Scientists in this field often work in a multidisciplinary setting, which suggests a need for educational content unlike that currently offered in single-discipline high school and college science courses. Instructors are faced with the daunting task of accurately describing nanoscience in the context of their discipline, while inspiring students to explore careers in nanoscale science and engineering. The Molecular Foundry, a Department of Energy nanoscience user facility located at Lawrence Berkeley National Laboratory, offers opportunities for high school and college students, along with science and engineering educators interested in learning basic concepts and research developments in nanoscience. Successful partnering with the Nanoscale Informal Science Education Network also provides opportunities for scientists to interact informally with the general public. These interactions convey the role of national laboratories in helping lay audiences understand the breakthroughs, potential issues and societal impact of nanoscience.

9:48AM P5.00004 Marshalling Corporate Resources for Public and K-12 Technical Education Outreach and Engagement , JAMES WYNNE, IBM TJ Watson Research Center — In 1988, the Education Task Force of the Business Roundtable recommended that American corporations invest in pre-college education. Prior to that date, corporate investment was targeted at higher education. IBM and other corporations responded by encouraging their employees and their corporate philanthropic organizations to develop programs aimed at enhancing pre-college education. The IBM TJ Watson Research Center initiated a Local Education Outreach program, active for these past 23 years, that marshals the resources of our science-rich institution to enhance STEM education in our local schools. We have broad and deep partnerships between the Research Center and local school districts, including New York City. We have just completed our 19th consecutive year of Family Science Saturdays, which brings 4th and 5th grade children, along with their parents, to our Research Center for hands-on workshops in topics like States of Matter, Polymer Science, Kitchen Chemistry, and Sound and Light. The workshops are staffed by IBM volunteers, assisted by local high school student "Peer Teachers." Since 1990, the IBM Corporation has joined with a coalition of other companies, professional engineering societies, and government agencies to sponsor the annual Engineers Week (EWeek) campaign of technical education outreach, serving as Corporate Chair in 1992, 2001, and 2008. In recent years, we have annually recruited around 5000 IBM volunteers to reach out to more than 200,000 K-12 students in order to increase their awareness and appreciation of technical careers and encourage them to continue their studies of STEM (science, technology, engineering, and mathematics). The speaker, who helped found the APS Forum on Education (FED) and served as FED Councillor for 8 years, will review these and other programs for Public and K-12 Technical Education Outreach and Engagement.

10:24AM P5.00005 University Research Center Resources and Partnerships for Public and K-12 Outreach and Engagement[1] , GRETA M. ZENNER PETERSEN, University of Wisconsin-Madison — Collaboration and partnerships are essential to successful outreach and engagement in science. Through working together across disciplines and institutions, we can take advantage of a broad range of skills and expertise to strengthen a project and its outcomes. Additionally, building upon outreach and engagement resources developed by others is equally important to efficiently increasing impact and reducing redundancy. Research centers based at universities and other institutions of higher education commonly serve as both partners and resources for those active in education and outreach. This talk will share successful examples of public and K-12 outreach and engagement efforts that partner with a research center and/or use resources developed by a research center. A thorough discussion of strategies and recommendations for fostering such collaborations, as well as a broad survey of partnership models that exist, will help those at all levels of outreach and engagement experience pursue their science education ideas and goals.

[1]This material is based upon work supported by the National Science Foundation through the University of Wisconsin-Madison's Materials Research Science and Engineering Center on Nanostructured Interfaces (DMR-0520527).

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P6 DAMOP: Creating and Probing Exotic Optical Lattices Ballroom C2

8:00AM P6.00001 Quantum Gas Microscope - Simulating the Bose-Hubbard model and beyond[1] , MARKUS GREINER, Harvard University — The Quantum Gas Microscope enables high fidelity detection of single atoms in a Hubbard-regime optical lattice, bringing ultracold atom research to a new, microscopic level. I will report on investigating the Bose-Hubbard model by directly measuring number statistics and correlations across the superfluid - Mott insulator quantum phase transition. I will then give an outlook on how this enables creating novel phases in optical lattices and realizing quantum magnetism.

[1]This work was supported by ARO DARPA, AFOSR MURI, and NSF.

8:36AM P6.00002 Probing Mott insulators with single atom resolution , STEFAN KUHR, MPI Garching — This abstract not available.

9:12AM P6.00003 The Dicke quantum phase transition with a superfluid gas in an optical cavity , KRISTIAN BAUMANN, ETH Zurich — A phase transition describes the sudden change of state in a physical system, such as the transition between fluid and solid. Quantum gases provide the opportunity to establish a direct link between experiment and generic models which capture the underlying physics. A fundamental concept to describe the collective matter-light interaction is the Dicke model which has been predicted to show an intriguing quantum phase transition. We have realized the Dicke quantum phase transition in an open system formed by a Bose-Einstein condensate coupled to an optical cavity, and have observed the emergence of a self-organized supersolid phase. The phase transition is driven by infinitely long-ranged interactions between the condensed atoms, which are induced by two-photon processes involving the cavity mode and a pump field. We have shown that the phase transition is described by the Dicke Hamiltonian, including counter-rotating coupling terms, and that the supersolid phase is associated with a spontaneously broken spatial symmetry. The boundary of the phase transition is mapped out in quantitative agreement with the Dicke model.

9:48AM P6.00004 Strongly Correlated Quantum Gases Trapped in 3D Spin-Dependent Optical Lattices , BRIAN DEMARCO, University of Illinois — Optical lattices have emerged as ideal systems for exploring Hubbard model physics, since the equivalent of material parameters such as the ratio of tunneling to interaction energy are easily and widely tunable. In this talk I will discuss our recent measurements using novel lattice potentials to realize more complex Hubbard models for bosonic ^{87}Rb atoms. In these experiments, we adjust the polarization of the lattice laser beams to realize fully three-dimensional, spin-dependent cubic optical lattices. We demonstrate that atoms can be trapped in combinations of spin states for which superfluid and Mott-insulator phases exist simultaneously in the lattice. We also co-trap states that experience a strong lattice potential and no lattice potential whatsoever. I will discuss recent measurements revealing a mechanism similar to Kapitza resistance that leads to thermal decoupling in this latter combination. The implications for sympathetic cooling and thermometry using species-dependent lattices will be outlined.

10:24AM P6.00005 Excitons and Polaritons for Optical Lattice Ultracold Atoms in Cavity QED[1] , HASHEM ZOUBI, Institute for Theoretical Physics, Innsbruck University, Technikerstrasse 25, A-6020 Innsbruck, Austria — The quantum phase transition from the superfluid to the Mott insulator phase is predicted by the Bose-Hubbard model and realized for optical lattice ultracold atoms. We extend the model to include excited atoms and their coupling to cavity photons. In applying a mean field theory we calculate the phase diagram, where the Mott insulator reappears for deeper optical lattices [1]. In the Mott insulator we consider the system as an artificial crystal similar to molecular crystals with advantages due to the controllability of the system parameters. In such a system electronic excitations are delocalized due to resonance dipole-dipole interactions and in exploiting the lattice symmetry they form collective electronic excitations termed excitons [2]. We show that excitons in low dimensional systems include dark and bright modes, and in free space they can be metastable or superradiant, which deviates from the case of a single atom, the fact that implies the use of resonators [3]. We suggest optical lattice ultracold atoms as new frontiers of matter for cavity QED. In the strong coupling regime excitons and cavity photons are coherently mixed to form new quasiparticles called polaritons [4]. We suggest polariotons as a nondestructive observation tool for the different phases and properties of the system. We present different set-ups that have the potential to realize optical lattice ultracold atoms within a cavity. We emphasize the recent experiment in using tapered nanofibers, which are simultaneously used to trap and optically interface cold atoms through evanescent fields [5]. This system constitutes a hybrid quantum system combining both atomic and solid state devices.

[1] H Zoubi, H Ritsch, *PRA* **80**, 053608 (2009).
[2] H Zoubi, H Ritsch, *PRA* **76**, 013817 (2007). [3] H Zoubi, H Ritsch, *EPL* **90**, 23001 (2010).
[4] H Zoubi, H Ritsch, *EPL* **87**, 23001 (2009).
[5] H Zoubi, H Ritsch, *NJP* **12,** 103014 (2010).

[1]Austrian Science Funds (FWF).

Wednesday, March 23, 2011 8:00AM - 11:00AM –
Session P7 DBP GSNP: System Biology II: The Physics of Morphogenesis Ballroom C3

8:00AM P7.00001 Contractile forces driving embryonic development , MATTHIAS KASCHUBE, Princeton University — Proper development of an organism requires an orchestrated interplay of large sets of components. Recent developments in live fluorescent imaging methods allow the visualization of many key proteins in cells and tissues. Developing quantitative image analysis methods to measure the dynamics of shape changes in individual cells is central for understanding how a tissue gets sculpted, what molecular machineries are driving this process, and what interactions between cells are regulating it. In this talk, I will present recent advances in our understanding of the dynamical processes during morphogenesis, focusing on the example of tissue folding and invagination at the beginning of gastrulation in Drosophila. I show that this process is driven by a contractile multicellular actomyosin meshwork that dynamically forms within a few minutes at the cell surfaces. In individual cells, contraction is pulsed, with phases of contraction interrupted by pauses in which the cell size is maintained, i.e. a ratchet type dynamics that reduces the surface area of cells incrementally. Measuring the dynamics of whole cell shape changes in 2-photon live imaging data reveals that contraction pulses drive cell lengthening and relocation of cell nuclei, two transformations that are essential for successful invagination of tissue. This analysis further shows that over subsequent stages of invagination, during which cells undergo an elaborate sequence of shape changes, the volume of individual cells is a preserved quantity. These results shed new light on the forces and cellular dynamics driving tissue morphogenesis and are a step towards a quantitative understanding of how an organism's shape and internal structure arises in development.

8:36AM P7.00002 From Global Stresses to Local Cell Packing During Development[1] , DAVID LUBENSKY, University of Michigan — To perform their functions, cells in epithelial tissues must often adopt highly regular packings. It is still not fully understood how these ordered arrangements of cells arise from disordered, proliferative epithelia during development. I will use experimental and theoretical studies on an attractive model system, the cone cell mosaic in fish retina, to illustrate some ways that mechanical forces and cell signaling can interact to produce this transformation. Experiments examining the response to surgical lesions suggest that the correct mechanical environment at the tissue scale is essential to induce cone cells to rearrange into a rectangular lattice. Starting from this observation, I will argue that large-scale mechanical stresses naturally couple to and orient cell polarization and that this coupling can lead cells to line up in regular rows, as observed in the fish retina. This model predicts that cells in the rows will adopt characteristic trapezoidal shapes and that fragments of rows will persist even in tissue where the mosaic pattern is disrupted by lesions; these predictions are borne out by an analysis of cell packings at the level of the zonula occludens in wildtype and lesioned retinas.

[1]Supported by NSF grant IOS-0952873

9:12AM P7.00003 Emergence and Dynamics of Polar Order in Developing Epithelia , REZA FARHADIFAR, Harvard University — Planar Cell Polarity (PCP) is a conserved process in many vertebrate and invertebrate tissues, and is fundamental for the coordination of cell behavior and patterning. A well-studied example is the orientational pattern of hairs in the wing of the adult fruit fly Drosophila, which is an important model organism in biology. The Drosophila wing is an epithelium, i.e., a two-dimensional sheet of cells, which grows from a few cells to thousands of cells during the course of development. In the wing epithelium, planar polarity is established by an anisotropic distribution of PCP proteins within cells. The distribution of these proteins in a given cell affects the polarity of neighboring cells, such that at the end of wing development a large-scale PCP orientational order emerges. Here we present a theoretical study of planar polarity in developing epithelia based on a vertex model, which takes into account cell mechanics, cell adhesion, and cell division, combined with experimental results obtained from time-lapse imaging of the wing development. We show that in experiment, polarity order does not develop de novo at the end of wing development, but rather cells are initially polarized at an angle with respect to their final polarity axis. During wing development, the polarity axes of cells reorient towards their final direction. We identify a basic mechanism to generate such a large-scale initial polarization, based on the growth of a small number of cells with an initially random PCP distribution. Finally, we study the effect of shear and oriented cell division on dynamics of PCP order, showing that these two processes can robustly reorient the polarity axes of cells.

9:48AM P7.00004 Simple Physics in Diseases and Embryonic Development of the Eye[1] , ABBAS SHIRINIFARD, Biocomplexity Institute, Indiana University — While molecular-level regulation within cells during embryonic development is highly complex, the physical mechanisms which translate this intracellular information into multicellular physical structure at the tissue level are often surprisingly simple. I will discuss an example where regulation of cell-cell contact energies is primarily responsible for robust and evolvable regular patterns, the organization of the ommatidia and supporting cells into the regular tiling characteristic of the Drosophila eye and another example where adhesion failures in the human retina result in choroidal neovascularization leading to blindness. In both cases, simulations based on materials-science techniques can help us understand the patterning mechanisms and the reasons for their robustness and failures. Such simulations are easy to extend to other developmental phenomena and to development-related diseases like cancer.

[1]EPA grant "The Texas-Indiana Virtual STAR Center" and NIH grants R01 GM76692 and R01 GM077138.

10:24AM P7.00005 Morphogenesis of walled cells , OTGER CAMPAS, Harvard University — Walled cells have the ability to remodel their shape while sustaining an internal turgor pressure that can reach values up to 10 atmospheres. This requires a tight and simultaneous regulation of cell wall assembly and mechanochemistry, but the underlying mechanisms by which this is achieved remain unclear. In this talk I will discuss the interplay between growth and mechanics in shaping a walled cell, in the particularly simple geometry of tip-growing cells, which elongate via the assembly and expansion of cell wall in the apical region of the cell. Using only conservation laws and describing the observed irreversible expansion of the cell wall during growth as the extension of an inhomogeneous viscous fluid shell under the action of turgor pressure, we determine theoretically the radius of the cell and its growth velocity in terms of the turgor pressure and the secretion rate and rheology of the cell wall material. Moreover, we derive simple scaling laws for the geometry of the cell and find that a single dimensionless parameter, which characterizes the relative roles of cell wall assembly and expansion, is sufficient to explain the observed variation in shapes of tip-growing cells. Our work shows that the physics of cell wall expansion tightly constrains cell shape, providing a unified explanation of the characteristic morphologies of tip-growing cells across species that span several kingdoms, even though their underlying molecular mechanisms of cell morphogenesis are very different. More generally, our description provides a general framework to understand cell growth and remodeling in plants (pollen tubes, root hairs, etc.), fungi (hyphal growth and fission and budding yeast) and some bacteria.

Wednesday, March 23, 2011 8:00AM - 10:24AM –

Session P8 FPS FIAP: The Physics, Technology and Future of Robotics Ballroom C4

8:00AM P8.00001 Finding Fun and Fame in Physics with Robots , RANDY DUMSE, University of Northern Iowa — Physicist are often sought outside their immediate field for difficult solutions. Perhaps this is not surprising. However it might be unexpected how great the needs for physicists in the broadly cross discipline fields as robotics truly are. In this talk the author will describe being lured to Hollywood, by the need to uncover one of those principles, to find the deeper physical issues behind Panavision's needs for motion control. Then later describe using robotics as a tool to introduce students to physical concepts. Robots are excellent tools to focus student interest, both in General Ed courses, and graduate level electronics courses. In this vein, the author will try to highlight, "Where's the Physics in Robotics?"

8:36AM P8.00002 Recent Advances in Robotics and Career Opportunities for Physicists[1] , PAUL BOUCHIER, Dallas Personal Robotics Group — Some of the most significant advances in robotic systems over the last year are shown in this talk, which covers both autonomous and partly autonomous robots. A few robotic employers, both in Texas and elsewhere are profiled, with an emphasis on opportunities of interest to physicists.

[1]The presenter is president of the Dallas Personal Robotics Group

9:12AM P8.00003 Physics and Robotic Sensing – the good, the bad, and approaches to making it work , BRIAN HUFF, The University of Texas at Arlington — All of the technological advances that have benefited consumer electronics have direct application to robotics. Technological advances have resulted in the dramatic reduction in size, cost, and weight of computing systems, while simultaneously doubling computational speed every eighteen months. The same manufacturing advancements that have enabled this rapid increase in computational power are now being leveraged to produce small, powerful and cost-effective sensing technologies applicable for use in mobile robotics applications. Despite the increase in computing and sensing resources available to today's robotic systems developers, there are sensing problems typically found in unstructured environments that continue to frustrate the widespread use of robotics and unmanned systems. This talk presents how physics has contributed to the creation of the technologies that are making modern robotics possible. The talk discusses theoretical approaches to robotic sensing that appear to suffer when they are deployed in the real world. Finally the author presents methods being used to make robotic sensing more robust.

9:48AM P8.00004 Robot Competitions Around the World , STEVE RAINWATER, Network Cybernetics Corp. — This abstract not available.

Wednesday, March 23, 2011 8:00AM - 11:00AM –
Session P9 DFD: Liquid Crystals: Smectics, Nano-mixtures D220

8:00AM P9.00001 Achiral structure of B4 phase in a Bent-Core Liquid Crystal[1] , DONG CHEN, MICHAEL-SCOTT HEBERLING, JOSEPH MACLENNAN, MATTHEW GLASER, NOEL CLARK, Liquid Crystal Materials Research Center, University of Colorado at Boulder, HIDEO TAKEZOE, Department of Organic and Polymeric Materials, Tokyo Institute of Technology — Bent-core smectic layers have a tendency to exhibit spontaneous saddle-splay curvature, driven by the intra-layer structural mismatch. In the chiral B4 phase, the tendency for twist in the orientation of neighboring molecules coupled with the saddle-splay curvature lead to the formation of helical nanofilaments with either clockwise or anticlockwise twist. In addition to the helical nanofilament structure, we observe another microscopic structure in P12OPIMB, which is achiral, with no helical twist. This coffee-bean-like microstructure is dominated by saddle-splay curvature, like the dark conglomerate phase, but appears to have three dimensional order. The origin of these structures will be discussed.

[1]This work is supported by NSF MRSEC Grant DMR0820579 and NSF Grant DMR0606528.

8:12AM P9.00002 Two ferroelectric phases in a bent-core liquid crystal , C. ZHANG, N. DIORIO, B.K. SADASHIVA, A. JÁKLI — We report electro-optical, polarization current, dielectric and SAXS studies on novel bent-core materials that contain four ester groups; three in one arm and only one in the other. These materials differ from each other only by the number of carbons (n) in the alkyloxy chain terminating the one ester containing arm: in Ar 35 n=14, while in Ar 39 n=18. The phase sequences of Ar 35 and 39 are very similar to each other. Both have two mesophases, M1 and M2, with M1 in the 115°C-140°C temperature range, and M2 in between about 100°C and 115°C. Polarization current measurements indicate polarization current and optical switching in the M_1 phase with spontaneous polarization and switching time in the Ps$\sim$2.5-3mC/m^2 and τ $\sim$200μs range, respectively. While in Ar 35 the M2 phase cannot be switched, in the AR 39 we could detect polarization switching with a polarization value of about 5-6 mC/m^2 and switching time over a millisecond. Dielectric and X-ray scattering studies were employed to reveal the fine structure of the M_1 and M_2 phases.

8:24AM P9.00003 Surface Induced Reduction of Twisting Power in Liquid Crystal Films , LIDONG PAN, University of Minnesota, CHENG-CHER HUANG — Null transmission ellipsometry was employed to study the temperature evolution of the helical structure in smectic liquid crystal films. Free standing films with thickness ranging from 31 to more than 400 layers were prepared and studied. The experimental results show a reduced twisting power in thin films. A simple model was constructed to explain the results. Surface effect was found to be the reason for this phenomenon. Our findings are consistent with the studies of helically ordered magnetic films.

8:36AM P9.00004 Evolution of the isotropic to smectic-A phase transition in liquid crystal and acetone binary mixtures , KRISHNA SIGDEL, GERMANO IANNACCHIONE, Worcester Polytechnic Institute — The first-order transition from the isotropic (I) to smectic- A(SmA) phase in the liquid crystal 4-cyano-4'-decylbiphenyl (10CB) doped with the polar solvent acetone (ace) has been studied as a function of solvent concentration by high- resolution ac-calorimetry. Heating and cooling scans were performed for miscible 10CB+ace samples having acetone mole fractions from $x_{ace} = 0.05(1$ wt.%) to $0.36(10\%)$ over a wide temperature range from 310 to $327K$. Two distinct first-order phase transition features are observed in the mixture whereas there is only one transition (I-SmA) in the pure 10CB for that particular temperature range. Both calorimetric features reproduce on repeated heating and cooling scans and evolve with increasing x_{ace} with the high temperature feature relatively stable in temperature but reduced in size while the low temperature feature shifts dramatically to lower temperature and exhibits increased dispersion. Polarizing optical microscopy supports the identification of a smectic phase below the high-temperature heat capacity signature indicating that the low-temperature feature represents an injected smectic-smectic phase transition. These effects may be the consequence of screening the intermolecular potential of the liquid crystals by the solvent that stabilizes a weak smectic phase intermediate of the isotropic and pure smectic-A.

8:48AM P9.00005 The Power of Poincaré: Elucidating the Hidden Symmetries in Focal Conic Domains , ELISABETTA A. MATSUMOTO, GARETH P. ALEXANDER, BRYAN GIN-GE CHEN, RANDALL D. KAMIEN, Department of Physics and Astronomy, University of Pennsylvania — Focal conic domains are typically the "smoking gun" by which smectic liquid crystalline phases are identified. The geometry of the equally spaced smectic layers is highly generic but, at the same time, difficult to work with. We develop an approach to the study of focal sets in smectics which exploits a hidden Poincaré symmetry revealed only by viewing the smectic layers as projections from one-higher dimension. We use this perspective to shed light upon the concentric cyclides of Dupin and several classic focal conic textures which exhibit a more widespread level of geometric organization as in Friedel's law of corresponding cones, the networks and trellises expounded by Bouligand, or Apollonian packings.

9:00AM P9.00006 Phase behavior of platelets at different aspect ratios , ANDRES MEJIA, YA-WEN CHANG, Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX 77843, DAZHI SUN, Department of Mechanical Engineering, Texas A&M University, College Station, TX 77843, AGUSTIN DIAZ, ABRAHAM CLEARFIELD, Department of Chemistry, Texas A&M University, College Station, TX 77843, HUNG-JUE SUN, Department of Mechanical Engineering, Texas A&M University, College Station, TX 77843, ZHENGDONG CHENG, Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX 77843 — Suspensions of α -ZrP monolayer plates have recently been found to exhibit an isotropic to nematic (I-N) and nematic to smectic (N-S) phase transition. In the past, computer simulations have been developed to study the phase diagrams of platelets. In order to experimentally investigate the phase transitions and rheological behaviors of these particles, it is necessary to be able to manipulate their size, thickness and reduce their size distribution. We demonstrate here the strong dependency of the I-N transition on the aspect ratio (diameter/thickness) via the control of pristine α -ZrP platelets. We confirmed that the I-N transition volume fraction decrease monotonically with the aspect ratio as shown in previous simulations by J.A.C. Veerman and D. Frenkel. Furthermore, we found additional isotropic and gel phases by increasing the polydispersity of platelet sizes.

9:12AM P9.00007 Liquid Crystal-ZnO Nanoparticle Potential Photovoltaics: Role of LC Order and ZnO Particle Size and Concentration[1] , LUZ J. MARTINEZ-MIRANDA, JANELLE BRANCH[2], ROBERT THOMPSON, JEFFERSON W. TAYLOR, LOURDES SALAMANCA-RIBA, University of Maryland — We investigate the role order plays in the transfer of charges in ZnO nanoparticle - 8CB liquid crystal system for photovoltaic applications as well as the role the nominally 5x7nm^2 ZnO nanoparticles play in improving that order. Our results for the 5nm nanoparticles show an improvement in the alignment of the liquid crystal with increasing weight percentage of ZnO nanoparticles, up to a concentration of 30% wt for the 5nm particles accompanied by an increase by three orders of magnitude in the current generated.[3] Our results for the 5 x 7 nm^2 sample show that the current is larger than the current obtained for the 5 nm samples. The photocurrent can be expressed as the conductivity as a function dependent in the order in the sample times the portion of the electric field that is absorbed and transformed into the current.

[1]This work was supported by NSF-DMR- MRSEC-0520471, and its REU program, and in part by NSF-DMR-0906433.

[2]UMCP REU participant from Florida Institute of Technology

[3]L. J. Martínez-Miranda, Kaitlin M. Traister, Iriselies Meléndez-Rodríguez, and Lourdes Salamanca-Riba, Appl. Phys. Letts, 97, in press (2010).

9:24AM P9.00008 Interaction of a Bi-molecular Liquid Crystal Film With Functionalized Nanoparticles[1] , JEFFERSON W. TAYLOR, LUZ J. MARTINEZ-MIRANDA, University of Maryland, LYNN K. KURIHARA, Naval Research Labs — We investigate the properties of a nominally bi-molecular film of liquid crystal mixed with a magnetic nanoparticle (CoFe) that was functionalized with an organic compound (MHDA or APTS) with the atomic force microscope (AFM). We seek to investigate if the functionalization compound has an effect on the ordering of the liquid crystal in the vicinity of the nanoparticle. Studies in bulk liquid crystals have shown that the functionalization compound influences how the liquid crystal will reorganize.[2] The results of this investigation are compared to the results of work done on phospholipids in close contact with uncovered silica nanoparticles.[3] There seems to be a relation between the way that the two functionalizations behave in the bulk 8CB. The two functionalizations studied behave differently for particles larger than 22 nm, and apparently for the smaller particles.

[1]This work was supported by NSF-DMR-0906344.

[2]L. J. Martínez-Miranda, and Lynn Kurihara, *J. Appl. Phys, 105,* p. 084305 (2009).

[3]Yuri Roiter, Maryna Ornatska, Aravind R. Rammohan, Jitendra Balakrishnan, David R. Heine, and Sergiy Minko, *Langmuir*, 25, 6287-6299 (2009).

9:36AM P9.00009 Directed assembly of CdSe/ZnS quantum dots in cholesteric liquid crystal matrix , ANDREA RODARTE, LINDA S. HIRST, SAYANTANI GHOSH, University of California, Merced — Controlled self assembly of quantum dots (QDs) over macroscopic scales is important to realizing the potential for new applications such as photovoltaic devices and sensors. Here, we suspend CdSe/ZnS core/shell QDs in a cholesteric liquid crystal (LC) and investigate the dispersion and collective emission of the QDs when loaded into a Grandjean-Cano wedge cell. We use polarized optical microscopy and scanning photoluminescence microscopy to generate spatial and spectral maps of the QD-liquid crystal samples. We find that the LC forms Grandjean steps approximately 200um in width and the spectral effects of the QD emission correlate to the stripe formation. We also find that the cholesteric LC modulates the spectral emission of the QDs, creating a wavelength gradient dependant on the orientation of the collection polarizer with the director axis of the liquid crystal molecules.

9:48AM P9.00010 ABSTRACT WITHDRAWN –

10:00AM P9.00011 Diffusion-controlled Aggregation of Bucky Balls on Freely Suspended Smectic Liquid Crystal Films , ZOOM NGUYEN, TATYANA MALININA, CHEOL PARK, JOSEPH MACLENNAN, MATTHEW GLASER, NOEL CLARK, University of Colorado-Boulder, LIQUID CRYSTAL MATERIALS RESEARCH CENTER TEAM — Bucky balls (BB) have the tendency to clump together, making it hard to have them suspended in a solvent. We find that in highly viscous bulk 8CB, a smectic liquid crystal at room temperature, the aggregation happens more slowly. As the result, a freely suspended film made from the 8CB-BB mixture contains mostly small BB clumps. The diffusion coefficients of the clumps in thin films are much bigger than in the bulk, however, accelerating the aggregation process. We measure, via video microscopy, the decrease of the clumps' diffusion coefficients over time, indicating that their sizes increase towards a terminal size determined from the rate of diffusion. The terminal-sized clumps still diffuse around and stick to each other when they meet, forming the classic fractal pattern.

10:12AM P9.00012 Investigation of the lyotropic liquid crystal phase of Graphene Oxide solution[1] , YUE SHI, RIZWAN MAHMOOD, DONG CHEN, NOEL CLARK — Graphite Oxide spontaneously exfoliates into single-layer Graphene Oxide flakes in water. As the concentration becomes higher, Graphene Oxide solution shows a phase transition from the isotropic to the lyotropic liquid crystal phase. In the liquid crystal phase, the Graphene Oxide flakes can be ordered spontaneously by flow and shearing forces. We will report the investigation of the liquid crystal phase of the Graphene Oxide solution. In addition, the light scattering studies give dynamic information of the Graphene Oxide solution. Both the translational and rotational diffusion properties are investigated corresponding to different phases formed by Graphene Oxide at different concentrations.

[1]Supported by NSF MRSEC Grant DMR0820579.

10:24AM P9.00013 Defect dynamics in monodomain formation of a lyotropic chromonic liquid crystal under confinement , XUXIA YAO, Georgia Tech, ALEJANDRO REY, McGill University, JUNG PARK, MOHAN SRINIVASARAO, Georgia Tech — Lyotropic chromonic liquid crystals are a relatively new class of liquid crystals. We have studied the process of monodomain formation and the associated defect dynmaics of an anionic dye, Sunset Yellow FCF(SSY), under confinement in a flat capillary. SSY solutions were filled into a flat capillary by capillary action in isotropic phase and subsequently cooled to nematic state. Defect coarsening processes due to confinemnet include growth of small uniform domains, splitting of a center disclination line (+1) into two lines (+1/2), merging of uniform domains, and relaxation of defect curvature after pinch-off. Previously we studied the kinematics of a branch point involving a +1 and two +1/2 intersecting lines. Here we report on the collision of two such branch points and the subsequent emergence of two curved +1/2 lines that eventually coarsen into two paralell lines close to the edge of the capillary. A model that includes bending and tension line elasticity describes the branch point post collision and provides the means to asses viscoleatic moduli.

10:36AM P9.00014 Thermotropic Gold Nanorod Liquid Crystal Phases[1] , PAUL LUCHETTE, PETER PALFFY-MUHORAY, Liquid Crystal Institute - KSU — Large scale, oriented arrays of gold nanorods (Au NR) are of interest for a variety of applications, such as negative index materials and hyperbolic dispersion lenses. We report a method for preparing lyotropic, nematic LC phases of Au NR by combining polymer coated Au NR with a low molecular weight ($<$ 3200) polymers solvent. The solvent system was prepared by reacting hydroxymethyl siloxane and styrene via a hydrosilylation reaction. At appropriate ratios, these mixtures exhibit liquid crystalline phase behavior. Lyotropic LC phases of Au NR were observed for Au NR with aspect ratio above 4, diameter $\sim$15nm, using either linear or cyclic siloxane-styrene polymers as the solvent. Compared with other preparation methods such as lithography or evaporative deposition that produce static films, these self-assembled thermotropic LC phases of Au NR may be re-oriented in response to thermal or electric stimulus.

[1]This work was supported by the AFOSR under MURI grant FA9550-06-1-0337

10:48AM P9.00015 Organic-Inorganic Liquid Crystalline Composites , PETR SHIBAEV, Department of Physics, Fordham University, New York — Design of novel liquid crystalline composites consisting of organic liquid crystals, metal oxides (titanium oxide, zinc oxide, etc.) and "interface" layer covering inorganic materials is presented and discussed. The composites respond to light irradiation by changing orientation of liquid crystalline molecules, resulting in the changes of transmission and reflection properties of cells made of composite materials. The interaction of composite materials with light results from a complex chain of physico-chemical processes inside both the inorganic component and the "interface" layer. The processes that play the major role in the re-orientation of liquid crystalline molecules in the surface layer include: i. light-induced formation of electron-donor pairs inside metal oxides, ii. energy transfer of electron excitations to molecules inside the "interface" layer, iii. breaking of hydrogen bonds and conformational changes of molecules inside the "interface" layer. The experimental study of the processes resulting in re-orientation of liquid crystals by light is accompanied by theoretical calculations of conformational changes inside the "interface" layer and molecular re-orientation on the surface of inorganic materials.

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P10 DMP: Focus Session: Growth, Structure, Dynamics, and Function of Nanostructured Surfaces and Interfaces – Metals D221

8:00AM P10.00001 Interplay between Quantum Size Effect and Strain Effect on Growth of Nanoscale Metal Thin Film[1] , MIAO LIU, University of Utah, YONG HAN, Iowa State University, FENG LIU, University of Utah — Quantum Size Effect (QSE) has been shown to be a dominant factor in the growth of metal nanofilms on semiconductor substrates in the so-called electronic growth regime. On the other hand, the strain effect is ubiquitous in heteroepitaxial growth of semiconductor and metal thin films. Most time, however, these two important effects have been studied separately focusing on one while neglecting the other. Here, we develop a theoretical framework to investigate the interplay between QSE and strain effect on the stability of metal nanofilms. The QSE and strain effect are shown to be coupled through the concept of "quantum stress". First-principles calculations reveal large quantum oscillations in the surface stress of metal nanofilms as a function of film thickness, which adds extrinsically additional strain-coupled quantum oscillations to surface energy of strained metal nanofilms. Our theory enables a quantitative estimation of the amount of strain in experimental samples from the measured stability patterns, explaining a possible origin for some outstanding discrepancies between the existing theories and experiments.

[1]Supported by NSF (DMR-0909212)

8:12AM P10.00002 Contrasting growth modes of Ru thin film nano-structures on Si and Pd[1] , XIANGSHI YIN, AO TENG, The University of Tennessee, MUSTAFA ÖZER, Oak Ridge National Laboratory, HANNO WEITERING, The University of Tennessee, PAUL SNIJDERS, Oak Ridge National Laboratory — We have studied Ruthenium thin film growth on both Si (111) and Pd (111) surfaces. The films were deposited at low (LN2) temperature and at room temperature, and subsequently annealed at elevated temperatures, up to 600C. The surface structure, morphology, and chemical composition were investigated by LEED, STM, AES and XPS. Upon deposition at low temperature, nanoclusters are formed on both Si and Pd. Remarkably, the nanoclusters are approximately 3 nm in diameter and exhibit narrow size distributions on both substrates. In the case of Ru on Si, XPS spectra indicate silicide formation at the interface above 300C, but the nanocluster surface morphology survives up to 600C. On the other hand, nanoclusters on Pd smoothen into atomically flat films above 200C. The striking difference in adatom mobilities on these substrates is surprising in light of the very high melting temperature of Ru (2400C).

[1]Research (PCS) sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U. S. Department of Energy.

8:24AM P10.00003 Temperature-dependence of Ni+Al co-deposition on NiAl(110): Atomistic-level modeling of deviations from perfect alloy ordering , YONG HAN, DAPENG JING, BARIS UNAL, P.A. THIEL, J.W. EVANS, Institute for Physical Research and Technology; Departments of Chemistry, MSE, Mathematics, Physics and Astronomy; Ames Lab, ISU, Ames, Iowa 50011 — Stoichiometric co-deposition of Ni and Al on NiAl(110) for high enough temperatures (below the order-disorder transition for NiAl) must produce near-perfect alloy islands and overlayers. However, at 300K, island structure is far from perfectly ordered and depends strongly on the deposition protocol (e.g., simultaneous vs. sequential). Realistic atomistic-level modeling of this non-equilibrium behavior must provide an accurate description of not just alloy thermodynamics (through adatom adsorption and interaction energies), but also of diffusion kinetics (for adatom attachment-detachment at and transport along island edges). This is achieved by multi-site lattice gas modeling with DFT input for adsorption and interaction energies for adatoms both at adsorption sites and at transition states for hopping [T. Duguet, Y. Han et al., Proc. Nat. Acad. Sci. 107 (2010) Special Issue on Surface Chemistry; Y. Han et al., submitted (2010)]. Model analysis by KMC simulation shows a transition from poor alloy order at 300K to almost perfect order at 600K.

8:36AM P10.00004 Electronic origin of kinetic and dynamic processes at atomic steps on vicinal metal substrates[1]

, WENGUANG ZHU, University of Tennessee & Oak Ridge National Laboratory — Single-atomic-layer steps play an important role in the kinetics and dynamics of morphological evolution and structural formation at surfaces. In this talk, we will attempt to elucidate the importance of the electronic nature in determining the bonding of adatoms and the activation barriers for adatom descent at step edges. The insights gained through first-principles case studies have timely and important impacts in understanding the evolution of many nanostructured surfaces and prevention of electrical breakdown in nanodevices. In the first case [1], we establish a clear correlation between the preferred diffusion mechanism and step-edge barrier and the relative degree of electronic shell filling of the adatom and the substrate. We also find an approximate linear relation between the adatom step-edge hopping barrier and the adatom-surface bonding strength with a slope roughly proportional to the number of the nearest neighbors of the adatom in the initial state. These results can serve as simple guiding rules for predicting precise atomic surface morphologies and designing desirable surface nanostructures, such as atom wires [2]. In the second case [3], we discover an optimal surface electromigration inhibitor on the technologically important Cu(111) surface, characterized by energetically favoring and binding strongly at the kink of step edges. Finally, we will briefly discuss how the electronic bonding strengths influence the nucleation and growth behavior of carbon atoms at the step edges of various transition-metal surfaces, a crucial insight in designing optimal kinetic pathways for mass production of quality epitaxial graphene [4].

[1] Y. Mo, W. G. Zhu, E. Kaxiras, and Z. Y. Zhang, Phys. Rev. Lett. 101, 216101 (2008).
[2] Y. Mo, K. Varga, E. Kaxiras, and Z. Y. Zhang, Phys. Rev. Lett. 94, 155503 (2005).
[3] K. H. Bevan, W. G. Zhu, H. Guo, and Z. Y. Zhang, Phys. Rev. Lett. (submitted).
[4] H. Chen, W. G. Zhu, and Z. Y. Zhang, Phys. Rev. Lett. 104, 186101 (2010).

[1]Work done in collaboration with Zhenyu Zhang, Efthimios Kaxiras, Yina Mo, Kirk H. Bevan, Hua Chen, and Hong Guo, and supported by USDOE, USNSF, and NNSF of China.

9:12AM P10.00005 Bilayer islands in heteroepitaxy of transition metals: insights from first principles[1]

, TALAT S. RAHMAN, MARISOL ALCANTARA ORTIGOZA, SERGEY STOLBOV, Department of Physics, University of Central Florida, Orlando, FL32816 — Although not in equilibrium configuration, bilayer islands have been observed in the heteroepitaxy of some transition metals for four decades. Its physical origin, however, was investigated experimentally recently for Ru on Pt(111) [1]. By introducing an energy-gain criterion (upon adlayer formation) and by analyzing the density of electronic states of 1 to 3 Ru adlayers on Pt(111), we show that, even though no bonding stronger than that of atoms in bulk Ru is involved, the energy gain for the formation of the second layer is the largest. We find that the effect of the lattice mismatch is not trivial to elucidate from experiment since the electronic structure of a clean substrate changes in the presence of strain and/or chemical bonding with other species. The lattice mismatch, however, is the key factor for the instability in the formation of a third-layer. We extend the model to explain the well-known case of Co/Cu(111) and to predict other possible bilayer systems.

[1] A. Bergbreiter et al., Vacuum **84** 13 (2010)

[1]Work supported by DOE Grant No. DE-FG02-07ER15842

9:24AM P10.00006 Collective Super-Diffusive Motion of the Pb Wetting Layer on Si(111)

, MICHAEL ALTMAN, K.L. MAN, M.M.T. LOY, Hong Kong University of Science and Technology, M.C. TRINGIDES, Iowa State University — An unusual mass transport behavior has been discovered in the Pb/Si(111) wetting layer. Mass transport is studied by observing non-equilibrium coverage profile evolution with low energy electron microscopy (LEEM). Equilibration of an initial coverage step profile does not exhibit the profile broadening and gradual, $x \sim t^{1/2}$, time-dependent evolution that is expected from classical considerations. Instead, the profile edge is displaced linearly in time, $x \sim t$, much faster than expected for thermally activated hopping and without dispersal. LEEM also reveals a wave-like disturbance in the wetting layer that propagates in the direction opposite the step profile motion. The Pb coverage that is left in the wake of this disturbance can be determined accurately and with high lateral resolution using selected-area LEED due to the Devil's Staircase (DS) phases in this system. The expanding wave converts an initial homogeneous DS phase with coverage $\theta > \theta_c$ to a final phase with $\theta_c = 1.25$ ML, thereby conserving mass across the initial step profile position. This identifies a collective super-diffusive motion of the Pb layer that can extend rapidly over macroscopic distances. Such motion may facilitate the remarkably efficient self-organization of uniform height, quantum size effect-induced Pb islands on Si(111).

9:36AM P10.00007 Crossover from concerted motion to periphery diffusion for Cu clusters on Cu(111): Application of Fine Grid On-Lattice SLKMC[1]

, SYED ISLAMUDDIN SHAH, GIRIDHAR NANDIPATI, University of Central Florida, ALTAF KARIM, Lawrence Berkeley National Laboratory, ABDELKADER KARA, TALAT S. RAHMAN, University of Central Florida — The "fine grid on-Lattice" Self-Learning Kinetic Monte Carlo (SLKMC) technique combines the ideas embedded in the SLKMC [1] method with a new pattern recognition scheme which incorporates both fcc and hcp sites to characterize and store configurations. Application of methods for saddle point searches have revealed several new mechanisms involving multiple atoms which contribute to cluster migration. We present results for the diffusion of 2D Cu islands on Cu(111), using semi-empirical interatomic potentials [2], at three temperatures (300K, 500K and 700K). Long time simulations show a trend in crossover from concerted motion to periphery diffusion for clusters containing more than 14 atoms. The calculated trends in effective energy barriers and diffusion constants are compared with those obtained earlier from the SLKMC Method [1] which allowed only surface fcc site occupancy.

[1] A. Karim et al. Phys. Rev. B 73, 165411 (2006)
[2] S. M. Foiles et al. Phys. Rev. B 33, 7983 (1986)

[1]Work supported by NSF-ITR 0840389.

9:48AM P10.00008 Shape transitions in strained islands: kinetics versus energetics[1]

, YUNSIC SHIM, YEVGEN KRYUKOV, JACQUES AMAR, University of Toledo — Recently, it has been argued that the shape transition from compact to ramified islands observed experimentally in submonolayer Cu/Ni(100) growth is not due to kinetics but can be understood in terms of energetic arguments. In order to determine the responsible mechanisms we have carried out temperature-accelerated dynamics (TAD) simulations as well as energetics calculations. Surprisingly, our results indicate that the strain-energy contribution to the dependence of island-energy on shape is relatively weak. In contrast, our TAD simulations indicate that unexpected concerted motions occurring at step edges may be responsible. The energy barriers for these concerted motions are significantly lower than for Cu/Cu(100) and Ni/Ni(100), decrease with increasing island size, and appear to saturate for islands larger than 300 - 400 atoms. These results suggest that the shape transition is of kinetic origin but is strongly mediated by strain.

[1]Supported by NSF-DMR 0907399

10:00AM P10.00009 Temperature-induced crossovers in the static roughness of a one-dimensional interface[1] , ELISABETH AGORITSAS, DPMC-MaNEP - University of Geneva (Switzerland), VIVIEN LECOMTE, Laboratoire de Probabilite et Modeles Aleatoires, University Paris Diderot (France), THIERRY GIAMARCHI, DPMC-MaNEP - University of Geneva (Switzerland) — At finite temperature and in presence of disorder, a one-dimensional elastic interface displays different scaling regimes at small and large lengthscales. Using a replica approach and a Gaussian variational method (GVM), we explore the consequences of a finite interface width ξ on its small-lengthscale geometrical fluctuations. We compute analytically the static roughness $B(r)$ of the interface as a function of the distance r between two points on the interface, in the specific case of short-range elasticity and random-bond disorder. We find that for a finite ξ two temperature regimes exist, and we determine the corresponding different roughness regimes and their crossover lengthscales. In addition, using a directed polymer description, we study via a second GVM procedure and generic scaling arguments, a modified toy model that provides further insight on those results, which apply to experimental interfaces such as e.g. ferromagnetic domain walls in thin films, subjected to a quenched uncorrelated disorder.

[1]This work was supported in part by the Swiss SNF under MaNEP and division II.

10:12AM P10.00010 Mean field approach to fluctuations of surface line defects[1] , DIONISIOS MARGETIS, Department of Mathematics, University of Maryland — Below the roughening transition temperature, the dynamics of crystal surfaces are driven by the motion of line defects (steps) of atomic size. According to the celebrated Burton Cabrera-Frank (BCF) model, the steps move by mass conservation, as adsorbed atoms (adatoms) diffuse on terraces and attach/detach at step edges. The resulting deterministic equations of motion incorporate nonlinear couplings due to entropic and elastic-dipole step-step interactions. In this talk, I will discuss a formal theory for stochastic aspects of step motion by adding noise to the BCF model in 1+1 dimensions. I will define systematically a "mean field" that enables the conversion of the coupled, nonlinear stochastic equations for the distance between neighboring steps (terrace widths) to a single Langevin-type equation for an effective terrace width. In the course of my study, I invoke the Bogoliubov-Born-Green Kirkwood-Yvon (BBGKY) hierarchy for joint terrace-width probability densities and a decorrelation ansatz for terrace widths. By using an example drawn from epitaxial growth (with material deposition from above), I will compare the mean field approach to an exact result from a linearized growth model. [D. Margetis, J. Phys A: Math. Theor. 43, 065003 (2010).]

[1]This work was supported by NSF under Grant DMS-0847587.

10:24AM P10.00011 Spacing distribution functions for 1D point island model with irreversible attachment[1] , DIEGO GONZALEZ, THEODORE EINSTEIN, University of Maryland, ALBERTO PIMPINELLI, University of Maryland and Science Attache, French Consulate, Houston — We study the configurational structure of the point island model for epitaxial growth in one dimension. In particular, we calculate the island gap and capture zone distributions. Our model is based on an approximate description of nucleation inside the gaps. Nucleation is described by the joint probability density p_n^{xy} (x,y), which represents the probability density to have nucleation at position x within a gap of size y. Our proposed functional form for p_n^{xy} (x,y) describes excellently the statistical behavior of the system. We compare our analytical model with extensive numerical simulations. Our model retains the most relevant physical properties of the system.

[1]This work was supported by the NSF-MRSEC at the University of Maryland, Grant No. DMR 05-20471, with ancillary support from the Center for Nanophysics and Advanced Materials (CNAM).

10:36AM P10.00012 Capture zone area distributions for homogeneous nucleation and growth of islands during deposition[1] , JIM EVANS, YONG HAN, Iowa State University, MAOZHI LI, Renmin University — The size distribution of islands formed by homogeneous nucleation and growth during deposition is known to encode information about the nucleation mechanism. The same was recently proposed for the distribution, g(A), of areas, A, of capture zones (CZ) surrounding islands [1], where most atoms landing within a CZ aggregate with the associated island. We have developed a precise theory for g(A) whose evolution is driven by the nucleation of new islands [2]. g(A) has a complicated form controlled by details of the spatial aspects of nucleation. However, it is reasonably approximated by a Generalized Gamma distribution, $g(A) \sim A^{\beta} \exp[-cA^{n}]$. For compact 2D islands, one has n $\sim$ 1.5, and $\beta \sim 3(i+2)/2$ for critical size i. Here, β follows from analysis of the creation of new small capture zones between nearby pairs of islands, and n from analysis of the likelihood that a new CZ overlaps an existing large CZ.

[1] Pimpinelli & Einstein, PRL 99 (2007) 226102; 104 (2010) 149602;
[2] Li, Han & Evans, PRL 104 (2010) 149601.

[1]Supported by NSF grant CHE-0809472

10:48AM P10.00013 Modeling Island-Growth Capture Zone Distributions (CZD) with the Generalized Wigner Distribution (GWD): New Developments in Theory and Experiment[1] , ALBERTO PIMPINELLI[2], T.L. EINSTEIN, DIEGO LUIS GONZÁLEZ, RAJESH SATHIYANARAYANAN[3], AJMI BH. HAMOUDA[4], U. Maryland — Earlier we showed [PRL 99, 226102 (2007)] that the CZD in growth could be well described by $P(s) = as^{\beta}\exp(-bs^2)$, where s is the CZ area divided by its average value. Painstaking simulations by Amar's [PRE 79, 011602 (2009)] and Evans's [PRL 104, 149601 (2010)] groups showed inadequacies in our mean field Fokker-Planck argument relating β to the critical nucleus size. We refine our derivation to retrieve their $\beta \approx i+2$ [PRL 104, 149602 (2010)]. We discuss applications of this formula and methodology to experiments on Ge/Si(001) and on various organics on SiO_2, as well as to kinetic Monte Carlo studies homoepitaxial growth on Cu(100) with codeposited impurities of different sorts. In contrast to theory, there can be significant changes to β with coverage. Some experiments also show temperature dependence.

[1]Supported by NSF-MRSEC at UMD, Grant DMR 05-20471.
[2]Also Science Attaché, French Consulate, Houston; Rice U.; and U. Blaise Pascal Clermont-2, France
[3]Now at IBM-Bangalore, India
[4]Also U. Monastir, Tunisia

Wednesday, March 23, 2011 8:00AM - 11:00AM –
Session P11 FIAP: Electronic Structure: Theory and Spectra I D222

8:00AM P11.00001 Hybrid functional calculations for defects in TiO_2[1] , CHRIS VAN DE WALLE, Materials Department, University of California, Santa Barbara, JOEL VARLEY, Department of Physics, University of California, Santa Barbara, ANDERSON JANOTTI, Materials Department, University of California, Santa Barbara — Density functional theory (DFT) has proven its value as an immensely powerful tool for assessing structural properties of defects in semiconductors or insulators. Frequently, however, information about electronic structure is required, i.e., the position of defect levels in the band gap. Since DFT in the LDA or GGA severely underestimates the band gap, the position of defect levels is subject to large error bars. Here we show that the use of hybrid functionals allows us to overcome this problem. We illustrate the power of the approach with the example of point defects in TiO_2, a material of high interest for electronics, optoelectronics, and photocatalysis. Unintentional n-type conductivity in TiO_2 has often been attributed to oxygen vacancies (V_O). We find that V_O is indeed a shallow donor [1]. Our calculated formation energies allow us to assess whether vacancy concentrations are consistent with experimental observations of unintentional conductivity.

[1] A. Janotti, J. B. Varley, P. Rinke, N. Umezawa, G. Kresse, and C. G. Van de Walle, Phys. Rev. B 81, 085212 (2010).

[1]Work supported by the NSF MRSEC Program.

8:12AM P11.00002 Bandgap properties of amorphous TiO2 (aTiO2) , M. KYLEE UNDERWOOD, West Virginia University, BINAY PRASAI, BIN CAI, DAVID A. DRABOLD, Ohio University, JAMES P. LEWIS, West Virginia University — In photocatalytic and photovoltaic applications, TiO_2 is a convenient material due to its stability, abundance, and functionality. The natural bandgap of TiO_2 is very wide thus limits its usability to the UV region of the solar spectrum. Previous research has indicated that these limitations may be overcome by doping with anionic nonmetal elements such as carbon or nitrogen. However, both experimental and theoretical research suggests that these dopants tend to act more as recombination centers rather than truly enhance the functionality of TiO_2. Although naturally occurring in crystalline form, the initial processing of TiO_2 for the production of thin films and powders results in mostly amorphous materials and further processing locks the material into a particular crystalline or poly-crystalline form. The properties of anatase and rutile crystalline structures of bulk and nanophase TiO_2 have been studied in detail; however, amorphous TiO_2 ($aTiO_2$) lacks a similar depth of study. We show, through ab initio density functional theory calculations, that $aTiO_2$ exhibits a bandgap almost identical to crystalline TiO_2. We will further discuss our results for anionic nonmetal dopants in $aTiO_2$.

8:24AM P11.00003 Evidences for Ti-N anchoring in organic dyes on TiO2 and its influence on photovoltaic performance[1] , YANG JIAO, SHENG MENG, Inst. Physics, Chinese Academy of Sciences, SEEC LAB TEAM — New metal-free organic dyes with a novel donor-pi-acceptor design produce efficiencies exceeding 10% for dye-sensitized solar cells (DSSC) applications since 2010. Based on state-of- the-art electronic structure calculations and real time time- dependent density functional theory (TDDFT) simulations, we present consolidated evidences for novel Ti-N anchoring at the interface for such a broad group of new dyes, inferred from energetics, vibrational recognition, and electronic and optical data. This fact is contrary to what people usually believed and assumed in previous experiments and was largely ignored. We further demonstrate that the presence of interface Ti-N bonds largely benefit the electronic level alignment and photoelectron injection dynamics, greatly contributing to the improved efficiencies of DSSC based on cost-effective, environment-friendly organic dyes.

[1]We acknowledge supports from NSFC and hundred-talent program of CAS.

8:36AM P11.00004 First Principles Study on Ta_2O_5 Polymorphs[1] , YUNING WU, HAI-PING CHENG, Department of Physics, University of Florida, USA, LAN LI, College of Arts and Sciences, Kent State University, USA — Using density functional theory (DFT) with generalized gradient approximations (GGA) and the projector-augmented wave method, we have investigated structure, energetics, elastic tensors and mechanical properties of four crystalline forms of Ta_2O_5 with exact stoichiometry and a model amorphous structure. A virtual crystal potential has also been constructed to address partial oxygen occupancy and compared to models of explicit oxygen vacancies and the oxygen-rich system. Calculations show that mechanical properties of these polymorphs are highly anisotropic. By comparison with experimental data, we find that all crystalline phases and the simulated amorphous phase have Young's modulus higher than the amorphous thin film that is measured experimentally, but the variation among crystalline structures is as high a factor of 2. Electronic properties of three Ta_2O_5 polymorphs have been calculated using a hybrid DFT and Hartree-Fock functional method that improves gap size obtained by GGA. We suggest that further experimental measurements on tantala crystals are needed to understand physical properties of this import material.

[1]Funding support from NSF/PHY-0855292 and NSF/DMR-0804407, computers from NERSC and UF/HPC.

8:48AM P11.00005 What is the G^0W^0 band gap of ZnO? , M. STANKOVSKI, G. ANTONIUS, D. WAROQUIERS, A. MIGLIO, H. DIXIT, P. RINKE, H. JIANG, M. GIANTOMASSI, X. GONZE, M. CÔTÉ, G.-M. RIGNANESE — Recently, there has been considerable attention on ZnO as a candidate material for low-cost transparent conducting oxides. Even in its natural wurtzite bulk phase, it is numerically difficult to evaluate G^0W^0 quasiparticle (QP) corrections for ZnO. Therefore we have a wide range of theoretical QP gaps quoted in the literature (from $\sim$1.6 eV to $\sim$3.6 eV to be compared with 3.44 eV experimentally). Typically, many approximations are used *en route*. To find the correct theoretical gap, we have performed calculations of unprecedented accuracy. First, we study the G^0W^0 band gap given different ground-state DFT starting point approximations (LDA and GGA) and the effect of including scalar-relativistic corrections. Second, we present a study of results for norm-conserving pseudopotentials vs. all-electron techniques (both PAW and FP-LAPW). Four different plasmon-pole models are compared with the more accurate contour-deformation approach. Finally, a Hubbard U parameter for the 3d-states of Zn is shown to depend on the exact details of application. This work shows that the band-gap of ZnO is indeed underestimated in the G^0W^0 approach.

9:00AM P11.00006 Energies of formation and electronic band structure of Zn-IV-N_2 semiconductors , ATCHARA PUNYA, WALTER R.L. LAMBRECHT, Case Western Reserve University — The II-IV-N_2 semiconductors are expected to have properties closely related to those of the III-N semiconductors. We focus on Zn-IV-N_2 semiconductors with the group IV-element Si, Ge and Sn. The formation energies of the compounds in this series were calculated by the full-potential linearized muffin-tin orbital method with LDA and GGA. Zero point motion corrections were included. Furthermore, the energies of formation of competing Zn_3N_2, Si_3N_4, Ge_3N_4, Sn_3N_4 compounds were also calculated to determine the allowed ranges of the chemical potentials of the elements where the compounds are stable at zero temperature. For comparison, we also calculated the energy of formation of GaN, which is found to be in good agreement with experimental values. All compounds in the series are found to have a large region of stability. The electronic band structures are calculated using the QSGW method. The band gaps span the region from 1.65 - 5.30 eV, increasing from $ZnSnN_2$ to $ZnSiN_2$, with the bandgap of $ZnGeN_2$ close to that of GaN. While $ZnGeN_2$ and $ZnSnN_2$ are direct band gaps semiconductors, $ZnSiN_2$ is found to have an indirect gap slightly smaller than its lowest direct gap. The states near the valence band maximum at Gamma are symmetry labeled and their splittings analyzed in terms of two crystal field parameters. Spin-orbit coupling is found to have negligible effect on these states.

9:12AM P11.00007 Structural and Electronic properties of β-In_2X_3 (X = O, S, Se, Te) using *ab initio* calculations[1] , S.V. KHARE, S. MARSILLAC, N.S. MANGALE, V. GADE, University of Toledo — Several III-VI body-centered tetragonal layered compounds belonging to space group $I4_1/amd$ have been a subject of interest recently because of their potential applications in high efficiency and environmentally friendly copper-indium-gallium-selenide (CIGS) solar cells and molecules. Here we have studied the structural, energetic, and electronic properties of four compounds β-In_2X_3 (X = O, S, Se, Te), in this space group. Using first principles computations, we have fully determined the lattice constants *a* and *c*, as well as 10 internal parameters that define this unique structure of primitive unit cells of 40 atoms. For β-In_2S_3 our computed values are found to be consistent with experimental measurements. The bulk modulus B, local electronic density of states (LDOS), total density of states (DOS), and band gap E_f of these phases have been investigated.

[1]Supported by Ohio Supercomputing Center, National Center for Supercomputing Applications, Wright Center for PVIC, National Science Foundation, DARPA.

9:24AM P11.00008 ABSTRACT WITHDRAWN –

9:36AM P11.00009 The surface passivation effects on the optical response of small CdTe quantum dots , OSMAN BARIS MALCIOGLU, JEAN-YVES RATY, University of Liege — In this work, the optical properties of various small-sized CdTe based quantum dots are investigated using time dependent density functional formalism. `turboTDDFT`, an implementation of the Lanczos-Liouville approach to linearized time-dependent density-functional theory, designed to simulate the optical spectra of molecular systems made of up to several hundreds atoms and distrubuted as a part of the open source QUANTUM ESPRESSO project is used. The response of the clusters at ambient temperature is estimated by performing averages of the optical spectra along the molecular dynamics trajectories. Different types of surface passivation schemes are considered in forming the quantum dot structures. Solvent effects on the surfaces that result from different passivation schemes are considered in detail using an explicit solvent approach.

9:48AM P11.00010 First-principles study of the electronic structure of NiS and NiO[1] , JOAQUIN NOYOLA, MENG TAO, QIMING ZHANG, University of Texas at Arlington — First-principles calculations of the electronic structure of NiS and NiO are performed. The exchange-correlation schemes of GGA, DFT+U and hybrid functional have been applied. The resulting band structures for each scheme are compared and analyzed to assess the reliability of the GGA, DFT+U, and hybrid functional.

[1]supported by the U.S. DOE, Office of BES, under No. DE-SC0002062.

10:00AM P11.00011 Tight-binding based alloy scattering calculations in $Si_{1-x}Ge_x$, SAUMITRA MEHROTRA, ABHIJEET PAUL, GERHARD KLIMECK — Role of alloy scattering in SiGe device performance has been up for debate since long time. The main source of confusion stems from the choice of alloy scattering potential parameter ΔU_{fit}. We present a theoretical model within tight-binding representation for treating alloy scattering in SiGe devices. The approach is shown to inherently capture the alloy scattering potential parameter(s) which otherwise are experimentally fitted or determined from first principles calculations for different band edges. It is shown that both onsite (variation in atom type) and off-diagonal (variation in bond type) blocks are important in estimating the potential value. The extracted scattering potential is then used to estimate bulk alloy scattering limited mobility in atomistic SiGe representation. The results show good agreement for both n-type and p-type experimental bulk mobility values.

10:12AM P11.00012 Predicting the Direct to Indirect Transition in III-V Alloys , JEREMY NICKLAS, JOHN WILKINS, The Ohio State University — The screened hybrid functional, HSE, used in density functional theory (DFT) has been gaining traction recently for its predictive powers of the band structure in bulk semiconductors. It is natural to assume that these accurate results would carry over to alloy semiconductors, but little work has been done to confirm this. We recently investigated the compositional dependence on the electronic band structure for a range of III-V semiconducting alloys (AlGaAs, InAlAs, AlInP, InGaP, and GaAsP) [1]. These alloys have a critical composition where the band gap crosses over from a direct band gap (having optoelectronic uses) to an indirect band gap (window layers in solar cells). A direct comparison of this critical composition is made between HSE and the standard density functional, PBE, revealing crossover compositions within 12% atomic composition when compared to experiment while PBE overestimates by as much as 39% atomic composition. Such results give merit that HSE is a reliable functional for tuning the electronic properties of semiconducting alloys.

[1] Jeremy W. Nicklas and John W. Wilkins, Appl. Phys. Lett. 97, 091902 (2010)

10:24AM P11.00013 Hybrid DFT computes accurate band offsets of semiconductor alloy heterostructures[1] , AMITA WADEHRA, JEREMY NICKLAS, JOHN WILKINS, The Ohio State University — Semiconductor alloy heterostructures are the backbone of optoelectronic devices. Among the most important parameters that determine the utility of heterostructure devices are the valence and conduction band offsets. Although DFT with standard functionals such as LDA or PBE does an acceptable job for valence band offsets, it fails to predict accurate conduction band offsets on its own due to the well-known band gap problem. We demonstrate the accuracy of HSE (Heyd-Scuseria-Ernzerhof) hybrid functional for computing the band gaps and band offsets of a broad selection of technologically important semiconductor alloys and their heterostructures, e.g., AlInAs/GaInAs, GaInP/AlGaAs, AlInP/GaInP [1]. The highlight of this study is the computation of conduction band offsets with a reliability that has eluded standard density functional theory. These results demonstrate predictive power of HSE for band engineering of relevant devices.

[1]. A. Wadehra, J. W. Nicklas and J. W. Wilkins, Appl. Phys. Lett. 97, 092119 (2010)

[1]Acknowledgements: DOE, NERSC, OSC

10:36AM P11.00014 Electronic Structure of Random Alloys , CHAD WAXLER, BYOUNGHAK LEE, Department of Physics, Texas State University at San Marcos, XAVIER CARTOIXÁ, Departament d'Enginyeria Electrónica, Universitat Autónoma de Barcelona — We present a theoretical investigation of the evolution of the electronic properties of the random alloys as they undergo a transition from one pure crystal to another. For random substitutional alloys the Bloch wavevector is not a good quantum number due to the lack of translational invariance. In spite of this obvious fact the conventional methods used for random alloys calculations, e.g., Virtual Crystal Approximation and Coherent Potential Approximation, assume a medium that pertains the same symmetries of the parent compounds. The question we ask is how well the band structures from such effective medium theories agree with the real electronic structures. We address this issue using direct simulations of randomly distributed (Al,Ga)As and (In,Ga)P atom structures.

10:48AM P11.00015 Atomic-scale evolution of interfacial electronic band alignment in epitaxial Gd_2O_3 on GaAs (100) , B.C. HUANG, Y.P. CHIU, M.C. SHIH, Department of Physics, National Sun Yat-Sen University, Kaohsiung, 80424, Taiwan, J.Y. SHEN, P. CHANG, T.H. CHIANG, Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, 30013, Taiwan, C.S. CHANG, Institute of Physics, Academia Sinica, Taipei, 10617, Taiwan, M.L. HUANG, National Taiwan University, and National Tsing Hua University, Taiwan, M. HONG, Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, 30013, Taiwan, J. KWO, National Taiwan University, and National Tsing Hua University, Taiwan — Direct imaging of the atomic-scale configuration and interfacial electronic band alignment in epitaxial Gd_2O_3 high κ oxides grown on GaAs (100) has been demonstrated using cross sectional scanning tunneling microscopy and spectroscopy. Measurements of the local density of states characteristics with atomic precision enabled us to determine the evolution of electronic properties in passivating the Gd_2O_3/GaAs hetero-interface. Close examinations suggested excellent electrical passivation at this interface, with low interfacial states and low leakage current density. In addition, from the local electronic states across the gate oxides, the spatial extent of the GaAs wavefunctions extended into the gate dielectric situates a minimum thickness of 0.8 nm for the Gd_2O_3 gate capacitance.

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P12 DMP: Focus Session: Dopants and Defects in Semiconductors: Hyper Doping D223/224

8:00AM P12.00001 Limits of doping $In_{0.53}Ga_{0.47}As$ with Si and Be , SANGEETHA VIJEYARAGUNATHAN, TETSUYA D. MISHIMA, MICHAEL B. SANTOS, University of Oklahoma — We report on a study of doping efficiency in $In_{0.53}Ga_{0.47}As$ layers grown on InP (001) substrates by molecular beam epitaxy. Si and Be effusion cells were used to provide n- and p-type dopants, respectively. In epilayers grown at 0.63 monolayers per second with a substrate temperature of 500°C, doping cell temperatures below T_{Si}=1260°C (T_{Be}=907°C) resulted in electron (hole) concentrations that followed an Arrhenius relation with an activation energy of 5.0 eV (4.0 eV). At higher cell temperatures, the carrier concentration saturated at approximately n=3.1×10^{19}cm^3 (p=2.6×10^{19}cm^3). For T_{Si}=1300°C (T_{Be}=928°C), the carrier concentration was increased to n=4.2×10^{19}cm^3 (p=3.3×10^{19}cm^3) through use of a lower substrate temperature of 400°C (470°C). The maximum carrier concentration achieved through lowering the substrate temperature was n=4.8×10^{19}cm^3 (p=9.1×10^{19}cm^3). For Be doping, the maximum hole concentration was increased to 1.3×10^{20}cm^3 by using a lower growth rate. We will compare our results with the doping of GaSb and InAs, and discuss attempts to increase the maximum concentration through delta-doping and migration enhanced epitaxy.

8:12AM P12.00002 Se-precipitation in ZnSe under moderate-power laser-irradiation at high-pressure , G.P. LINDBERG, R.E. TALLMAN, Dep. of Physics, Univ. at Buffalo, Buffalo, NY, USA, R. LAUCK, M. CARDONA, Max Planck Institut für Festkórperforschung, Stuttgart, Germany, B.A. WEINSTEIN, Dep. of Physics, Univ. at Buffalo, Buffalo, NY, USA — We report evidence for the formation of Se inclusions in ZnSe under laser-irradiation during pressure-Raman experiments. Spectra of high-quality $^{68}Zn^{76}Se$ crystals are recorded at 300K for pressures of 0-13GPa using 647nm excitation at powers of 10 and 100 mW (focal spot $\sim$ 50μm.) For runs at the higher power a new Raman peak appears at 1.8 GPa, and shifts to lower energy at the rate –3.5 cm^{-1}/GPa with further increase of pressure. Its frequency, 228cm^{-1} at 1.8GPa, is within 7 cm^{-1} of the A1 and E$''$ Raman peaks in trigonal Se, which both exhibit negative, strongly non-linear, pressure shifts.[1] In particular, the pressure-shift of the new ZnSe peak gives a reasonable fit to the average dependence of the Se A1 peak over the range 2-8 GPa. No assignment to any of the ZnSe acoustic modes (one- or two- phonon) that also soften with pressure is feasible for the new peak. It is most likely related to the Se A1-mode in Se-inclusions, whose tendency to precipitate appears to increase with pressure.

[1]W. Richter, *et. al.*, phys. stat. sol. (b)56, 223(1993); K. Aoki, *et. al.*, J. Phys. Soc. Japan 48, 906 (1980).

8:24AM P12.00003 Band Renormalization in Mn Doped TiS_2 , TIMOTHY KIDD, PAUL SHAND, LAURA STRAUSS, University of Northern Iowa, JON RAMEAU, TONICA VALLA, PETER JOHNSON, Brookhaven National Laboratory — Titanium disulphide is a narrow gap semiconductor with a highly 2D layered structure. Mn dopants can be used to transform the band structure into being truly metallic via a rigid band shift of the electronic states. The system also begins to exhibit a variety of low temperature magnetic phases at Mn concentrations above 5%. We have performed angle resolved photoemission measurements of this system that clearly the transformation of the band structure from semiconducting to metallic. Furthermore, it can be seen that states near the valence band maxima become strongly modified beyond the rigid band shift approximation. The degeneracy of these states is lifted and they show behavior much like the spin splitting classically seen in surface states of gold and more recently in those of topological insulators. This behavior was quite unexpected as the states probed should be essentially bulk bands for this inert material. While no signs of temperature dependence were found to correlate these changes in electronic structure with any magnetic phase transition, it seems likely that this novel behavior arises from magnetic interactions with the Mn dopants.

8:36AM P12.00004 Persistent Photoconductivity and Magnetotransport in Dilute Nitride Semiconductor Alloys , R.L. FIELD III, Y. JIN, C. KURDAK, Physics Department, R.S. GOLDMAN, Department of Material Science and Physics Department, University of Michigan, Ann Arbor, MI 48109 — Nitrogen related defects, such as N interstitials and Si-N complexes, are known to dominate electrical and optical properties of dilute nitride semiconductor alloys [1,2]. We investigate the dependence of these defects on N incorporation for MBE grown Si and Te-doped dilute $GaAs_{1-x}N_x$ (x = 0.75-1.9) alloys. Persistent photoconductivity was observed for these heterostructures as high as 160 K, with photo-capture barriers from 216-350 meV. Also, carrier concentrations extracted from Hall measurements reveal a T-independent regime above 150 K and a strong thermally-activated regime below 150 K. These two phenomena are reminiscent of the behavior of n- type AlGaAs, suggesting the presence of similar N-induced DX- center-like states in GaAsN. We will discuss the dependence of these energies on both N composition and annealing temperature.

[1] Y. Jin *et al.*, Appl. Phys. Lett. 95, 092109 (2009).
[2] Y. Jin *et al.*, Appl. Phys. Lett. 95, 062109 (2009).

8:48AM P12.00005 ABSTRACT WITHDRAWN –

9:00AM P12.00006 Magnetic properties of Mn doped zinc selenide clusters: First principles calculations[1]

, SACHIN NANAVATI, Department of Electronic Science, University of Pune, Pune 411007 India, SUNDARARAJAN V., Centre for Development of Advanced Computing (C-DAC), Pune University campus, Pune 411007, India, SHAILAJA MAHAMUNI, Department of Physics, University of Pune, Pune 411007, India, SUBHASH GHAISAS, Department of Electronic Science, University of Pune, Pune 411007, India, VIJAY KUMAR, Dr. Vijay Kumar Foundation, 1969, Sector 4, Gurgaon 122001, India — We report the result of our study on magnetic properties of Mn doped ZnSe clusters within the pseudopotential based density functional theory (DFT). In the present work, we substituted one or two Mn atoms at different cationic sites of small ZnSe clusters and the corresponding stable geometrical configurations are obtained. In general, we find a large magnetic moment of 5 μ_B magnetic moment when one Mn atom is substituted. For the case of doping of two Mn atoms, calculations were performed for both parallel and anti-parallel spin-configurations. The variations in the density of state (DOS), the gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), the binding energy, and the magnetic moment have been analyzed as a function of the cluster size. This paper will discuss the preferred sites of the dopants, type of magnetization and their bonding characteristics for the above mentioned clusters.

[1]The authors would like to thank C-DAC for the funding and the computing time on its PARAM supercomputers.

9:12AM P12.00007 Sub-bandgap absorptance in chalcogen-hyperdoped silicon[1]

, BONNA NEWMAN, Massachusetts Institute of Technology — It has been shown that optical doping with pulsed lasers can achieve non-equilibrium concentrations up to one atomic % of heavy chalcogens in silicon. Compared to intrinsic silicon, this material exhibits near-unity absorption of sub-bandgap photons and has potential use in silicon infrared photodetectors and high-efficiency photovoltaics. Successful application of this material, however, requires better understanding of the exact mechanism responsible for sub-bandgap absorptance. Using a variety of techniques, we probe the chemical structure of this material system. We find that the short range structure of the dopant atom is correlated to the amount of sub-bandgap absorptance. We also compare the structure of different dopant species (S and Se) as well as different hyperdoping mechanisms (fs-laser doping vs. ion implantation followed by pulsed laser melting). In conjunction with theoretical modeling of expected chalcogen defect states, we identify dominant structural characteristics related to the observation of sub-bandgap absorptance. Expanding on previous results, we demonstrate control of sub-bandgap absorptance through thermal processing. In addition to suggesting a method to engineer the optical properties of the material, this result provides further insight into the thermodynamics of formation of a possible dopant-related defect state. We compare the thermodynamics measurements to the dopant structural measurements and posit a model of sub-bandgap absorptance and defect dynamics. These results provide a better understanding of the phenomena of sub-bandgap absorptance in chalcogen-hyperdoped silicon and a pathway to explore other hyperdoped semiconductors.

[1]We acknowledge the support of the Clare B. Luce Foundation and the Chesonis Family Foundation.

9:48AM P12.00008 Supersaturated Silicon-Chalcogen Alloys for Thin-film Photodetectors

, DANIEL RECHT, AURORE SAID, SI HUI PAN, MICHAEL AZIZ, Harvard School of Engineering and Applied Sciences, JEFFERY WARRENDER, US Army ARDEC - Benet Laboratories, THOMAS CRUSON, DAVID HUTCHINSON, PETER PERSANS, Rensselaer Polytechnic Institute, JOSEPH SULLIVAN, MARK WINKLER, TONIO BUONASSISI, Massachusetts Institute of Technology — Supersatured silicon-chalcogen alloys are known to have strong infrared optical absorption and the ability to detect light with energy less than silicon's bandgap. The range of infrared wavelengths these alloys absorb is much broader than the range over which photodiodes made from these alloys respond. We have recently performed several experiments to understand the disconnect between optical absorption and photodetection in thin, monocrystalline films of these alloys fabricated by ion implantation followed by nanosecond laser melting. When subjected to sensitive tests of photoconductivity, these alloys show no optoelectronic response at several absorbed sub-bandgap wavelengths. Furthermore, measurements on photodiodes made from silicon chalcogen alloys suggest that these materials are in fact a potent low-voltage photodetection gain medium. These results, along with temperature dependent transport measurements and sensitive optical spectroscopy, indicate that the mechanism of sub-bandgap response could be substantially more complex than is commonly thought.

10:00AM P12.00009 Non-radiative Recombination in Intermediate Band Photovoltaics[1]

, JACOB KRICH, ALÁN ASPURU-GUZIK, Harvard University — Intermediate band photovoltaics (IBPV) promise to absorb low energy photons while maintaining large open circuit voltages, breaking the Shockley-Queisser efficiency limit. Proposals for IBPV include hyperdoping semiconductors with impurities forming mid-gap states, creating a band entirely contained inside the larger semiconductor bandgap. For such devices to function, the electronic states in the middle of the band gap must be extended and thus not contribute to multiphonon recombination. Since the intermediate band is produced by randomly placed impurities, however, there is an inherent disorder in the electronic structure, which produces localized states inside the band gap due to Anderson localization, even at high impurity concentrations. We use a finite size scaling analysis to find the localization properties of a non-interacting intermediate band and its resultant contribution to non-radiative recombination.

[1]We acknowledge support from the Harvard University Center for the Environment.

10:12AM P12.00010 A Metal-Insulator Transition in Silicon Hyperdoped with Chalcogens

, ELIF ERTEKIN, MARK WINKLER, MIT, AURORE SAID, MICHAEL AZIZ, Harvard, TONIO BUONASSISI, JEFFREY GROSSMAN, MIT — Hyperdoped Silicon, the material resulting from the laser doping of Silicon to impurity concentrations orders of magnitude beyond the room temperature solubility limit, can exhibit unique properties. For example, "Black Silicon", formed from laser doping with chalcogens S, Se, or Te, exhibits anomalous sub band gap optical absorption at photon energies as low as 0.5 eV and a flat absorption spectrum. While this has piqued interest in the use of Black Silicon for optoelectronics and photovoltaics, there has not yet been a clear explanation for the enhanced optical properties. Focusing on the Se doped systems, we use Density Functional Theory to show that the optical absorption results from an impurity induced insulator to metal transition. Our calculations indicate that an isolated Se impurity introduces a localized electronic state in the band gap. At higher defect concentrations, the transition to the metallic state is demonstrated by an increase in the defect level bandwidth and the eventual merging of the defect state with the conduction bands. The concentration at which this occurs corresponds very well with experimental low temperature Hall effect measurements.

10:24AM P12.00011 Dopant effects on dislocation width of dislocations in Si

, YUTAKA OHNO, Institute for Materials Research, Tohoku University, TOSHINORI TAISHI, Institute for Materials Research, Tohoku Unviersity, YUKI TOKUMOTO, ICHIRO YONENAGA, Institute for Materials Research, Tohoku University — Impurities interact with dislocations in semiconductor crystals, resulting in variations of dynamical activities of dislocations such as mobility and immobilization, and also in leading to inhomogeneity of electrical and optical properties of microelectronic and PV devices. Especially in Si in demanded trend of heavily doping for miniaturized transistors, basic knowledge of dislocation-dopant impurity interaction increases the importance. In CZ-Si doped with n-type impurities of P, As, and Sb, dislocations freshly induced at 1173 K extended their dissociation width with increasing duration of subsequent annealing at the same temperature. The width increased by annealing when the concentration of n-type impurities was high. On the other hand, the dissociation width was unchanged during annealing in Si undoped and doped with p-type impurities of B and Ga. These results suggest that the energy of stacking fault bound to partial dislocations is strongly affected by the number of n-dopant impurities segregated nearby them via their thermal migration, irrespective of atomic size of the dopant impurities; i.e., n-dopant impurities segregate nearby a stacking fault so as to reduce the stacking fault energy.

10:36AM P12.00012 Entropic Influence on the Aggregation Physics of Interstitial Point Defects in Silicon , TALID SINNO, SUMEET KAPUR, ALEX NIEVES, University of Pennsylvania — The evolution of self-interstitials and their aggregates during the annealing of ion-implanted silicon has received a tremendous amount of attention because of their strong, non-linear effects on the diffusion of dopants. The implantation process leads to extensive lattice damage, which must be healed by thermal annealing. Also generated by the implantation process is a large number of self-interstitials which lead to enhanced dopant diffusion during annealing known as Transient Enhanced Diffusion, or TED. A major obstacle to understanding and quantitatively predicting TED is the formation of a variety of self-interstitial aggregates, which range from small amorphous three-dimensional clusters, to planar stacking-faults with various crystallographic orientations. In the present study, we use large-scale constant-stress MD simulations to dynamically simulate the evolution of an ensemble of highly supersaturated self-interstitials at various temperatures and pressures. We show that the simulated interstitial clustering into various types of planar structures exhibits a complex thermodynamic-kinetic phase diagram that is sensitively controlled by entropic factors. The observations are studied with a recently developed approach that maps out the potential energy landscape in the vicinity of the defect cluster and allows for the total (classical) free energy to be analyzed.

10:48AM P12.00013 The chemical trends of a new defect cluster: DDX centers , JIE MA, SU-HUAI WEI, National Renewable Energy Laboratory, Golden, Colorado 80401, USA — DX center is a major "killer" defect limiting n-type doping in group II-VI and III-V semiconductors. It converts a shallow donor to deep one, which is a major reason for the saturation of free-electron carriers in the doping process. Several structure models of isolated DX centers have been proposed in the literatures, such as the broken-bond model (BB-DX), and the α and β cation-cation bond model (CCB-DX). All these DX centers can be stabilized with hydrostatic pressure or reduced dimensionality and size. In group III-V and II-VI semiconductors, it has been common believe that cation-site induced DX centers are easier to form than anion-site induced ones. Because DX centers trap an extra electron, therefore, another defect in the system must donate the electron and form a positive charged defect. We show, using GaAs as an example, that in heavily doped semiconductor, the negative charged DX center and positive charged donor can couple strongly through the Coulomb interaction, forming the dominant DDX center. The DDX centers are still deep level defects. However, unlike the DX center, the DDX centers have different chemical trends, i.e., anion-site DDX center is easier to form than cation-site DDX centers. A simple model is proposed to explain the new trends.

Wednesday, March 23, 2011 8:00AM - 9:30AM –

Session P13 APS: Tutorial for Authors and Referees D225/226

8:00AM P13.00001 Tutorial for Authors and Referees —Editors from Physical Review Letters and Physical Review will provide information and tips for our less experienced referees and authors. This session is aimed at anyone looking to submit to or review for any of the APS journals, as well as anyone who would like to learn more about the authoring and refereeing processes. Topics for discussion will include advice on how to write good manuscripts, similarities and differences in writing referee reports for PRL and PR, and other ways in which authors, referees, and editors can work together productively. Following a short presentation from the editors, there will be a moderated discussion. Refreshments will be served.

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P14 DMP GSNP DCOMP: Focus Session: Friction, Fracture and Deformation Across Length Scales II: Plasticity and Rupture D227

8:00AM P14.00001 Scaling theory of continuum dislocation dynamics in two and three dimensions , YONG S. CHEN, WOOSONG CHOI, STEFANOS PAPANIKOLAOU, JAMES P. SETHNA, Cornell University — When crystalline materials deform plastically, complex dislocation structures have been observed experimentally.[1] We provide a continuum plasticity theory to study the emergent self-similar morphologies.[2] We analyze the self-similarity in terms of critical exponents for correlation functions of dislocation density, crystalline orientation and plastic distortion, and explore the connection to the power spectrum of the total free energy. In two and three dimensions, we apply anisotropic loadings, and observe little anisotropy in the critical properties. We explore the addition of quenched disorders to our continuum theory, to investigate the relation between dynamics (plasticity avalanches) and static dislocation morphologies.

[1]P. Hahner et al., Phys. Rev. Lett. 81, 2470, 1998.
[2]Y.S.Chen et al., Phys. Rev. Lett. 105, 105501, 2010.

8:12AM P14.00002 Saddle node scaling on approach to dislocation nucleation , AKANKSHA GARG, ASAD HASAN, CRAIG MALONEY, Carnegie Mellon University — We study the process of dislocation nucleation in a perfect 2D hexagonal crystal under nano-indentation loading in a numerical model using energy minimization techniques and analysis of the energy eigenmodes. The nucleation event takes the form of a saddle-node catastrophe and is governed by associated scaling laws. In particular, on approach to nucleation, a single energy eigenmode descends through the spectrum and its eigenvalue vanishes as the square root of the distance to the nucleation point. The velocity of the system shows the same scaling behavior, and its normal mode decomposition demonstrates that it is dominated by the critical mode responsible for nucleation.

8:24AM P14.00003 Dislocation dynamics at zero temperature and at finite temperature: analytics and simulations[1] , KARIN DAHMEN, GEORGIOS TSEKENIS, Department of Physics, University of Illinois at Urbana Champaign, PAK YUEN CHAN, THOMAS FEHM, JONATHAN DANTZIG, NIGEL GOLDENFELD, JONATHAN UHL — Crystalline materials are known to deform in an intermittent way with avalanches. Power laws govern the statistics of the avalanches. In this work we are studying plasticity as a member of the universality class of depinning phase transition. Results from our Discrete Dislocation Dynamics simulations agree with analytical mean field predictions for distributions of avalanche sizes, durations, power spectra, and avalanche shapes. Results from phase field crystal simulations agree with analytical predictions for the depinning phase transition at finite temperature. Both numerics and analytics indicate that the dynamics of edge dislocations in sheared crystals belong to the mean field universality class of depinning transitions, both at zero temperature and at finite temperature.

[1]We acknowledge support from the NSF funded Materials Computation Center (MCC) and NSF DMR 1005209.

8:36AM P14.00004 Size Matters: size-dependent strength and nucleation-governed deformation mechanisms in nano-scale Cu pillars , JULIA GREER, Caltech — Uniaxial compression and tension tests on single crystalline micro and nanopillars have revealed a strong size effect. For face-centered cubic metals, this size effect is characterized by a power-law: where n is between .5 - .7. The majority of these micro-mechanical tests have been performed on pillars produced by the focused-ion-beam (FIB), a process known to introduce surface damage into the material and to limit the smallest attained pillar diameter to $\sim$150nm while maintaining its shape integrity. In order to overcome these detriments, we developed a new technique combining electroplating and electron beam lithography to create single crystalline Cu nano-pillars with diameters down to 50 nm. We find the mechanical response of these samples to exhibit the same power-law strengthening behavior as other fcc metals down to the diameter of 100nm, as revealed by *in-situ* uniaxial compression and tension tests conducted in a custom-built in-situ mechanical deformation instrument, SEMentor. TEM investigations of the microstructure of pillars produced by the FIB and by electroplating show similar initial dislocation densities of $\sim 10^{14}$ m^{-2} implying that size-dependent strength at the nano-scale is a strong function of initial microstructure and not of fabrication method. We examine the limits of this power-law trend down to diameters of 50nm, as at these small sizes, deformation behavior has been theoretically predicted to change due to the activation of surface dislocation sources and the increasing influence of the surface stress. Furthermore, we find that these single crystalline Cu nano-pillars show a remarkable strain-rate dependence that increases with decreasing diameter further revealing the thermally activated nature of dislocation sources and corresponding changes in activation volume. HRTEM investigations of post-mortem structures will be presented in the context of dislocation-based phenomenological modeling.

9:12AM P14.00005 Effect of Inertia and Damping on Avalanche Distributions in Sheared Amorphous Solids[1] , K. MICHAEL SALERNO, Johns Hopkins University, CRAIG MALONEY, Carnegie Mellon University, MARK O. ROBBINS, Johns Hopkins University — Avalanches occur in a variety of contexts from magnets to granular materials. Molecular dynamics simulations of a sheared binary Lennard-Jones glass are used to explore the effect of inertia and damping on avalanche distributions. We find that the energy dissipation rate is one of the key factors in determining the size of an individual avalanche as well as the distribution of avalanche energies. There are three distinct regimes: an overdamped regime where the distribution has an exponential cutoff that varies with dissipation rate, a critical regime where avalanches follow power-law statistics and large events are limited by simulation size, and a run-away regime where inertia leads to a peak at large energies. The same regimes are found for Langevin type viscous damping and Galilean-invariant Kelvin damping. While inertia determines how an avalanche evolves, some properties of the avalanche are predetermined. Weakening of the average shear modulus prior to an avalanche is a good indicator that a large, system-spanning event may occur.

[1]This material is based upon work supported by NSF Grant DMR 108474.

9:24AM P14.00006 Nonclassical Nucleation and Growth of Cohesive Tensile Cracks , JOSEPH GRAN, UC Davis, JOHN RUNDLE, UC Davis, Santa Fe Institute, WILLIAM KLEIN, Boston University — We analyze the nucleation and growth of cohesive tensile cracks using a Hamiltonian which is written as a functional of the crack separation (offset field). We simulate the nucleation events on a square lattice using a Metropolis Monte Carlo algorithm. Several modes of crack propagation are seen in the simulations. Our results indicate that for certain materials, crack nucleation and growth proceed through the formation and extension of a diffuse "halo" surrounding the classical portion of the crack. This is similar to nonclassical nucleation near the spinodal in magnetic systems. Theoretical considerations and numerical calculations strongly suggest that the diffuse halo can be identified with the fracture "process zone" seen in laboratory studies of advancing cracks. We are investigating scaling exponents associated with this apparent phase transition.

9:36AM P14.00007 Enhanced Strength via crack friction and Pressure[1] , DONALD WIEGAND, ARDEC Picatinny USA, KEVIN ELLIS, CLAIRE LEPPARD, AWE Aldermaston — The effect of pressure on the mechanical response of particulate polymer composites is being studied. Between about 0.1 and 7 MPa for one composite the results indicate that slow crack growth is the dominant failure mode. With continuously creasing strain at low pressures the stress initially increases to a maximum, the compressive strength, then decreases indicating work softening and them becomes approximately constant at a plateau value. Both the compressive strength and the plateau stress increases linearly with pressure but the plateau stress increases with a steeper slope such that at higher pressures work softening is not observed. The results are analyzed in terms of shear cracks with friction between the crack surfaces. The model predicts a threshold stress for crack growth which increases linearly with pressure and further predicts that the compressive strength increases linearly with pressure as observed and with the same slope as the threshold stress. These results clearly indicate that the pressure dependence of the compressive strength is due to the pressure dependence of the threshold stress for crack growth. The changes in the plateau region can also be attributed to frictional effects.

[1]Supported by AWE Aldermaston.

9:48AM P14.00008 Irreversible Damage in Amorphous Silica , CINDY ROUNTREE, CEA,DSM,IRAMIS,SPCSI, DAMIEN VANDEMBROUCQ, Laboratoire PMMH, ESPCI, STEPHANE ROUX, LMT, ENS-Cachan, ELISABETH BOUCHAUD, CEA,DSM,IRAMIS,SPEC — Glass touches every aspect of our lives including the glass dishes which we cook with to the storage of nuclear waste. The extensive use of oxide glasses can be attributed to optical transparency, electrical and heat insulation, and large hardness. However, oxide glasses have a major drawback: brittleness. Even small flaws in the structure can lead to the ultimate failure of the material. Recent Atomic Force Microscope experiments and Molecular Dynamics simulations revealed a process zone ahead of the crack tip where damage nucleates, augments, and finally merges with the advancing crack front. Furthermore, when a-SiO_2 samples are nanoindented, one finds permanent damage under the indenter in the form of densified silica. To shed light on the origin of irreversible deformation in amorphous media, we have expanded our studies to examine what happens to an oxide glass when subjected to shear. MD simulations have been performed in a-SiO_2 systems which are subject to a shearing force at room temperature. The system was initially isotropic and as long the maximum shear deformation remains under 5% the system remains isotropic upon unloading. However if the system is sheared to a point greater than 5% permanent plastic deformation sets in and the system is no longer isotropic upon unloading.

10:00AM P14.00009 Molecular dynamics study of the contact strengths between clean metallic surfaces with nanoscale asperities , HOJIN KIM, ALEJANDRO STRACHAN, School of Materials Engineering, Purdue University, West Lafayette, Indiana, USA — A fundamental understanding of the mechanical behavior of contacting surfaces with nanoscale asperities including their adhesion and friction is critical for MEMS and other applications. We characterize the tensile strength of contacts formed between various clean Pt surfaces such as commensurate contacts between (001) and (111) surfaces and incommensurate (001) ones by using MD simulations over wide range of asperity size. In cyclic closing and opening, the first contact shows significant plastic deformation, leading to a considerable reduction in the contact area. After few cycles, steady state is achieved both contact size and the pullout force. The strength of bridges in both commensurate and incommensurate contacts exhibits strong size effects. Their strength increases with decreasing size until a length of approximately 5 nm below which weakening is observed. Commensurate contacts are stronger than incommensurate ones but only during the initial contacts, after steady state is achieved commensurate and incommensurate (001) surfaces lead to similar strengths.

10:12AM P14.00010 Friction and Sliding of Polystyrene Micro Spheres in the Presence and Absence of Capillary Adhesion[1] , IYAM LYNCH, JACQUELINE KRIM, North Carolina State University — Quartz crystal microbalance (QCM) response to varying load geometries, particularly micro particles, is a rapidly growing field of research.[2,3] This no doubt is due to its varied applications involving the study of textiles, DNA and viruses[3], micro adhesion[2,3], micro sorting[3], and friction. There are many challenges that must be overcome in this field. One major difficulty is capillary adhesion, which is difficult to quantify. We have created an experiment to greatly reduce the impact of capillary adhesion by employing the shaking motion of a 5MHz QCM to eject micro spheres (15μm) from its surface, which subsequently land on the surface of a nearby 8 MHz QCM. The experiment is performed in a vacuum chamber to include different environments such as air, vacuum, and dry nitrogen. During the experiment we monitor the behavior of the unloaded QCM by measuring the change in frequency and quality factor as a result of the newly landed spheres. Particle motion and dynamics are observed using a microscope with a camera attached.

[1]We would like to acknowledge NSF and NTC for funding this project.
[2]Dybwad, G.L. J. Appl. Phys. **1985**, 58, 2789
[3]Dultsev, F.N. et al. Langmuir **2000**, 16, 5036.

10:24AM P14.00011 Cooperative adhesion and friction of compliant nanohairs[1] , ALI DHINOJWALA, LIEHUI GE, The University of Akron, LIJIE CI, ANUBHA GOYAL, PULICKEL AJAYAN, Rice University, L. MAHADEVAN, Harvard University — The adhesion and friction behavior of soft materials, including compliant brushes and hairs, depends on the temporal and spatial evolution of the interfaces in contact. For compliant nanofibrous materials, the actual contact area of individual fibers make with surfaces depends on the preload applied upon contact. Using in-situ microscopy observations of preloaded nanotube hairs, we show how nanotubes make cooperative contact with a surface by buckling and conforming to the surface topography. The overall adhesion of compliant nanohairs increases with increasing preload as nanotubes deform and continuously add new side-wall contacts with the surface. Electrical resistance measurements indicate significant hysteresis in the relative contact area. Contact area increases with preload (or stress) and decreases suddenly during unloading, consistent with strong adhesion observed for these complaint nanohairs.

[1]National Science Foundation

10:36AM P14.00012 The effect of Coulombic friction on spatial displacement statistics[1] , ANDREAS MENZEL, NIGEL GOLDENFELD, University of Illinois at Urbana-Champaign — We study the effect of Coulombic (dry) friction on the spatial displacement statistics of one-dimensional stochastic motions. In other words, one of the simplest forms of nonlinear friction is added to the Fokker-Planck equation for conventional viscous Brownian motion, and its consequences are investigated. First, we find the eigenfunctions to the problem that includes the velocity component only. This problem can be mapped on the case of a quantum mechanical harmonic oscillator in the presence of a delta potential. Then we show numerically that a crossover from exponential to Gaussian displacement statistics results from the Coulombic frictional contribution. A transient regime of multiscaling is identified for the spatial distribution function. Our results are important for the interpretation of recent experiments in the field of soft matter physics: it turns out that, for practical purposes, higher order moments of the spatial distribution function must be determined to identify the presence of effective Coulombic frictional forces.

[1]This work was supported by the Deutsche Forschungsgemeinschaft.

10:48AM P14.00013 Understanding frictional duality and bi-duality: Sb-nanoparticles on HOPG[1] , JAN BRNDIAR, ROBERT TURANSKY, IVAN STICH, Inst. of Physics, Slovak Academy of Sciences, Bratislava, Slovakia — We have simulated [1] the behavior of motion of Sb_n nanoparticles on HOPG with the quest to elucidate the experimentally observed frictional bi-duality [2]. The first duality was observed for clean Sb-nanoparticles deposited under UHV conditions. Both frictionless and "normal" behavior was observed. Another dual behavior was found for Sb-nanoparticles exposed to ambient conditions, both scaling linearly with contact area. The vanishing friction branch is due to incommensurability of the Sb-HOPG. The non-vanishing friction branch can be accounted for by contaminants due to imperfect UHV, such as water, hydrocarbons, oxygen, etc., including small Sb_n clusters. The large friction forces after exposition to ambient conditions result from presence of mobile oxidized multiasperities. The simulations allow for quantitative estimates of impurity concentrations and understanding of the molecular mobility.

[1] J. Brndiar et al. submitted (2010).
[2] D. Dietzel et al. Phys.Rev.Lett. **101**, 125505 (2008), Phys.Rev. **B 82**, 035401 (2010).

[1]Financial support from APVT ESF-EC-0007-07 under ESF FANAS and ERDF OP R&D, Project CE QUTE ITMS 26240120009 are acknowledged.

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P15 DMP GMAG FIAP: Focus Session: Spins in Semiconductors - Quantum Computing with Defects D171

8:00AM P15.00001 Quantum computing with defects[1] , JOEL VARLEY, Department of Physics, University of California, Santa Barbara — The development of a quantum computer is contingent upon the identification and design of systems for use as qubits, the basic units of quantum information. One of the most promising candidates consists of a defect in diamond known as the nitrogen-vacancy (NV^{-1}) center, since it is an individually-addressable quantum system that can be initialized, manipulated, and measured with high fidelity at room temperature. While the success of the NV^{-1} stems from its nature as a localized "deep-center" point defect, no systematic effort has been made to identify other defects that might behave in a similar way. We provide guidelines for identifying other defect centers with similar properties. We present a list of physical criteria that these centers and their hosts should meet and explain how these requirements can be used in conjunction with electronic structure theory to intelligently sort through candidate systems. To elucidate these points, we compare electronic structure calculations of the NV^{-1} center in diamond with those of several deep centers in 4H silicon carbide (SiC). Using hybrid functionals, we report formation energies, configuration-coordinate diagrams, and defect-level diagrams to compare and contrast the properties of these defects. We find that the $N_C V_{Si}^{-1}$ center in SiC, a structural analog of the NV^{-1} center in diamond, may be a suitable center with very different optical transition energies. We also discuss how the proposed criteria can be translated into guidelines to discover NV analogs in other tetrahedrally coordinated materials.

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

[1]This work was performed in collaboration with J. R. Weber, W. F. Koehl, B. B. Buckley, A. Janotti, C. G. Van de Walle, and D. D. Awschalom. This work was supported by ARO, AFOSR, and NSF.

8:36AM P15.00002 ABSTRACT WITHDRAWN –

8:48AM P15.00003 Optical Control of Spatial Patterning of Nuclear Polarization in GaAs

, JONATHAN KING, University of California, Berkeley, YUNPU LI, LE PENG, MARIA TAMARGO, CARLOS MERILES, City College of New York, JEFFREY REIMER, University of California, Berkeley — We present new results on the optical polarization of nuclear spins in gallium arsenide. Previous work has identified the contact hyperfine interaction at shallow donors as the mechanism for helicity dependent nuclear polarization. We show a new regime, where donors are only partially occupied, where nuclear quadrupolar relaxation at shallow donors is the dominant mechanism. Since quadrupolar relaxation is helicity independent, the incident light polarization may be tuned such that the two relaxation mechanisms drive the nuclear spins to opposite signs of polarization. We show that incident light wavelength and power may be tuned to create spatial patterns of varying donor occupation in a single sample, which in turn creates a pattern of positive and negative nuclear polarization. We have developed an analytical mode which accurately describes the bulk NMR signal in terms of irradiation power and wavelength. We also present stray-field NMR imaging experiments showing direct observation of the patterned nuclear polarization.

9:00AM P15.00004 Spin Orbit Interaction in Inversion-Symmetric Semiconductors: SrTiO3 and group IV

, CUNEYT SAHIN, Optical Science and Technology Center and Department of Physics and Astronomy, University of Iowa, Iowa City, Iowa 52242, USA, GIOVANNI VIGNALE, Department of Physics, University of Missouri, Columbia, Missouri 65211, MICHAEL E. FLATTÉ, Optical Science and Technology Center and Department of Physics and Astronomy, University of Iowa, Iowa City, Iowa 52242, USA — Low-energy effective spin-orbit Hamiltonians have proved effective at describing the effect of spin-orbit interactions on populations of polarized carriers in direct-gap semiconductors such as gallium arsenide. No similar low-energy Hamiltonians are available for materials with inversion symmetry, such as cubic oxides or group-IV semiconductors. In order to construct such low-energy Hamiltonians we have calculated the electronic band structure of strontium titanate, a perovskite material which has recently been used to make high-density two-dimensional electron gases, using a tight-binding electronic structure with atomic spin-orbit interactions. We have also calculated the band structures of several group-IV semiconductors, including germanium, silicon, and diamond. An expression for the effective spin-orbit interaction in the conduction band of these materials has been derived, and calculated for these materials. The symmetry properties of this effective spin-orbit interaction tensor will also be discussed. This work was supported by an ARO MURI.

9:12AM P15.00005 Excited-State Spin Manipulation and Intrinsic Nuclear Spin Memory using Single Nitrogen-Vacancy Centers in Diamond[1]

, GREGORY FUCHS[2], Center for Spintronics and Quantum Computation, University of California, Santa Barbara — Nitrogen vacancy (NV) center spins in diamond have emerged as a promising solid-state system for quantum information processing and precision metrology at room temperature. Understanding and developing the built-in resources of this defect center for quantum logic and memory is critical to achieving these goals. In the first case, we use nanosecond duration microwave manipulation to study the electronic spin of single NV centers in their orbital excited-state (ES) [1]. We demonstrate ES Rabi oscillations and use multi-pulse resonant control to differentiate between phonon-induced dephasing, orbital relaxation, and coherent electron-nuclear interactions. A second resource, the nuclear spin of the intrinsic nitrogen atom, may be an ideal candidate for a quantum memory due to both the long coherence of nuclear spins and their deterministic presence. We investigate coherent swaps between the NV center electronic spin state and the nuclear spin state of nitrogen using Landau-Zener transitions performed outside the asymptotic regime [2]. The swap gates are generated using lithographically fabricated waveguides that form a high-bandwidth, two-axis vector magnet on the diamond substrate. These experiments provide tools for coherently manipulating and storing quantum information in a scalable solid-state system at room temperature.

[1] G. D. Fuchs, V. V. Dobrovitski, D. M. Toyli, F. J. Heremans, C. D. Weis, T. Schenkel, and D.D. Awschalom, *Nat. Phys.* **6**, 668 (2010).
[2] G. D. Fuchs, G. Burkard, P. Klimov, and D. D. Awschalom, *in preparation*.

[1]We gratefully acknowledge support from AFOSR, ARO, and DARPA.
[2]In collaboration with V. V. Dobrovitski, G. Burkard, D. M. Toyli, F. J. Heremans, P. Klimov, and D. D. Awschalom

9:48AM P15.00006 Dynamic Jahn-Teller Effect in Negatively Charged Nitrogen-Vacancy Center in Diamond[1]

, TESFAYE ABTEW, PEIHONG ZHANG — The negatively charged nitrogen-vacancy (NV) center in diamond has attracted much research interest recently owing to its desirable optical properties and long spin coherent lifetime. The ground state of NV^- center has a $^3A_2$ symmetry, which can be optically excited, to a ^3E state. The excited state is orbitally degenerate therefore should experience either static or dynamic Jahn-Teller (JT) effects. We use accurate first-principles methods to study structural and electronic properties of the NV^- center in diamond both in the ground and excited states. Our results indicate that the excited state of the NV^- center is indeed a dynamic JT system.

[1]We acknowledge the Center for Computational Research at the University at Buffalo, SUNY. This work is supported by the National Science Foundation under Grant No. DMR-0946404 and by the Department of Energy under GrantNo. DE-SC0002623.

10:00AM P15.00007 Using Adiabatic Pulses for the Control of Nitrogen Impurities in Diamond

, ZHI-HUI WANG, Ames Laboratory, USDOE, G. DE LANGE, R. HANSON, Kavli Institute of Nanoscience Delft, Delft University of Technology, Delft, The Netherlands, V.V. DOBROVITSKI, Ames Laboratory, USDOE — High-fidelity quantum control and dynamical decoupling of the NV center in diamond has been recently demonstrated [1]. Efficiently manipulating the spin bath of nitrogen atoms (P1 centers) can add new freedom to the control of NV centers, and can map out the properties of the bath. However, the electron spins of P1 centers have a broad spectrum, and it is difficult to implement accurate rotations uniformly over the whole spectrum. We show that the adiabatic pulses (AP) provide an efficient tool for the bath control. The internal bath dynamics imposes very moderate limitations on the AP parameters so that P1 centers can be controlled with good ($> 90\%$) fidelities. The shape of AP can be tailored to the spectral density of the bath for optimized performance. We show how, by manipulating P1 centers, spin echo and dynamical decoupling of the NV center can be achieved in efficient manner.

[1] G. de Lange et al., Science **330**, 60 (2010); B. Naydenov et al., arXiv:1008.1953 (2010); C. A. Ryan et al., arXiv:1008.2197 (2010).

10:12AM P15.00008 Nanofabrication of single spins and spin arrays in diamond[1]

, D.M. TOYLI, G.D. FUCHS, D.J. CHRISTLE, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA, C.D. WEIS, T. SCHENKEL, Lawrence Berkeley National Laboratory, Berkeley, CA — The properties of isolated nitrogen vacancy (NV) centers in diamond make them a promising solid-state qubit candidate for spin-based quantum information processing. However, scaling this system to multi-qubit NV center devices requires methods to accurately place single NV centers in pure diamond substrates. To address this challenge we have developed a method for fabricating single NV centers on 50 nm length scales based on ion implantation and electron beam lithography.[2] Secondary ion mass spectroscopy measurements facilitate depth profiling of the implanted nitrogen to provide three-dimensional characterization of the NV center spatial distribution. Finally, electron spin resonance measurements of single NV centers, including temperature-dependent spin coherence measurements, suggest a pathway for optimizing single spin coherence in future devices.

[1]This work is funded by AFOSR, ARO, DARPA, and DOE.
[2]D. M. Toyli *et al.*, Nano Lett. 10, 3168 (2010).

10:24AM P15.00009 Nuclear spin diffusion in semiconductor quantum wells[1] , IONEL TIFREA, TOM D. KIM, Cal State Fullerton — We analyze the nuclear spin diffusion effect in semiconductor quantum wells in connection with dynamical nuclear polarization under optical pumping. The natural confinement provided by the particular geometry of quantum well structures is responsible for a position dependent nuclear spin relaxation time and a reduced nuclear spin diffusion. In particular, we consider the case of GaAs quantum wells within GaAlAs barriers and analyze the nuclear spin diffusion for As nuclei. Our results, obtained for different nuclear spin diffusion constants, show that nuclear spin diffusion has a relatively small effect on the overall polarization of As nuclei in these structures.

[1]The authors would like to acknowledge finacial support from Research Corporation.

10:36AM P15.00010 Single-shot electrical readout of an ensemble nuclear spin memory in silicon , DANE R. MCCAMEY, School of Physics, University of Sydney, J. VAN TOL, National High Magnetic Field Laboratory, Florida State University, G. W. MORLEY, London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, C. BOEHME, Department of Physics and Astronomy, University of Utah — Storing information in spin is widely recognized as a promising technological driver. However, the ability to interact with, and thus control electron spin implies a reasonable coupling to the environment, and thus a limited spin lifetime. This problem can be overcome by using nuclear spins for long term information storage even though mapping nuclear spin information onto device currents has remained challenging. Here, we report on an electrically readable nuclear spin memory implemented using phosphorus donors in silicon [1]. Donor electron spins can be used to encode logical information, which is then transferred to the nuclei. The state can be stored in the nuclear spin and then read out electrically via the hyperfine coupling with the electron. We show that information can be stored in the nuclear spin for longer than 100 seconds, that the information can be read back single shot, and that repetitive measurement does not degrade the stored information. Other nuclei, such as the spin 1/2 ^{29}Si, can also be used, pointing to the possibility of a nuclear spin memory register. [1] D. R. McCamey, J. van Tol, G. W. Morley and C. Boehme. Science, in press (2010)

10:48AM P15.00011 Nuclear spin phase transition in the presence of interacting two-dimensional electrons , ROBERT ŻAK, University of Basel, DMITRII MASLOV, University of Florida, DANIEL LOSS, University of Basel — The recent study of the RKKY interaction between localized moments, e.g., nuclear spins of Ga and As atoms in a GaAs heterostructure, mediated by interacting two-dimensional electrons, has shown a possibility of polarizing nuclear spins at currently accessible temperatures [1]. This ferromagnetic phase transition is governed by: (i) anisotropy of the electron spin susceptibility, χ, in the presence of Rashba spin-orbit interaction (RSOI) and (ii) nonanalyticity in momentum dependence of χ. In this talk I will argue that on top of the anisotropy in χ caused by the RSOI at zero momentum [2], the momentum dependence of χ is anisotropic itself: while the linear scaling of χ_{zz} with momentum saturates at the energy scale set by the RSOI, that of the $\chi_{xx} = \chi_{yy}$ continues through this energy scale (in this way it resembles the temperature and magnetic field dependence of χ in the presence of the RSOI [2]). The effect of the renormalization of the backscattering amplitude in the Cooper channel will be taken into account as well. In the end I will elaborate on possible implications of our results for the stability and nature of the nuclear spin ordered phase. References: [1] P. Simon and D. Loss, PRL **98**, 156401 (2007), P. Simon, B. Braunecker, and D. Loss, PRB **77**, 045108 (2008); [2] R. A. Żak, D. Maslov, and D. Loss, PRB **82**, 115415 (2010).

Wednesday, March 23, 2011 8:00AM - 10:48AM –

Session P16 DMP GMAG: Focus Session: Magnetic Nanostructures, Vortices & Domain Walls

D173

8:00AM P16.00001 Tuneable remote pinning of domain walls in magnetic nanowires , L. O'BRIEN, University of Cambridge, D.E. READ, J. SAMPAIO, Imperial College London, D. PETIT, University of Cambridge, E.R. LEWIS, Imperial College London, A.-V. JAUSOVEC, H.T. ZENG, Imperial College London, R.P. COWBURN, University of Cambridge — Domain wall (DW) motion in ferromagnetic nanowires has received much attention for its potential technological applications and for probing fundamental physics. The role of DW pinning in nanowires is crucial for these investigations however it is in general a complex process. Distortions of the DW shape make quantitative agreement between modelling and experiment difficult. Here we demonstrate pinning using nanometre scale localised stray fields. This type of interaction gives well characterised, tailorable potential landscapes that do not appreciably distort the DW. Our experimental results are in excellent quantitative agreement with an Arrhenius-Néel model of depinning - a result only possible when the modelled potential profile agrees fully with that experienced by the DW.

8:12AM P16.00002 Measurements of nanoscale domain wall flexing in a ferromagnetic thin film , A.L. BALK, Physics Dept., Penn State University, University Park PA 16802, M.E. NOWAKOWSKI, Physics Dept., University of California, Santa Barbara CA 93106, M.J. WILSON, D.S. RENCH, P. SCHIFFER, Physics Dept., Penn State University, University Park PA 16802, D.D. AWSCHALOM, Physics Dept., University of California, Santa Barbara CA 93106, N. SAMARTH, Physics Dept., Penn State University, University Park PA 16802 — We use the anomalous Hall effect to probe the nanoscale behavior of a single magnetic domain wall (DW) in (Ga,Mn)As thin film devices with out-of-plane magnetic anisotropy. Video-rate magneto-optical Kerr microscopy is also used to confirm the variation of the AHE with DW position. Our all-electrical technique allows us to observe a low field flexing regime of DW motion, distinct from the stochastic creep regime that occurs at higher fields. This flexing regime is characterized by a larger DW mobility, linear response to applied field, and non-hysteretic motion which is repeatable within our ~ 5 nm experimental resolution. We then analyze the flexing and depinning behavior of the DW to estimate the density and strength of pinning sites. Supported by the ONR MURI program.

8:24AM P16.00003 Observation of two step magnetization reversal in $Fe_0.25TaS_2$, S. PARK, Department of Physics, Chung-Ang University-Seoul, South Korea, S.B. KIM, Laboratory of Pohang Emergent Materials and Department of Physics, Pohang University of Science and Technology - Pohang, South Korea, Y.J. CHOI, Y. HORIBE, S-W. CHEONG, WEIDA WU, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, 08854, USA — Understanding magnetic coercivity mechanisms in strong ferromagnets is crucial for new technologies. We studied domain wall pinning in a highly anisotropic ferromagnet of single crystalline $Fe_0.25TaS_2$ by utilizing variable temperature magnetic force microscopy (VT-MFM). Magnetic domain structure and the magnetization reversal were investigated in magnetic fields up to 8 tesla at several temperature. Our results revealed the existence of two step magnetization reversal in $Fe_0.25TaS_2$. The real space images of magnetic domains, showing this intriguing phenomenon, will be presented.

8:36AM P16.00004 Measurement of Annihilation Barriers for Magnetic Vortices[1] , JACOB BURGESS, University of Alberta and National Institute for Nanotechnology, DAVID FORTIN, University of Alberta, JOE LOSBY, University of Alberta and National Institute for Nanotechnology, DENYS GROMBACHER, JOHN DAVIS, University of Alberta, MARK FREEMAN, University of Alberta and National Institute for Nanotechnology — Measurements of the susceptibility of an array of 2 micrometer diameter Permalloy discs are made using the AC magneto-optical Kerr effect. Employing an extended version of the rigid vortex model, saturation magnetization as a function of temperature is extracted from the data. The model also allows extraction of the switching distribution of the array as the discs transition from the vortex state to the quasi single-domain state. Tuning of temperature or sweep rate shows shifts in the distribution peak that confirm vortex annihilation is governed by a thermally activated mechanism. Using the measured saturation magnetization data in conjunction with the measured peak shifts, quantitative extraction of energetic parameters used in semi-empirical models of the annihilation energy barrier is possible. Several models are considered in the context of qualitative observations made in the experiment.

[1]We acknowledge support from NSERC, CIFAR, NINT, CRC, iCORE and Alberta Innovates.

8:48AM P16.00005 Pinning Mechanisms for Vortices in Ferromagnetic Films , TE-YU CHEN, MICHAEL ERICKSON, CHRIS LEIGHTON, PAUL CROWELL, University of Minnesota — In ferromagnetic materials, domain wall motion is generally discontinuous and stochastic in the presence of pinning sites. The pinning energy is typically quantified via a single experimental parameter - the coercivity of the hysteresis loop. We show here that in magnetic structures supporting a vortex, the vortex dynamics provide quantitative information about both the strength and range of the interaction between the vortex and individual pinning sites. Using time-resolved Kerr microscopy, we have measured the defect-induced pinning energy and length scales for magnetic vortices in micron-sized NiFe disks. We find that the pinning length scale matches the size of vortex core, and is insensitive to film thickness and growth conditions. This suggests that the dominant mechanism of vortex pinning is directly associated with the core region. The pinning energy however, is strongly dependent on microstructure. Specifically, we observe large pinning energies in NiFe films that have large roughness on lateral length scales commensurate with the core size (10 nm). The dependence of pinning energy on thickness provides further insight into the relative role of surface roughness versus bulk disorder. The strength as well as the spatial distribution of pinning sites suggest that roughness at this length scale is the dominant source of pinning in these films.

9:00AM P16.00006 Enhanced current-induced domain wall motion by tuning perpendicular magnetic anisotropy , SATORU EMORI, GEOFFREY BEACH, Department of Materials Science and Engineering, Massachusetts Institute of Technology — The effect of perpendicular magnetic anisotropy (PMA) on current-induced domain wall (DW) motion is investigated by micromagnetic simulations. The critical current density Jc to drive DWs into periodic transformation and continuous motion by adiabatic spin transfer torque decreases with increasing PMA. Also, with optimized PMA that almost exactly compensates the demagnetizing field, the adiabatic displacement of DWs driven by currents less than Jc is strongly enhanced. Since PMA can be controlled easily in multilayer films (e.g. Co/Pt), this technique of enhancing current-induced DW motion may be practical for device applications.

9:12AM P16.00007 Geometrically Confined Spin Vortices: from Fundamental Physics to Biomedical Applications , VALENTYN NOVOSAD, Argonne National Laboratory — The magnetic ground state of magnetically soft thin film ferromagnets in confined geometries (on the micrometer scale) consists of a curling spin configuration, known as a magnetic vortex state. We have recently demonstrated that the magnetic vortex microdisks can be successfully used as multifunctional magnetic carriers for biomedicine [1]. In particular, we will report on successful interfacing of ferromagnetic nanomaterials with a spin vortex ground state and biomaterials (antibody, whole cell). Namely, the gold-coated lithographically defined microdisks with an Fe-Ni magnetic core were biofunctionalized with anti-human-IL13a2R antibody for specifically targeting human glioblastoma cells. When an alternating magnetic field is applied the vortices shift, leading to the microdisks oscillation that causes a mechanical force to be transmitted to the cell. Cytotoxicity assays, along with optical and atomic force microscopy studies, show that the spin vortex-mediated stimulus creates two dramatic effects: (a) membrane disturbance and compromising, and (b) cellular signal transduction and amplification, leading to robust DNA fragmentation and, finally, programmed cell death [2]. The experiments reveals that by employing biofunctionalized magnetic vortex microdisks the magnetic fields of low frequency of a few tens of Hz and of small amplitude of < 100 Oe applied during only 10 minutes was sufficient to achieve $\sim$90% cancer cells destruction.

[1] E. A. Rozhkova, et al., J. Appl. Phys. Vol. 105, (2009) 07B306.
[2] D.-H. Kim, et al., Nature Materials, vol. 9, pp. 165 - 171 (2010).

9:48AM P16.00008 Fast transport of superparamagnetic beads by field-driven magnetic domain walls , ELIZABETH RAPOPORT, GEOFFREY BEACH, Massachusetts Institute of Technology — The manipulation of superparamagnetic (SPM) beads with magnetic domain walls (DWs) is of interest for biomedical applications [1, 2]. We present data supporting fast, continuous transport of SPM beads by field-driven DWs along straight magnetic nanowires. If the magnetostatic binding force (F_b) between a DW and an SPM bead exceeds the Zeeman force (F_Z) from a driving field, DW velocity is limited by the hydrodynamic drag force on the bead [3], and a wall-bead pair can be propelled at high speeds. We have combined micromagnetic simulations and numerical calculations to determine F_b, covering the parameter space of bead radius, wire width and thickness, and domain wall type. Comparing F_b and F_Z for different applied fields, we find that the field, H_{crit}, at which the Zeeman force separates the wall from the bead, is maximized by the same wire width, independent of bead size. Optimal conditions for continuous bead transport are achieved with 150 nm wide wires, which can transport 500 nm radius beads in driving fields up to 90 Oe, corresponding to transport velocities of up to 8 mm/s. These results suggest that fast, long-distance transport of SPM beads is possible using simple linear magnetic guide-wire structures. [1] M. Donolato, et al., Nanotechnology 20 (2009) [2] G. Vieira et al., Phys. Rev. Lett. 103, 128101 (2009) [3] M.T. Bryan et al., Appl. Phys. Lett. 96,192503 (2010)

10:00AM P16.00009 Domain wall pinning in magnetic structures with perpendicular magnetic anisotropy[1] , DANIEL GOPMAN, DANIEL BEDAU, New York University, S. PARK, DAFINE RAVELOSONA, Institut d'Electronique Fondamentale, Université Paris Sud, Orsay, France, ANDREW KENT, New York University — An experimental technique has been designed to trap domain walls in ferromagnetic nanostructures. Spin valve nanowires and nanopillars with perpendicularly magnetized free and reference layers were engineered with lithographically defined notches of varying depths and lengths. The influence of notch geometry in domain wall pinning has been compared with intrinsic domain wall pinning sites. Thermally activated jumping between metastable states has been observed under rf excitation along with telegraph noise. Coercive fields have been determined to vary linearly with applied direct currents.

[1]Supported by NSF-DMR-1006575.

10:12AM P16.00010 Breather states in magnetic domain wall racetrack memory samples , JOHN EVES, REMO HUGLI, NAOISE GRISEWOOD, BENI BRAUN, UCD — Proposed magnetic domain wall(DW) racetrack memory [1] exploits controlled motion of magnetic DWs along magnetic nanowires, and the sequence of DWs encodes the bit states. Here we investigate the possibility of the existence of dynamically bound states of pairs of DWs. We show that by the choice of suitable initial conditions for two DWs in a racetrack geometry, such dynamical states can be prepared by a suitable applied field. The breather states correspond to two DWs which have the same chirality and which oscillate around their common center of mass.

[1] S.S.P. Parkin, Science 320, 190 (2008)

10:24AM P16.00011 Reversible helicity and higher harmonics in spin textures: stripes and skyrmions , XIUZHEN YU, Japan Science and Technology Agency(JST), YUSUKE TOKUNAGA, YOSHIO KANEKO, JST, YOSHIO MATSUI, National Institute for Materials Science, YOSHINORI TOKURA, Tokyo Univ., JST and RIKEN — The magnetic bubbles viewed as skyrmions have long been attracting attention because of possible application to spintronics. The bubble configuration has been revealed by versatile microscopic techniques such as magnetic-force microscopy, scanning Hall microscopy, and Lorentz transmission electron microscopy (TEM). However, their topological properties, such as topological spin texture and helicity, have not been sufficiently unraveled in spite of possibly important implication in the novel magneto-transport phenomena. In this study, we have scrutinized the spin texture of the thin films of Sc-doped hexagonal barium ferrite with controlled magnetic anisotropy; we have demonstrated the generation of the bubble lattice under external magnetic fields which are applied perpendicular to the film plane. The magnetic component distributions in strips, bubbles and Bloch lines have been successfully achieved by means of high-resolution Lorentz TEM observations and quantitative analyses of the local magnetizations. The results indicate the reversible helicity and higher harmonics in spin textures of stripy and bubble domains.

10:36AM P16.00012 Domain Growth Behavior in the Compressible Ising Model[1] , MENG MENG, DAVID LANDAU, Center for Simulational Physics, University of Georgia — We perform large scale Monte Carlo simulations to study long-time domain growth behavior in a compressible, spin-exchange, two-dimensional triangular-lattice Ising model with continuous particle positions and zero total magnetization. To investigate the effects of compressibility on domain growth behavior, we include an elastic energy term in the Hamiltonian of our model to adjust the rigidity. The system is quenched below the critical temperature from a homogenous disordered state to an ordered phase where multiple domains coexist. Theory expects the domain size $R(t)$ grow as a power law $R(t) = A + Bt^n$, where t is the time after quench, and n is the domain growth exponent. Lifshitz and Slyozov have predicted n to be $\frac{1}{3}$ at late-time, but earlier studies[2] suggested that n could be affected by compressibility. We observe the domain growth exponent to be significantly smaller than the Lifshitz-Slyozov value of $n = \frac{1}{3}$.

[1]Research supported by NSF.

[2]S. J. Mitchell and D. P. Landau, Phys. Rev. Lett. **97**, 025701(2006).

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P17 DMP GMAG: Focus Session: Bulk Properties of Complex Oxides - 3d Oxides D174

8:00AM P17.00001 Surprises in low dimensional spin 1/2 magnets - from crystal chemistry to microscopic magnetic models of complex oxides , HELGE ROSNER, MPI CPfS Dresden — A microscopic understanding of the structure-properties relation in crystalline materials is a main goal of modern solid state chemistry and physics. Due to their peculiar magnetism, low dimensional spin 1/2 systems are often highly sensitive to structural details. Seemingly unimportant structural details can be crucial for the magnetic ground state of a compound, especially in the case of competing interactions, frustration and near-degeneracy. Here, we present for selected, complex Cu^{2+} systems that a first principles based approach can reliably provide the correct magnetic model, especially in cases where the interpretation of experimental data meets serious difficulties or fails. We demonstrate that the magnetism of low dimensional insulators crucially depends on the magnetically active orbitals which are determined by details of the ligand field of the magnetic cation. Our theoretical results are in very good agreement with thermodynamic and spectroscopic data and provide deep microscopic insight into topical low dimensional magnets.

8:36AM P17.00002 Spin Waves and Magnetic Interaction in the Multiferroic Antiferromagnet MnWO4 , J.A. FERNANDEZ-BACA, FENG YE, ORNL, R.S. FISHMAN, A. PODLESNYAK, G. EHLERS, H.A. MOOK, ORNL, Y.Q. WANG, B. LORENZ, C.W. CHU, Univ of Houston — The spin wave excitations of the multiferroic MnWO4 have been measured in the low-temperature collinear commensurate phase using high-resolution inelastic scattering. The spin excitations can be well described by a Heisenberg model with competing exchange interactions up to 11th nearest neighbors. We find the magnetic exchange couplings are highly frustrated within each zigzag spin chain along c-axis and between chains along the a-axis. However, the magnetic interactions are much weaker between chains along the b-axis. Our measurements suggest that the delicate balance of long range magnetic couplings is subject to small perturbations that can lead to a complex magnetic configuration exhibiting magnetoelectric behavior.

8:48AM P17.00003 Field-induced slow spin relaxation in monoclinic $Nd_2Ti_2O_7$ single crystals[1] , HUI XING, Department of Physics, Zhejiang University, GEN LONG, Department of Physics, SUNY at Buffalo, HANJIE GUO, CHUNMU FENG, GUANGHAN CAO, Zhejiang University, HAO ZENG, SUNY at Buffalo, ZHUAN XU, Zhejiang University — We report the ac susceptibility measurement in the paramagnetic state of the monoclinic $Nd_2Ti_2O_7$ single crystals. An unexpected slow spin relaxation is observed in the presence of a nonzero magnetic field. Such behavior is absent in zero field. Distinct features of the relaxation, including the intrinsic frequency on the order of 1 Hz, the field-, temperature- and spin dilution dependence, and its evolution under positive and negative pressures, indicate that the relaxation is associated with an unusual cooperative behavior involving spin correlations.

[1]Work supported by the NSFC (No. 10634030), NSF DMR-0547036 and National Basic Research Program

9:00AM P17.00004 The d-band manifold in $SrTiO_3$: high mobility Shubnikov–de Haas effect in magnetic fields to the quantum limit. , S. JAMES ALLEN, Physics Dept., BHARAT JALAN, Materials Dept., UCSB, GURU KHALSA, ALLAN MACDONALD, Physics Dept., UT Austin, JAN JAROSZYNSKI, National High Magnetic Field Lab, FSU, SUSANNE STEMMER, Materials Dept., UCSB — The molecular beam epitaxial growth of high mobility ($>$ 30,000 cm^2/volt.sec), low electron density ($\sim 10^{17}$ - $10^{18} cm^{-3}$) La doped $SrTiO_3$ has provided an opportunity to explore the lowest conduction band states, which are derived from the Ti d-band. Despite the long history of experiments on these d-band states, including magneto transport, we are left without a firm quantitative model of the manifold at the conduction band minimum. But, these states form the basis of quantum confined 2D electron systems at oxide interfaces with $SrTiO_3$ and delta doped layers, both the subject of current interest. To remedy this, we have performed magneto transport at temperatures down to $\sim$ 0.4 K, in magnetic fields to 31 Tesla, which is sufficient to reach the quantum limit, in high mobility samples and with carrier densities that tune the Fermi energy through the energy splitting caused by the low temperature tetragonal distortion. In close analogy to hole states in conventional semiconductors, we use 5 "Luttinger" parameters and the splitting energy, to describe these results and compare with the current understanding of the $SrTiO_3$ d-band structure.

9:12AM P17.00005 Low Energy Conduction Band Structure of SrTiO3 , GURU KHALSA, Department of Physics - University of Texas at Austin, BHARAT JALAN, Materials Department, UCSB, S. JAMES ALLEN, Department of Physics - UCSB, SUSANNE STEMMER, Materials Department, UCSB, ALLAN MACDONALD, Department of Physics - University of Texas at Austin — The recent observation of a high mobility 2DEG, and truly two-dimensional superconductor, at oxide interfaces with SrTiO3 (STO) and in delta-doped layers of STO have thus far gone without a clear theoretical description. The starting point for any quantitative theory of these systems is a reliable low energy parameterization of the Ti d-band in the bulk parent compound. Here we present a five parameter symmetry constrained model of the t2g band in STO near the conduction band minimum. We use this model to describe a recent high field (up to 31 Tesla), low temperature, angular magneto-transport study of lightly La doped STO and compare our results with other available experimental data. We will also discuss the relation between orbital density and matrix element effects in photoemission experiments of d0 Perovskites.

9:24AM P17.00006 ABSTRACT WITHDRAWN –

9:36AM P17.00007 Unconventional Electronic Transport in Doped $SrTiO_3$, C. LEIGHTON, A. SPINELLI, M.A. TORIJA, C. LIU, C. JAN, University of Minnesota — Resistivity, Hall effect, and magnetoresistance are reported on a large set of semiconducting $SrTiO_{3-\delta}$ single crystals doped n-type (by reduction or Nb substitution) over a broad range of carrier density (10^{15} to $>10^{20}$ cm^{-3}). Temperature-independent densities, strongly temperature-dependent mobilities (up to 22,000 $cm^2V^{-1}s^{-1}$ at 4.2 K), and a remarkably low critical carrier density for the metal-insulator transition are observed, and interpreted in terms of the quantum paraelectricity of the host. We argue that an unusual, high mobility, low density, metallic state is thus established at carrier densities at least as low as 8.5 x 10^{15} cm^{-3}. At low temperatures the temperature dependence of the mobility and resistivity exhibit a non-monotonic carrier density dependence and an abrupt change in character near 2 x 10^{16} cm^{-3}, indicating a distinct crossover in conduction mechanism, perhaps associated with a transition from impurity band to conduction band transport. The results provide a simple framework for the understanding of the global transport behavior, and suggest some potential applications. Work supported by NSF.

9:48AM P17.00008 Pseudogap in metallic layered nickelate $R_{2-x}Sr_xNiO_4$, MASAKI UCHIDA, K. ISHIZAKA, Y. ISHIDA, Y. ONOSE, R. ARITA, S. SHIN, Y. TOKURA, University of Tokyo, P. HANSMANN, A. TOSCHI, K. HELD, Vienna University of Technology, Y. KANEKO, ERATO-MF, X. YANG, O.K. ANDERSEN, Max-Planck-Institut, R. KUMAI, AIST — We have investigated charge dynamics and electronic structures for single crystals of metallic layered nickelates $R_{2-x}Sr_xNiO_4$. Angle-resolved photoemission spectroscopy (ARPES) on the barely-metallic $Eu_{0.9}Sr_{1.1}NiO_4$ has revealed a large hole surface of x^2-y^2 character with a high-energy pseudogap of the same symmetry and comparable magnitude with those of underdoped cuprates, although the antiferromagnetic interactions are one order of magnitude smaller. Our findings strongly indicate that the high-energy momentum-dependent pseudogap (or Fermi arc) is not unique to the high-T_c cuprates but commonly develops in the anomalous quasi-two-dimensional metallic state near the Mott transition reflecting the real-space charge correlation.

10:00AM P17.00009 Density wave driven metal-insulator transition in nickelates , SUNGBIN LEE, RU CHEN, University of California, Santa Barbara, LEON BALENTS, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, BALENTS GROUP TEAM — The Mott transition in nickelates, RNiO3, shows unusual magnetic ordering and charge ordering in the insulating phase. For the more itinerant nickelates, one may argue that these unusual density waves are actually driven by Fermi-surface nesting, originated from the large flat regions of Fermi surfaces. Using a tight-binding model of the band derived from doubly degenerate eg orbitals, we obtain the density wave induced metal- insulator transition phase diagram in the presence of on-site Coulomb interaction and Hund's coupling, treated in Hartree-Fock approximation. Furthermore, motivated by recent success in layer by layer growth of nickelates, the thin film effects in nickelates are also studied. Finally we calculate the optical conductivity for the various states in our phase diagram, suggesting experimental measurements to check the theory.

10:12AM P17.00010 Molecular correlated insulating state in low-valence layered nickelates , VICTOR PARDO, WARREN E. PICKETT, University of California Davis — In recent years, there has been an effort on artificially creating Fermi surfaces that resemble those of the superconducting cuprates. A Ni^{3+}:d^7 (one e_g electron) configuration can be made into the electron-like analog of the d^9 (one e_g hole) cuprate electronic structure.[1] Another cleaner alternative would be to grow low-valence Ni^{+}:d^9 compounds, which have recently become available through synthesis[2] of members of the series $La_{n+1}Ni_nO_{2n+2}$. We present LDA+U calculations on the layered compounds $La_4Ni_3O_8$ [3] and $La_3Ni_2O_6$, with three and two NiO_2 layers, respectively. Electron count implies very low Ni formal valencies: 1.33+ and 1.5+, respectively. If charge order is present, Ni^{+}:d^9 could occur in a geometry similar to that of the cuprates. However, this is not the case. Both compounds are insulators, which we can attribute to quantum confinement in the NiO_2 tri/bi-layers. The only states close to the Fermi level are Ni $d_{3z^2-r^2}$, which couple along the c-axis (Ni trimers or dimers). The insulating behavior must be viewed from a molecular orbital viewpoint, after AFM order within layers has narrowed the bands. Insulating behavior is that of a "molecular" Mott insulator rather than a charge-ordered insulator.
[1] J. Chaloupka and G. Khaliullin, *PRL* **100**, 016404 (2008).
[2] V. V. Poltavets *et al.*, *Phys. Rev. Lett.* **102**, 046405 (2009).
[3] V. Pardo and W.E. Pickett, arXiv:1008.2707.

10:24AM P17.00011 Search for structural fluctuations in the disordered stripe state of $Nd_{1:67}Sr_{0:33}NiO_4$[1] , A.M. MILINDA ABEYKOON, EMIL BOZIN, GENDA GU, JOHN HILL, JOHN TRANQUADA, SIMON BILLINGE, Brookhaven National Laboratory — We present a temperature series PDF and a Rietveld analysis of $Nd_{1:67}Sr_{0:33}NiO_4$ system to study the local structural response in the state above the charge-ordered state that has not been characterized in detail to date. We observed NiO_6 octahedral tilting patterns of different magnitude for short and long-range structure of the system. A sequential Rietveld refinement, and a T-series PDF analysis on the length scale (5-20)Å were carried out to characterize the long-range order of the system. A PDF analysis on the length scale (0-4.2) Å revealed a different magnitude local octahedral tilt pattern as a function of temperature. The correlation length of short-range ordered charge stripes existing above T_{co} was estimated using a Box-Car type PDF model. Combining this information with the refined isothermal atomic displacement parameters (ADPs) yields a much more complete picture of the nature of both atomic displacements and how they are correlated with each other in the system.

[1]This work was supported by US-DOE-BES.

10:36AM P17.00012 Lattice normal modes and electronic properties of the correlated metal $LaNiO_3$, GAOYANG GOU, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104, USA, JAMES RONDINELLI, X-Ray Science Division, Argonne National Laboratory, Argonne, IL 60439, USA, ILYA GRINBERG, ANDREW RAPPE, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104, USA — We present results from density functional calculations of lattice vibrations and electronic properties of the correlated metal $LaNiO_3$. Using the landau theory of phase transitions and *ab initio* derived phenomenological coefficients obtained from local-spin density approximation (LSDA) calculation, we examine the evolution of the Raman-active phonon modes with temperature and find that the LSDA results give excellent agreement with experiments. To study the electronic structure of $LaNiO_3$, we extend to the post-LSDA functional methods, including the local spin density+Hubbard U (LSDA+U) method, and two hybrid exchange-correlation functionals, PBE0 and HSE. By comparing the results obtained from the various functionals with the experimental photoelectron spectroscopy (PES) and X-ray photoelectron spectroscopy (XPS) data, we argue that the screening effect coming from the delocalized O-2p and Ni-t_{2g} electrons will be strong enough to reduce the electron correlation of $LaNiO_3$.

10:48AM P17.00013 Time-Dependent Recovery of Charge and Spin Order in Stripe-Ordered Nickelates[1] , Y.F. KUNG, A.F. KEMPER, W.-S. LEE, B. MORITZ, A.P. SORINI, Z.-X. SHEN, T.P. DEVEREAUX, Stanford Institute for Materials and Energy Science, SLAC National Accelerator Laboratory and Stanford University — Using time-dependent Ginzburg-Landau theory, we study the melting and recovery of charge and spin order in striped nickelates ($La_{2-x}Sr_xNiO_4$) in response to an ultrashort pump pulse that destroys the order. We find that the critical temperature for onset of spin order varies with increasing coupling between charge and spin order. Solving the Gross-Pitaevskii equations to model the time evolution, we explore the temporal dynamics of charge and spin order parameters, to be compared to experimental observations at LCLS.

[1]National Defense Science and Engineering Graduate Fellowship

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P18 GMAG DMP: Focus Session: Low D/Frustrated Magnetism - Triangular Lattices

D172

8:00AM P18.00001 Neutron Scattering Studies of the S=1/2 Triangular Lattice Magnets $NaNiO_2$ and $LiNiO_2$, J. PATRICK CLANCY, McMaster University — $NaNiO_2$ and $LiNiO_2$ are isostructural quantum magnets based on a stacked triangular lattice in which magnetism arises from S=1/2 magnetic moments carried by Ni^{3+} ions. Surprisingly, while these compounds are structurally and electronically very similar, the magnetic properties they exhibit are dramatically different. $NaNiO_2$ undergoes a cooperative Jahn-Teller phase transition at 480K and magnetically orders below $T_N \sim 23$K, adopting a structure which consists of ferromagnetic sheets of S=1/2 moments stacked in an antiferromagnetic fashion. In contrast, $LiNiO_2$ undergoes a spin glass transition at $T_g \sim 9$K and remains disordered down to the lowest measured temperatures. Understanding the absence of long-range magnetic order in $LiNiO_2$ is a problem which has attracted considerable interest for more than twenty five years. Among many potential explanations, the answer has most notably been attributed to geometric frustration caused by inherent mixing of the Li and Ni sublattices, or orbital degeneracy resulting from the lack of a coherent Jahn-Teller distortion. In this talk I will describe time-of-flight neutron scattering measurements performed on polycrystalline samples of $NaNiO_2$ and $LiNiO_2$ using the wide Angular-Range Chopper Spectrometer (ARCS) at ORNL and the Disk Chopper Spectrometer (DCS) at NIST. These measurements provide a thorough characterization of the excitation spectra for these two compounds, probing the inelastic scattering over energy scales ranging from $\sim$ 0.1 meV to 1.5 eV. In $NaNiO_2$, our measurements reveal two sets of well-defined spin excitations, which we associate with ferromagnetic spin waves mediated by in-plane interactions and antiferromagnetic spin waves mediated by out-of-plane interactions. In $LiNiO_2$, we observe similar, albeit much broader, excitations consistent with short-range two-dimensional magnetic correlations. In the case of $NaNiO_2$, we have developed a simple linear spin wave theory model to describe these excitations and extract the relevant magnetic exchange couplings for this system.

8:36AM P18.00002 Magnetic order and glassiness in distorted triangular lattice materials, $Cu_{2(1-x)}Zn_{2x}(OH)_3NO_3/(C_7H_{15}COO)$, JIAN WU, FLETCHER WERNER, JULIA S. WILDEBOER, ALEXANDER SEIDEL, ZOHAR NUSSINOV, S.A. SOLIN, Washington University in St. Louis — We have synthesized two series of distorted triangular lattice materials $Cu_{2(1-x)}Zn_{2x}(OH)_3M$, where M = NO_3^- or $C_7H_{15}COO^-$, by hydrothermal reaction. The powder X-ray diffraction measurements show that the substitution of Zn for Cu leads to a series of isostructural doped compounds [1]. The $C_7H_{15}COO^-$ long chain intercalated samples display a series of intense (00*l*) reflections, which signals their enhanced 2D structures with an almost doping-independent interlayer distance 24.2Å. In the DC magnetic susceptibility data for all NO_3^- samples, we observe clear evidence of transitions from a paramagnetic to antiferromagnet phase. The onset of long-range order is further proven by the prominent features in specific heat data. However, all the long chain intercalated samples were found to display several spin-glass-like behaviors. A clear bifurcation between the ZFC and FC data was observed at T $<$ 15K. The time evolution of isothermal remnant magnetization M_{ZFC}(t) has a linear dependence on $\ln(t)$. No peak features or broad maximum have been discovered in the specific heat measurements. Further analysis of the above results suggest that the long chain intercalated samples are cluster spin glasses at low temperature.
[1] J.Wu et al, J. Phys. Condens. Matter. 22, 334211(2010).

8:48AM P18.00003 Spin glassiness and power law scaling in anisotropic triangular spin-1/2 antiferromagnets , ALEXANDER SEIDEL, JIAN WU, JULIA S. WILDEBOER, FLETCHER WERNER, ZOHAR NUSSINOV, S.A. SOLIN, Washington University in St. Louis — We discuss the magnetic properties of a class of spin $S = 1/2$ antiferromagnetic quasi-triangular lattice materials, both in the clean limit and in the presence of non-magnetic Zn impurities. These systems are long organic chain intercalated derivatives of copper hydroxy nitrate, with a very large c-axis separation of 24Å. In these compounds, we find that a spin glass phase is universally preceded by two different power law regimes in the temperature dependence of the DC magnetic susceptibility, separated by a sharp crossover. This is seen both in the presence as well as in the absence of non-magnetic Zn impurities, where the power law exponents are surprisingly unperturbed by the compositional disorder. We argue that these findings may be consistent with a picture based on a self-generated spin glass in the clean undoped compound, where frustration is the driving mechanism of the glassiness rather than disorder. While AC measurements and time dependent magnetization follow traditional spin glass paradigms, the power law structure found in the DC susceptibility is argued to deviate in various ways from scenarios expected based on Griffiths type physics, and may call for new explanations. [1] J. Wu et al., J. Phys. Condens. Matter, 22, 334211 (2010). [2] J. Wu et al., arXiv:1007.0442

9:00AM P18.00004 Competing interactions and continuum excitations in the spin-1 triangular lattice antiferromagnet $NiGa_2S_4$[1] , J. WEN, IQM, Johns Hopkins Univ, USA, Y. NAMBU, ISSP, Univ. of Tokyo, Japan, J. RODRIGUEZ, C. STOCK, NCNR, NIST, USA, S. NAKATSUJI, ISSP, Univ. of Tokyo, Japan, S. ONODA, RIKEN, Japan, Y. MAENO, Kyoto Univ., Japan, C. BROHOLM, IQM, Johns Hopkins Univ, USA — In some geometrically frustrated magnets, conventional long range order is replaced by static or dynamic short range order. Quasi-2D $NiGa_2S_4$ is the only known S=1 antiferromagnet with an exact triangular lattice. Recent neutron scattering experiment on high quality $NiGa_2S_4$single crystals revealed short range quasi-2D incommensurate spin correlation with a critical wavevector close to (1/6, 1/6, 0) [1]. Here we report a measurement of the dynamic spin correlation function through a volume of **Q**-E space for T<<J. A gapless spectrum was observed at the incommensurate critical wavevector while a softened but still gapped response was found at (1/3, 1/3, 0). This indicates dominant third nearest neighbor interaction and competing weaker near neighbor interactions. The excitation spectrum takes the form of a bounded continuum throughout the 2D Brillouin zone. The temperature dependence dynamic correlation length shows that short range correlation persist up to Θ_{cw}=-80(2)K.
[1] C.Stock, *et al,* Phys.Rev.Lett.105,037402 (2010)

[1]Supported by the DoE through DE-FG02-08ER46544.

9:12AM P18.00005 Quantum Antiferromagnet on an Anisotropic Triangular Lattice , SEDIGH GHAMARI, CATHERINE KALLIN, SUNG-SIK LEE, McMaster University — The effects of quantum fluctuations on the spin 1/2 Heisenberg antiferromagnet on a triangular lattice, with diagonal interchain exchange J' weaker than the intrachain exchange J, are studied. This model is of considerable interest because of its relevance to Cs2CuCl4, where experiments have been interpreted as evidence for a nearby two-dimensional spin liquid and because numerous theoretical studies have proposed that the incommensurate spiral spin density wave order is destroyed by quantum fluctuations well before the one-dimensional limit (J'=0) is reached.

9:24AM P18.00006 ESR as a probe of spinon excitations of the spin-1/2 antiferromagnet Cs_2CuCl_4 , K. POVAROV, A. SMIRNOV, Kapitza Institute for Physical Problems RAS, O. STARYKH, University of Utah, S. PETROV, Kapitza Institute for Physical Problems RAS, A. SHAPIRO, Shubnikov Institute for Crystallography RAS — We report dramatic manifestation of the uniform Dzyaloshinskii-Moriya (DM) interaction in the ESR response of quasi-one-dimensional spin-1/2 antiferromagnet Cs_2CuCl_4. We find the ESR response in the range 10-90 GHz to be strongly sensitive to the relative orientation of the magnetic field and DM axes. Most importantly, we observe splitting of the ESR line into two lines in the paramagnetic phase, upon lowering the temperature from 10 K to 1.3 K. The latter temperature is about twice the ordering temperature $T_N = 0.62$ K, and yet far below the Curie-Weiss temperature 4 K . The splitting occurs when the static magnetic field H is aligned with one of the DM axes of the material and is absent when H is oriented perpendicular to the axes. This novel phenomenon is a consequence of the critical nature of fractionalized spinon excitations of the individual antiferromagnetic chains in the paramagnetic phase. A uniform (along the spin chain direction) DM interaction provides an effective magnetic field, the sign of which is opposite for the right- and left-moving spinons. In the presence of external magnetic field this difference translates into a pair of ESR frequencies, making the experiment a novel probe of spinon excitations.

9:36AM P18.00007 Metallic magnetization plateau on triangular lattice[1] , ZHIHAO HAO, Department of Physics and Astronomy, Johns Hopkins University, OLEG STARYKH, Department of Physics and Astronomy, University of Utah — The $1/3$ magnetization plateau is well established for spin $1/2$ Heisenberg antiferromagnetic model on triangular lattice. The state is stable against a large range of spatial anisotropies and is observed in the triangular compound Cs_2CuBr_4. A natural question to ask is whether the plateau state remains stable if the on-site repulsion U is lowered for the underlying Hubbard model. In our work, we studied the one-band Hubbard model on triangular lattice. Through mean-field calculations, it is discovered that an up-up-down spin density wave state with $1/3$ of saturation magnetization is stablized for a range of U and magnetic field h. For $4.44t \leq U \leq 4.55t$, the state is a half metal: the spin up bands remain metallic while the spin down bands are insulating. For $U > 4.55t$, the spin up bands become gapped and the system is an insulator. It is speculated the plateau state remains stable for the entire range of $U \geq 4.44t$.

[1]Z. Hao is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-FG02- 08ER46544. O. Starykh is supported by NSF, Grant No. DMR-0808842.

9:48AM P18.00008 Phase Diagram of a Geometrically-Frustrated Triangular-Lattice Antiferromagnet in a Magnetic Field[1] , RANDY FISHMAN, Oak Ridge National Laboratory — The magnetic phase diagram of a geometrically-frustrated triangular-lattice antiferromagnet is evaluated as a function of magnetic field and anisotropy using a trial spin state built from harmonics of a fundamental ordering wavevector. A non-collinear incommensurate state, observed to be chiral and ferroelectric in $CuFeO_2$, appears above a collinear state with 4 sublattices (SLs). A previously unobserved collinear 5-SL phase may be accessible in a magnetic field for a non-stoichiometric compound with excess or deficient oxygen. The apparent absence of multiferroic behavior for predicted chiral, non-collinear 5-SL states poses a challenge to theories of the ferroelectric coupling in $CuFeO_2$.

[1]Research sponsored by the Division of Materials Sciences and Engineering, U.S. Department of Energy under contract with UT-Battelle, LLC.

10:00AM P18.00009 ABSTRACT WITHDRAWN —

10:12AM P18.00010 Phases of spatially anisotropic triangular antiferromagnet in high magnetic field , OLEG STARYKH, University of Utah, ANDREY CHUBUKOV, University of Wisconsin — We investigate phases of the Heisenberg spin model on a spatially anisotropic triangular lattice as a function of $J'/J < 1$ and a magnetic field H (J is the exchange along the horizontal bonds, and J' is the exchange along the diagonal bonds). The anisotropy of J's competes with quantum fluctuations and this competition leads to a rich phase diagram. Immediately below the saturation field H_s we find three phases: three-sublattice commensurate phase, incommensurate co-planar "fan" phase, and incommensurate non-coplanar "cone" phase. The former two are supersolids while the latter is a superfluid in the terminology of strongly interacting bosons. At a finite boson density ($H < H_s$) and on approach to the fan-cone phase boundary from within the cone phase with ordering momentum Q, we observe softening of the "roton" minima at momentum Q' different from $-Q$, which one would expect for a direct cone-fan transition. This points on the existence of the intermediate double-spiral state in which boson density exhibits incommensurate modulations with momenta Q and Q'. The extrapolation of our results to $H \sim H_s/3$ predicts that $Q' = Q$, and the intermediate state becomes similar to the "distorted umbrella" state that emerges out of up-up-down phase. We discuss the implications of our findings for the global phase diagram of the anisotropic triangular Heisenberg antiferromagnet.

10:24AM P18.00011 Theory of SU(2) invariant spin liquids on the triangular lattice with spinful Majorana excitations , RUDRO BISWAS, LIANG FU, CHRIS LAUMANN, SUBIR SACHDEV, Harvard — We present a theory of SU(2) invariant spin liquids on the 2D spin 1/2 triangular lattice described by a parton representation of the spin in terms of spin-1 Majorana particles. These spin liquids break time reversal symmetry and generically possess a novel Fermi surface consisting of three lines intersecting at $k = 0$ as well as an unconventional dynamic critical exponent $z = 3$. We also present calculations for observable quantities and discuss possible connections to recent experiments involving spin 1/2 Heisenberg triangular lattices.

10:36AM P18.00012 Phase Diagram of Classical Heisenberg Antiferromagnets with Four-Spin Interactions on Stacked Triangular Lattice under Magnetic field[1] , SHINTARO TAKAYOSHI, Institute for Solid State Physics, University of Tokyo, MASAHIRO SATO, Department of Physics, Aoyama-Gakuin University — Classical Heisenberg antiferromagnet (HAF) on stacked triangular lattice is a simple and important model of frustrated systems. Although there are some candidate materials for triangular HAF, they are not ideal ones and various kinds of perturbations should be present. While it is well known that the ground state of triangular HAF is 120-degree structure, how perturbations destabilize the structure has not been well studied. In this study, we consider effects of four-spin interactions on magnetic phase diagram of triangular HAF. In fact, some real mechanisms of generating four-spin interactions have been known: higher-order electron hopping processes in Mott insulators, spin-phonon couplings, etc. We complete the magnetic phase diagrams by using Monte Carlo simulation. We will report new phases induced by four-spin interactions.

[1]Grant-in-Aid for JSPS Fellows (Grant No. 09J08714)

10:48AM P18.00013 Magnetic ground state and excitation of SrV10O_{15} , JOOSEOP LEE, KAZUKI IIDA, University of Virginia, MATTHEW STONE, SNS, ORNL, MASAAKI MATSUDA, HFIR, ORNL, TOMOMASA KAZITA, TAKURO KATSUFUJI, Waseda University, SEUNGHUN LEE, University of Virginia, UNIVERSITY OF VIRGINIA TEAM, WASEDA UNIVERSITY COLLABORATION, SNS, OAK RIDGE NATIONAL LABORATORY COLLABORATION, HFIR, OAK RIDGE NATIONAL LABORATORY COLLABORATION — $SrV_{10}O_{15}$ has magnetic bilayers composed of triangular lattices with periodical missing, which can be an interesting playground for the study of frustration. In this new type of magnetic structure, using neutron powder diffraction, we find a magnetic ground state below 45K with ordering vector Q=(0 1/2 1), and study detailed spin configuration. Magnetic excitations have also been investigated using a single crystal at ARCS, a time-of-flight neutron chopper spectrometer at SNS. Our results show quite interesting highly dispersive dispersion relations: a gapless Goldstone mode is strongly dispersive along the a and c axis, and is less-strongly dispersive along the b axis. Another mode is dispersionless along the a and b axis, and is strongly dispersive along the c axis. We determine the spin hamiltonian that sheds light in understanding the interplay between orbital, spin, charge, and lattice degrees of freedom in this compound.

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P19 GMAG: Focus Session: Spin Transport & Magnetization Dynamics in Metals VI

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8:00AM P19.00001 Quantum Dynamics of Spin-torqued Nanomagnet , YONG WANG, YAOJUN ZHANG, L.J. SHAM, Department of Physics, University of California, San Diego — Nanomagnet is the key ingredient of many spintronics devices, such as hard disk read head, magnetoresistive random access memory(MRAM),etc. The underlying mechanisms in these structures are due to the interplay between the nanomagnet and spin-polarized electrons. Usually, the nanomagnet is characterized by the classical magnetization vector with its intrinsic quantum fluctuation neglected. By treating the nanomagnet as a huge atom with millions of energy levels, we are able to take account into the magnetization fluctuation, and study the interactions between nanomagnet and spin-polarized electrons on the same footing as quantum objects. We will show that the well-known giant magnetoresistance(GMR) effect and spin transfer torque(STT) effect are the consequences of continuous quantum measurements on the nanomagnet by spin-polarized electrons. We found that the quantum dynamics of nanomagnet is governed by a Fokker-Planck(FP) type equation in the atomic coherent state representation(P- representation). We will also discuss the correlation between the magnetization fluctuation and the electric current fluctuation.

8:12AM P19.00002 Minimum action paths for single domain ferromagnetic nanostructures under the influence of spin transfer torque , GABRIEL CHAVES-O'FLYNN, DANIEL STEIN, ANDREW KENT, ERIC VANDEN-EIJNDEN, New York University — Thermally induced magnetization reversal is an important issue for the design of magnetic storage devices. The problem is usually studied using Kramers' theory of reaction rates, which is applicable when the dynamics can be described as gradient forces. Spin Transfer Torque (STT) is an effect of technological importance which does not fall in this category. For Spin Transfer Torque an action minimization is required to find the most probable paths and transition states between metastable states. We calculate these most probable paths for ferromagnetic nanostructures under the influence of STT in the low noise limit for a variety of current strengths and magnetic fields. Previous action minimization were done in the absence of STT and provide a good basis for comparison [1]. We study thin films with an in-plane easy magnetization axis using the geometrical Minimum Action Method (gMAM) [2]. The action obtained using gMAM is in qualitative agreement with activation energy barriers on previous work by Li-Zhang [3].

[1] R.V. Kohn, M.G. Reznikoff, E. Vanden-Eijnden, J. Nonlinear Sci. 15, 223 (2005)
[2] M. Heymann, E. Vanden-Eijnden, Comm. Pure Appl. Math. LXI, 1052(2008)
[3] Z. Li, S. Zhang, Phys. Rev. B 69, 134416 (2004)

8:24AM P19.00003 Giant enhancement of microwave emission in magnetic tunnel junction oscillators by orientating in-plane field[1] , Z.M. ZENG, K.H. CHEUNG, H.W. JIANG, Department of Physics & Astronomy, UCLA, CA 90095, P. UPADHYAYA, P. KHALILI AMIRI, K.L. WANG, Department of Electrical Engineering, UCLA, CA 90095, J.A. KATINE, Hitachi Global Storage Technologies, San Jose, California 95135 — Recently spin-transfer nano-oscillators (STNOs) have attracted considerable attention because they are tunable over a wide frequency rang by varying the applied DC current or magnetic field. One main challenge for practical applications is to boost the relative low emitted power. MgO-based STNOs have exhibited a capability to deliver much larger power. However, they often show multiple emission peaks or broad linewidths. It is necessary to suppress the additional peaks and to reduce the central peak linewidth. In this talk, we present our microwave measurements in MgO-based STNOs as a function of in-plane field orientation. At an optimal orientation, emitted power of a single peak is largely enhanced, together with a significantly narrowed linewidth. The experiment shows that the understanding of intrinsic features of the oscillators as a function of in-plane orientation is important for optimizing the performances of MgO-based nano-oscillators.
[1] see for example, S. I. Kiselev, et.al., Nature 425, 308 (2003).

[1]This work was supported by the DARPA STT-RAM program.

8:36AM P19.00004 ABSTRACT WITHDRAWN –

8:48AM P19.00005 Spin-transfer oscillators in the effective planar approximation[1] , YA. B. BAZALIY[2], University of South Carolina — Spintronic devices with dominating easy plane anisotropy can be described in an effective planar approximation of the LLG equation. In particular, the effective equation can be used to study the spin-transfer oscillators. We use this approach to study the transitions of the oscillator excited by a combination of an AC and a DC electric currents between the small and large amplitude regimes.

[1]supported by NSF DMR-0847159
[2]also at the Institute of Magnetism, Kyiv, Ukraine

9:00AM P19.00006 High Speed Spin Torque Memory with Combined Perpendicular and In-Plane Polarizers , GRAHAM ROWLANDS, TOFIZUR RAHMAN, JORDAN KATINE, JUAN ALZATE, ALEXEY KOVALEV, YAROSLAV TSERKOVNYAK, KOSMAS GALATSIS, PEDRAM KHALILI AMIRI, KANG WANG, JIAN-PING WANG, ILYA KRIVOROTOV — The use of a perpendicular polarizing layer in combination with an in-plane free layer has been proposed [1] as a means of reducing the switching time and write energy of spin-torque MRAM cells. While these structures have been realized in nanopillars with metallic spacers [2-4], memory applications demand the use of magnetic tunnel junctions (MTJs) due to their higher magnetoresistance and better impedance matching to a write transistor. We augment standard in-plane CoFeB/ MgO/ CoFeB MTJs to include an additional fixed layer pulled out-of-plane by coupling to the adjacent [Co/Pd] multilayer designed to possess a strong perpendicular magnetic anisotropy. This additional polarizer generates spin torque with an out-of-plane component, resulting in a fast precessional switching with no incubation time or pre-switching oscillations. For a variety of sample sizes we observe switching times approaching 100 ps. References: [1] A. D. Kent et al. Appl. Phys. Lett. 84, 3897 (2004). [2] C. Papusoi et al. Appl. Phys. Lett. 95, 072506 (2009) [3] O. J. Lee et al. 95, 012506 (2009) [4] R. Sbiaa et al. J. Appl. Phys. 105, 013910 (2009)

9:12AM P19.00007 Noise in Spin Torque Oscillators , MARK KELLER — In a spin torque oscillator _(STO)_, a direct current passing through a reference magnetic layer becomes spin polarized and transfers angular momentum to a second magnetic layer that is excited into steady-state oscillation. The oscillating magnetization causes an oscillating device resistance, through either the giant magnetoresistance effect or the tunneling magnetoresistance effect, which in combination with the bias current generates an oscillating voltage as the output signal. Interest in potential applications of STOs in integrated microwave circuits is driven by their rapid frequency tunability, small size __(<100 nm)_, and compatibility with standard semiconductor processing techniques. For any oscillator, noise is both an important figure of merit for applications and a useful probe of internal physical processes. I will summarize the theoretical and experimental state of our understanding of frequency and phase noise in a variety of oscillators, considering both time domain and frequency domain measurements. Some aspects can be explained by the effects of thermal fluctuations. Others, such as frequency noise that varies as 1/f at low frequencies, are not yet understood.

9:48AM P19.00008 Optimal spin current pattern for fast domain wall propagation in nanowires[1] , PENG YAN, Physics Department, The Hong Kong University of Science and Technology, Hong Kong, ZHOUZHOU SUN, JOHN SCHLIEMANN, Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany, XIANGRONG WANG, Physics Department, The Hong Kong University of Science and Technology, Hong Kong — One of the important issues in nanomagnetism is to lower the current needed for a technologically useful domain wall (DW) propagation speed. Based on the modified Landau-Lifshitz-Gilbert (LLG) equation with both Slonczewski spin-transfer torque and the field-like torque, we derive an optimal temporally and spatially varying spin current pattern for fast DW propagation along nanowires. Under such conditions, the DW velocity in biaxial wires can be enhanced as much as tens of times higher than that achieved in experiments so far. Moreover, the fast variation of spin polarization can efficiently help DW depinning. Possible experimental realizations are discussed.

[1]This work is supported by Hong Kong RGC grants (#603508, 604109, RPC10SC05 and HKU10/CRF/08-HKUST17/CRF/08), and by Deutsche Forschungsgemeinschaft via SFB 689. ZZS thanks the Alexander von Humboldt Foundation (Germany) for a grant.

10:00AM P19.00009 Effects of Spin transfer torques on domain wall nucleation and propagation in perpendicular spinvalve nanopillars , STEPHANE MANGIN, JULIEN CUCCHIARA, THOMAS HAUET, Nancy Unversite, DAVID P. BERNSTEIN, SLAC - Stanford, ERIC E. FULLERTON, UCSD, ANDREW D. KENT, New York Univ, JORDAN KATINE, Hitachi-GST, JONATHAN Z. SUN, IBM — Controlled manipulation of magnetic domain wall (DW) propagation has spurred intensive research in recent years because of its fundamental interest and the potential impact in spintronic device technology such as racetrack memories. Both magnetic fields and electric currents may be used to control domain walls. Most of the studies have been performed on magnetic nanowires with in plane anisotropy. Here we study domain wall creation and propagation in spinvalve nanopillar composed of magnetic materials with perpendicular anisotropy such Co/Ni multilayers [1]. It is shown that DWs can nucleate and propagate in perpendicularly magnetized nanopillar spin valves as small as 50 $\times$ 100 nm^2 [2]. The study of the dynamics of DW nucleation and propagation driven by applied fields and injected currents is presented [3]. High domain wall velocities of about 100m/s are found.

[1] S. Mangin, et al , *Nat. Mater.* **5**, 210 (2006), S. Mangin, et al, *Appl. Phys. Lett.* **94**, 012502 (2009)
[2] D. Ravelosona, et al (2006)
[3] J. Cucchiara, et al *Appl. Phys. Lett. 94 102503 (2009)*

10:12AM P19.00010 Domain Wall Pumping with Spin-Transfer Torque , CARL BOONE[1], Hitachi Global Storage Technologies, ILYA KRIVOROTOV, University of California, Irvine — We numerically investigate the effects of current-perpendicular-to-the-plane (CPP), angularly asymmetric Slonczewski spin-transfer torque (ST) on transverse domain walls (DW) in nanowires. The CPP ST excites long-range domain wall motion in a direction independent of the current polarity and proportional to the square of the current amplitude. This symmetry with respect to current polarity creates the possibility of DW pumping – long range DW motion driven by an alternating current. The DW velocity becomes resonantly enhanced near a frequency that depends on the nanowire dimensions, corresponding to the eigenfrequency of a localized, spatially antisymmetric spin-wave mode that exists within the DW.

[1]The submitted work was done while at University of California, Irvine.

10:24AM P19.00011 Current-Perpendicular-to-Plane (CPP) Magnetoresistance at 4.2K of spin-valves with the half-metal Co(2)Fe(Al(0.5)Si(0.5)) and Permalloy[1] , RAKHI ACHARYYA, REZA LOLOEE, WILLIAM PRATT, JACK BASS, Physics Department, Michigan State University, East Lansing, MI 48824 — There is interest in current-perpendicular-to-plane (CPP) magnetoresistance (MR) in spin-valves containing half-metallic Heusler alloys such as Co(2)FeAl((0.5)Si(0.5)) (CFAS) [1]. Onto [001] oriented MgO substrates, we sputter epitaxially [001] oriented layers of 150-nm-thick Nb, 10-nm-thick Cu, and chosen thickness CFAS. We complete a spin-valve with 25 nm of Cu, 24 nm of Py = Ni(84)Fe(16), 10 nm of Cu, 25 nm of Nb, and 15 nm of a Au capping layer. With optical lithography and Ar-ion milling, we make 25 micron radius pillars insulated with in-situ deposited SiO. Finally, we lightly ion mill the Au surface and deposit a 150 nm thick Nb cross-strip, then covered by 5 nm of Au. The Nb strips superconduct at our measuring temperature of 4.2K, giving uniform current flow. We will describe how the CPP-MR varies with thicknesses of CFAS ranging from 2 nm to 20 nm. We hope to describe additional studies with Ag instead of Cu and with pinned Py layers.

[1] T.M. Nakatani et al., Appl. Phys. Lett. **96**, 212501 (2010).

[1]Research supported by NSF grant DMR 08-04126.

10:36AM P19.00012 Modulation of spin torque from spin transport through two nearby domain walls , ELIZABETH GOLOVATSKI, MICHAEL FLATTÉ, OSTC and Dept. of Physics and Astronomy, University of Iowa — The motion of domain walls due to the spin torque generated by coherent coherent carrier transport [1] is of considerable interest for the development of spintronic devices [2]. We model two π Néel walls [3] separated by a variable distance, and calculate transport characteristics and spin torque through the system [4]. We find that for large separations, the domain walls show the resonant transmission behavior of a spin-dependent double barrier; for small separations, the transmission spectrum resembles that of a 2π wall. We also find that the spin torque across the system initially increases as the separation between the walls increases from zero, then decreases slightly before reaching a saturation value that is larger than both the spin torque of a 2π wall and that of two individual π walls. This work is supported by an ARO MURI.

[1] M. Yamanouchi, D. Chiba, F. Matsukura, and H. Ohno, Nature 428, 539 (2004).
[2] S. Parkin,M . Hayashi, L. Thomas, Science 320, 190 (2008)
[3] G. Vignale and M. Flatté, Phys. Rev. Lett. 89 (2002).
[4] D. Ralph and M. Stiles, J.M.M.M. 320, 1190 (2008).

10:48AM P19.00013 Current-Induced Torques in the Presence of Spin-Orbit Coupling , M.D. STILES, PAUL M. HANEY, Center for Nanoscale Science and Technology, National Institute of Standards and Technology — In systems without spin-orbit coupling, the simple connection between spin transfer torque and the divergence of the spin current has provided a simple description of current induced torques. Here, we generalize this relationship for systems with strong spin-orbit coupling to a relationship between spin transfer torques, total angular momentum current, and mechanical torques. In such systems, the spin-orbit coupling modifies the behavior of the spin transfer torques. For example, the it can give rise to a persistent spin transfer torque in a spin valve: the spin transfer torque density approaches a constant value rather than decaying away from the interface. This approach also provides a formal expression for the mechanical torque at a single ferromagnetic-nonmagnetic interface.

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P20 FIAP/DMP GERA/DCOMP: Focus Session: Physics of Energy Storage Materials IV – Complex Hydrides and Methane D168

8:00AM P20.00001 $NaAlH_4$ – Carbon Aerogel: Kinetic Enhancement of a Complex Hydride by Nanoporous Carbon , FREDERICK PINKERTON, General Motors R&D Center — Complex hydrides promise high gravimetric and volumetric hydrogen storage densities, but considerable modification of their thermodynamic and kinetic properties will be required in order to make them feasible for on-vehicle applications. Catalyst additions to achieve fast hydrogen cycling kinetics have been studied for more than a decade. More recently, the concept of nanoconfinement has been explored as a means to improve kinetics, using melt infusion or solvent infusion to embed the hydride into nanoscale pores within a solid. We have achieved enhanced kinetic performance and reversibility of $NaAlH_4$ incorporated into nanoporous carbon aerogel by melt infusion, even in the absence of a catalyst. In fact, hydrogen cycling of uncatalyzed $NaAlH_4$ in aerogel is almost as good as unconfined $NaAlH_4$ catalyzed by addition of $TiCl_3$. It remains challenging, however, to obtain $NaAlH_4$-carbon aerogel infusions with high hydride loading and/or co-incorporated catalyst. We have therefore investigated combining $NaAlH_4$ with carbon aerogel and nanoporous activated carbon by ball milling. The kinetic performance is similar to that of melt-infused $NaAlH_4$ at the same loading, and importantly, higher $NaAlH_4$ loading can be easily achieved with only modest loss of kinetics. Furthermore, $TiCl_3$ catalyst can be easily co-incorporated. In the latter case, a small but significant improvement over $TiCl_3$-catalyzed $NaAlH_4$ without carbon is observed.

8:36AM P20.00002 Hydrogen release reactions in the {H,Li,B,Na,Al} system , ERIC DHALL, Graduate Student, VIDVUDS OZOLINS, Professor — A thermodynamic investigation of the {H,Li,B,Na,Al} system for new solid state hydrogen storage reactions is performed using first-principles DFT calculations and the the grand-canonical linear programming approach (Akbarzadeh, et al. Adv. Mater. 2007, 19, 3233). We report the static, zero-point, and T $>$ 0 K vibrational energies of all known compounds in this system. Enthalpies, entropies, and hydrogen release temperatures are calculated for all thermodynamically reversible dehydrogenation reactions occurring from 0-1000K. Several novel mixtures of reactants with high gravimetric hydrogen storage densities are found using the calculated {H,Li,B,Na,Al} phase diagrams.

8:48AM P20.00003 First-principles investigations of the quaternary Li-Zn-B-H hydrogen storage system , YONGLI WANG, CHRIS WOLVERTON, Northwestern University — Mixed metal borohydride hydrogen storage materials are a new class of materials which may possess better thermodynamic and kinetic properties than their separate phases. $LiBH_4$ has an undesirably high H_2 desorption temperature, while $Zn(BH_4)_2$ has a lower desorption temperature, but releases B_2H_6 upon desorption. We have used density functional theory, as well as Monte Carlo-based crystal structure prediction tools and phase diagram computational methods to explore the stability and decomposition reactions of mixed Li and Zn borohydrides to ascertain whether they possesses an intermediate decomposition temperature. Based on a combination of classical potentials, Monte Carlo optimization, and DFT calculations, we search for low-energy quarternary borohydrides as a function of the Li/Zn context. We find that this system has compounds that are lower in energy than the isolated borohydrides. In agreement with prior work, we confirm the existence of a $LiZn(BH_4)_3$ compound, which as yet has been unobserved. We find that this new mixed compound $LiZn(BH_4)_3$ decomposes via an initial decomposition of $Zn(BH_4)_2$, and a subsequent decomposition of $LiBH_4$. This sequential decomposition is favored due to the lack of stable intermediate products which involve both Li and Zn. Using this framework, we are searching for stable mixed metal borohydrides in a wide variety of other systems.

9:00AM P20.00004 First-principles studies of intermediate products in the decomposition of metal amidoboranes , YONGSHENG ZHANG, Department of Materials Science & Engineering, Northwestern University, TOM AUTREY, Pacific Northwest National Laboratory, CHRIS WOLVERTON, Department of Materials Science & Engineering, Northwestern University — Metal amidoboranes [MAB, M=metal cation] form an interesting class of recently-discovered hydrogen storage compounds. However, the decomposition products remain largely unknown. Armed with the combination of the prototype electrostatic ground state search and density-functional theory methodology (PEGS+DFT), we have searched for crystal structures of possible reaction products with $[NHBH_2]^-$, $[NBH]^-$, $[NBH_5]^-$, polymer-$[NHBH_2]$ anion groups in the decomposition of LiAB and CaAB. All these reaction pathways are significantly endothermic, which is in disagreement with the experimentally measured enthalpies in these systems, which are found to be nearly thermoneutral [$-3 \sim -5$ kJ/(mol H_2) in LiAB and 3.5 kJ/(mol H_2) in CaAB]. Using newly developed dianion group $[NHBHNHBH_3]^{2-}$, our PEGS+DFT methodology predicts structures and energies of Li/Ca-dianion compounds. Including vibrational thermodynamics and zero-point effects, we successfully obtain a nearly thermoneutral enthalpy of decomposition into these dianion compounds. This agreement lends strong support to the dianion phases as energetically preferred products in the decomposition of metal amidoboranes.

9:12AM P20.00005 Theoretical study of the vibrational properties of $\mathrm{NaAlH_4}$ with $\mathrm{AlH_3}$ vacancies , MEI-YIN CHOU, FENG ZHANG, YAN WANG, School of Physics, Georgia Institute of Technology — We investigate from first-principles calculations the vibrational properties in the presence of the $\mathrm{AlH_3}$ vacancy in both α and γ phases of $\mathrm{NaAlH_4}$. When $\mathrm{AlH_3}$ is removed from an $\mathrm{AlH_4^-}$ anion, the remaining H recombines with another neighboring $\mathrm{AlH_4^-}$ anion and forms an $\mathrm{AlH_5^{2-}}$ unit with slightly deformed D_{3h} symmetry. For both α- and γ-$\mathrm{NaAlH_4}$, the $\mathrm{AlH_3}$ vacancy induces several isolated phonon modes that are highly localized on the $\mathrm{AlH_5^{2-}}$ unit with frequencies within the band gap separating the Al-H stretching modes and Al-H bending modes in pure $\mathrm{NaAlH_4}$. Similar localized phonon modes also exist in the gap separating the Al-H bending modes and the modes involving the rotation of $\mathrm{AlH_4^-}$ anions for the γ phase. On the other hand, for both α and γ phases of $\mathrm{NaAlH_4}$ with charged $\mathrm{AlH_4^-}$ vacancies, no isolated phonon modes were found to be localized in the vacancy region with frequencies within the band gap of the pure crystal. These theoretical findings suggest further experimental studies to identify the defects that are involved in the decomposition of $\mathrm{NaAlH_4}$.

9:24AM P20.00006 Hexagonal Antiprismatic Metallacarborane Clusters for Hydrogen Storage , CÜNEYT BERKDEMIR, PING LIN, JORGE SOFO, Penn State — We investigated the adsorption properties of molecular hydrogen attached to hexagonal antiprismatic metallacarborane clusters, $RuNiC_2B_{10}H_{12}$ and $Ru_2C_2B_{10}H_{12}$, using density functional theory. These clusters have been recently synthesized using the reduction-metallation (RedMet) approach [1] and their structures have been resolved. The hydrogen molecules are sequentially attached to these clusters until the H_2 binding energies fall below 0.2 eV, which is the minimum value of ideal H_2 binding energy in the range of 0.2-0.4 eV/H_2 for the practical vehicle applications [2]. We included the van der Waals interactions between metallacarborane clusters and molecular hydrogens. We also evaluated the contribution of zero point vibrational energies to the H_2 binding energy. The kinetic stability of these clusters before and after hydrogen adsorption is discussed by analyzing the energy gap. The results show that $RuNiC_2B_{10}H_{12}$ and $Ru_2C_2B_{10}H_{12}$ clusters can bind up to 8.5 wt % and 9.8 wt % molecular hydrogen, respectively. These results suggest that these metallacarborane clusters are potential hydrogen storage materials to meet the targets of DOE for 2015.

[1] D. Ellis et al., Chem. Commu. **14**, 1917 (2005).
[2] http://www.sc.doe.gov/bes/hydrogen.pdf.

9:36AM P20.00007 Diffusion-limited Kinetic Pathway for Hydrogen Release from $\mathrm{LiNH_2/LiH}$, BILJANA ROLIH, VIDVUDS OZOLINS, UCLA — From experimental work on decomposition of hydrogen storage materials it has been suggested that bulk diffusion of metal species is the bottleneck for hydrogen release. In this work we study the underlying mechanism for diffusion reactions in the dehydrogenation of $LiNH_2$. Using first-principle, density functional theory methods we have calculated concentration gradients and diffusivities of neutral and charged defects in $LiNH_2$ and Li_2NH phases. The overall activation energy is obtained from these calculations. The calculated activation energies are found to agree well with experimental work on the kinetics of $LiNH_2$ decomposition, suggesting that diffusion of metal species is a possible method for dehydrogenation of Lithium Amide.

9:48AM P20.00008 Reaction Pathways in the Reactive Composite $\mathrm{Mg(NH_2)_2 + LiH}$, DENIZ CAKIR, University of Twente, GILLES A. DE WIJS, Radboud University Nijmegen, GEERT BROCKS — Chen *et al* [1] reported reversible hydrogen storage in a mixture of LiH + $LiNH_2$ with a storage capacity of 6.5 wt %. However, this system requires an operating temperature in excess of 250 C to achieve a hydrogen pressure of 1 bar. Several efforts including cation substitution have been considered in order to improve the operating conditions, which is necessary for onboard applications. For instance, replacing LiH with MgH_2 markedly reduces the operating temperature through the reaction $MgH_2 + 2LiNH_2 \rightarrow Li_2Mg(NH)_2 + 2H_2 \leftrightarrow Mg(NH_2)_2 + 2LiH$. Recent experimental results however indicate that the latter is not a simple one-step reaction and full hydrogenation of $Li_2Mg(NH)_2$ occurs in a two-step sequence via an intermediate $Li_2Mg_2(NH)_3$ [2]. In this work we examine the stability and structure of possible intermediates compounds, namely $Li_{2-2x}Mg_xNH$, $Li_{1-2x}Mg_xNH_2$, and $Li_{2-x}Mg(NH)_{2-x}(NH_2)_x$, by means of first-principles DFT calculations. All intermediate compounds are thermodynamically stable with respect to the elements. The hydrogenation reaction of $Li_2Mg(NH)_2$ via the intermediate imides $Li_{2-2x}Mg_xNH$ is energetically favorable compared to other intermediates.
Ref : [1] Nature **420**, 302 (2002). [2] J. Phys. Chem. C **113**, 15772 (2009).

10:00AM P20.00009 First-Principles Study of Native Defects in $\mathrm{Li_4BN_3H_{10}}$ Under Varied Chemical Conditions , DAVID FARRELL, CHRISTOPHER WOLVERTON, Northwestern University — Hydrogen desorption from many complex hydrides, such as $Li_4BN_3H_{10}$, is known to be kinetically limited. At temperatures below melting, the motion of point defects is one possible factor affecting chemical reactions. Therefore, an understanding of their formation and migration will yield insight into the kinetic limitation of hydrogen desorption. To explore this, we have determined the 0 K formation energy for a number of neutral and charged point defects in $Li_4BN_3H_{10}$ under a variety of chemical conditions via density functional theory calculations. We determined chemical potentials based on thermodynamically predicted hydrogen desorption reactions and provide a physical interpretation of the resulting equilibrium conditions. Our results indicate that: 1) The lowest energy defect varies with chemical conditions. 2) neutral defects are always lower energy than analogous pairs of oppositely charged defects. 3) Hydrogen defects are rarely the lowest energy defect.

10:12AM P20.00010 First-principles Modeling of Diffusion Reactions in the Hydrogenation of $\mathrm{NaAlH_4}$, KYLE MICHEL, VIDVUDS OZOLINS, University of California, Los Angeles — The hydrogenation of $NaAlH_4$ has been studied extensively since it was discovered that doping with Ti greatly increases its reversible hydrogen storage capacity. Experimental studies have suggested that diffusion of metal-containing defects may be the rate-limiting step in this reaction. We present a model to study the diffusion of defects during a solid-state reaction and apply it to this hydrogen storage reaction. The flux of defects in simple, model systems is calculated and from these values the activation energy for these processes is determined. We find that the activation energy for the diffusion of metal defects matches well to the experimental activation energy for the reaction when doped with Ti. The model that is presented can easily be applied to other systems in which a reaction takes place in the solid state.

10:24AM P20.00011 Catalytic effect of carbon nanomaterials on light metal hydride systems , ZHAO QIAN, RAJEEV AHUJA, Cond. Mat. Theory Group, Dept of Physics and Astronomy, Uppsala Univ; Dept of Mat. Sci. and Eng., Royal Inst. of Tech. (KTH), Stockholm, Sweden, C. MOYSES ARAUJO, ANDREAS BLOMQVIST, BISWARUP PATHAK, RALPH H. SCHEICHER, CMT Group, Uppsala University — Carbon nanomaterials are becoming recognized for their use in catalyzing hydrogen desorption from light metal hydride systems, in particular complex borohydrides and alanates. For example, it was shown by us that graphene, carbon nanotubes, and especially fullerenes can improve the hydrogen sorption properties of sodium alanate [Nano Lett. 9, 1501 (2009)]. In parallel to ongoing experimental investigations, we have carried out further theoretical studies in order to better understand the underlying catalyzing mechanism. Our most recent work is concentrated on the interaction of lithium borohydride with fullerene where a complete dehydrogenation process was simulated using the cluster approach. Furthermore, the catalytic effect of graphene nanofibres on sodium alanate has been experimentally demonstrated by our collaborators, and we have studied this system from first principles as well, to better understand the origin of its catalytic effect.

10:36AM P20.00012 Adsorbed Natural Gas Storage in Optimized High Surface Area Microporous Carbon , JIMMY ROMANOS, TYLER RASH, ERIK NORDWALD, JOSHUA SHAWN SHOCKLEE, CARLOS WEXLER, PETER PFEIFER, University of Missouri — Adsorbed natural gas (ANG) is an attractive alternative technology to compressed natural gas (CNG) or liquefied natural gas (LNG) for the efficient storage of natural gas, in particular for vehicular applications. In adsorbants engineered to have pores of a few molecular diameters, a strong van der Walls force allows reversible physisorption of methane at low pressures and room temperature. Activated carbons were optimized for storage by varying KOH:C ratio and activation temperature. We also consider the effect of mechanical compression of powders to further enhance the volumetric storage capacity. We will present standard porous material characterization (BET surface area and pore-size distribution from subcritical N_2 adsorption) and methane isotherms up to 250 bar at 293K. At sufficiently high pressure, specific surface area, methane binding energy and film density can be extracted from supercritical methane adsorption isotherms. Research supported by the California Energy Commission (500-08-022).

10:48AM P20.00013 On the reversibility of the adsorption of methane-mercaptan for natural gas storage[1] , M. GOLEBIOWSKA, U. Missouri, L. FIRLEJ, U. Montpellier 2, B. KUCHTA, U. Provence, M. ROTH, U. N. Iowa, C. WEXLER, U. Missouri — Methane is the main constituent of natural gas (NG). As fuel for vehicular applications NG requires sorbents that allow efficient, reversible and safe storage at room temperature and moderate pressure. To enable easy human detection of gas leaks the fuel gas should be added with compounds having low odor threshold, such as thiols (mercaptans). Thus a full understanding of the behavior of methane-mercaptan mixtures is necessary for the development of safe storage systems. In this talk we present results of molecular dynamics simulations in the temperature range 150–350 K and for a large range of methane partial pressures, up to the saturation pressure of methane. We observe the presence of 2D (and to a lesser degree 3D) diffusion of the thiols indicating that though thiols adsorb preferentially relative to methane, the adsorption is still reversible. We estimate that only a small increase in mercaptan concentration is necessary for the desorbed phase to be above the threshold for human detection.

[1]This work is supported by the California Energy Commission, Contract No. 500-08-022.

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P21 GIMS: Focus Session: Advances in Scanned Probe Microscopy III - Novel SPM of Spin, Force & Conductance D161

8:00AM P21.00001 A New Ultra-Low Temperature, High Magnetic Field STM in an Ultra-Quiet Laboratory , BRIAN B. ZHOU, SHASHANK MISRA, LUKAS URBAN, JUNGPIL SEO, ANDRAS GYENIS, Princeton University, SEJONG KAHNG, Korea University, ALI YAZDANI, Princeton University — We report progress in the construction of a new UHV STM capable of operating at the extremes of temperature (25 mK) and magnetic field (14 T), allowing atomically resolved studies in previously unexplored areas of phase space. Our novel design is based on a bottom-loading dilution refrigerator in which the entire dilution stage and mounted microscope are moved between measurement and sample transfer positions. Pumping for the dilution fridge and large magnetic fields introduce demanding challenges in vibration isolation, which we have addressed with an ultra-quiet laboratory setting and rigid microscope design. Our system is situated inside both acoustic and RF-shielded enclosures in complement with various stages of isolation for both pump and ambient vibration sources. We will discuss unique aspects of the microscope design, such as a two-in-one double sample holder, and assess preliminary system performance. Supported by the W. M. Keck Foundation. Infrastructure at Princeton Nanoscale Microscopy Laboratory is also supported by grants from DOE, NSF, and ARO.

8:12AM P21.00002 Low Temperature Scanning Tunneling Microscope for Spin Polarization Measurements[1] , SEONG HEON KIM, RYAN JAEHNE, LEUJEN CHEN, ALEX DE LOZANNE, Department of Physics, University of Texas at Austin — We describe a new design for a 4K scanning tunneling microscope (STM) with an 8 tesla superconducting magnet to be used for spin polarized measurements. The novel aspects include a compact design for the chamber and the STM, the use of a secondary STM for in-situ tip characterization, and new ideas for vibration isolation. We developed a new STM head unit with 1 inch diameter and 3.2 inch length. This microscope is small enough to be installed within the small space available in the 2 inch diameter bore of our superconducting magnet. To achieve this small size, we modified the typical Pan-type z-approach walker. We also developed new simple and inexpensive electronics to control any stick-slip walker.

[1]Supported by NSF DMR-0923231

8:24AM P21.00003 Compact probe design for Scanning Hall Probe Microscopy[1] , NELIZA LEON-BRITO, SEONGSOO KWEON[2], ALEX DE LOZANNE, Texas Materials Insitute, The University of Texas at Austin — In the search for new materials with desirable magnetic properties for applications such as spintronics the study of magnetic properties at the micro and nanoscale is necessary. Magnetic Force Microscopy (MFM) has been the technique of choice for these types of studies, but its invasive nature makes it unsuitable for low coercivity materials like diluted magnetic semiconductors. Scanning Hall Probe Microscopy (SHPM) is an alternative technique which provides a magnetically non-invasive, calibrated measurement of the stray fields above the sample with good resolution ($\sim$1um). We have built a compact cryogenic variable-temperature (4 - 300K) SHPM with unique features such as an inverted tapered seal that also performs as a heat sink for the microscope body and a new coarse approach mechanism. Details of this design will be presented in this talk.

[1]Supported by NSF-DMR and NSF-IGERT.

[2]Currently at Dongbu Hi-Tec, Korea

8:36AM P21.00004 Realizing Spin Logic Atom by Atom[1] , ALEXANDER KHAJETOORIANS, Institute of Applied Physics, Hamburg University — Scanning tunneling microscopy (STM) has emerged as a leading technique which can address single atom magnetism with high energy and spatial resolution. With the development of sub-Kelvin high-magnetic field STM, two complementary methods, namely spin-polarized scanning tunneling spectroscopy (SP-STS) and inelastic STS (ISTS), can address the fundamental properties of individual magnetic impurities at surfaces [1,2]. We use a map of the distance-dependent RKKY interaction between Fe atoms on Cu(111) obtained by SP-STS to engineer complex magnetic nanostructures with tailored magnetic properties with atomic manipulation. By combining constructed anti-ferromagnetic structures with spin frustration, we realize an atomic-scale logic device which functions solely on the spin-degrees of freedom of its magnetic constituents. This work was done in collaboration with J. Wiebe, S. Lounis, B. Chilian, A. T. Costa, L. Zhou, D. L. Mills, and R. Wiesendanger.

[1] A. A. Khajetoorians, B. Chilian, J. Wiebe, S. Schuwalow, F. Lechermann, and R. Wiesendanger, Nature 467, 1084 (2010).
[2] A. A. Khajetoorians, S. Lounis, B. Chilian, A. T. Costa, L. Zhou, D. Mills, J. Wiebe, and R. Wiesendanger, arXiv:1010.1284v2 (2010).

[1]We acknowledge funding from SFB668-A1 and GrK1286 of the DFG, from the ERC Advanced Grant "FURORE", and from the Cluster of Excellence "Nanospintronics."

9:12AM P21.00005 Visualizing spin-dependent scattering in strong spin-orbit systems , ANNA STROZECKA, Institute of Experimental Physics, Free University Berlin, Germany, ASIER EIGUREN, Dpto. Fisica de la Materia Condensada, Universidad del Pais Vasco, Bilbao, Spain, JOSE IGNACIO PASCUAL, Institute of Experimental Physics, Free University Berlin, Germany — For surfaces which exhibit spin-orbit coupling, electrons originating from spin polarized surface bands are protected against backscattering by time reversal symmetry. Electron interference patterns observed in STM confirm the chiral spin texture of the surface Fermi contours of such materials and reveal the dominant role of spin in the scattering processes. Using a combined experimental and theoretical approach, we distinguish the role of spin in the electron scattering processes on Bi(110). Utilizing spectroscopic imaging of the local density of states, we studied the energy dependence of the interference patterns formed around single adsorbates. Simulations based on Green's functions correctly reproduce the interference patterns, unveiling the role of spin in the interference process and allowing identification of the dominant scattering events.

9:24AM P21.00006 Cotunneling theory for STM spin-flip spectroscopy , F. DELGADO, J. FERNANDEZ-ROSSIER, Departamento de Fisica Aplicada, Universidad de Alicante, San Vicente del Raspeig, 03690 Spain — Scanning Tunneling Spectroscopy of both magnetic atoms and molecules adsorbed on surfaces is analyzed from the theoretical point of view. We show that cotunneling is the leading mechanism that explains the spin assisted inelastic conductance reported in recent experiments [1-4]. We describe the electronic transport between the scanning tip and the conducting surface through the magnetic system (MS) with a generalized Anderson model. The correlations in the MS are calculated exactly and transport is considered to fourth order in the tip-MS and MS-surface coupling. Our theory accounts for the observed [2,4] asymmetric conductance and provides an explanation of the large inelastic contribution.

[1] A. J. Heinrich et. al, Science 306, 466 (2004)
[2] Xi Chen, et al, Phys. Rev. Lett. 101, 197208 (2008)
[3] A. A. Khajetoorians et al, Nature 467, 1084 (2010)
[4] X. Chen et al, Phys. Rev. Lett. 101, 197208 (2008)

9:36AM P21.00007 Analysis of Tunneling Spectra in Constant-Current Distance-Voltage Mode , DANIEL DOUGHERTY, ALEX PRONSCHINSKE, DANIEL MARDIT, Department of Physics North Carolina State University — A technical challenge associated with the use of traditional constant height tunneling spectroscopy in current-voltage mode is that tunneling current increases very rapidly at even modest voltages. This can result in tip-induced damage or motion for soft or delicate materials like organic molecules. One solution to this problem is to measure tunneling spectra in constant current distance-voltage mode where the STM feedback loop maintains a constant small tunneling current. Using the standard integral expression for tunneling current with a WKB transmission function, it is possible to create a first order differential equation connecting distance-voltage spectra with sample density of electronic states. This can be used to experimentally extract density of states or to theoretically predict distance-voltage tunneling spectra from a known density of states. We illustrate the use of this approach with numerical and experimental examples.

9:48AM P21.00008 Quantitative force measurements with intermodulation atomic force microscopy , DANIEL PLATZ, DANIEL FORCHHEIMER, CARSTEN HUTTER, ERIK THOLÉN, DAVID HAVILAND, Royal Institute of Technology (KTH), Stockholm, Sweden — Dynamic atomic force microscopy (dynamic AFM) is a key tool for surface characterization on the nanoscale. Operation close to a cantilever resonance increases sensitivity and allows for the measurement of the phase of the cantilever response. This phase is traditionally interpreted as a measure of the energy dissipation due to the tip-sample interaction. However, a full understanding of dissipative processes remains a challenge in dynamic AFM. To address this problem we have developed Intermodulation AFM. With this multi-frequency technique we can tremendously increase the number of information carrying signals close to resonance. Using Fourier analysis and linear algebra we combine the amplitudes and phases of these signals to separately reconstruct the conservative and non-conservative tip-sample interactions. We have tested this method both on simulated and on experimental data. The method works at one tip-surface separation, providing quantitative high resolution maps of surface properties while imaging at normal rates.

10:00AM P21.00009 Nano-scale Strain Mapping using Near-field Microscopy , ANTONIO LLOPIS, ARKADII KROKHIN, University of North Texas, SERGIO PEREIRA, CICECO, University of Aveiro, IAN WATSON, University of Strathclyde, ARUP NEOGI, University of North Texas — Advances in nanophotonics are beginning to allow for the creation of nano-scale light emitting devices. Improving the quality of these next-generation emitters requires similarly advanced methods for characterization. These techniques need to be capable of imaging operational prototypes with nanometric resolution. We demonstrate here a new method for mapping strain capable of meeting the demands of next-generation device characterization. This technique makes use of near-field spectroscopy along with theoretical modelling to achieve non-destructive strain mapping with a resolution on the order of 10-100nm. An InGaN ELOG MQW sample is mapped using a SNOM, producing near-field maps of the intensity and Huang-Rhys parameter. Theoretical calculations are then used to obtain the relation between the Huang-Rhys parameter and the biaxial strain ε_{xx}, thereby allowing the production of a near-field map of the biaxial strain in the sample. Finally, to verify the efficacy of the method, we compare the results with those obtained using high-resolution XRD.

10:12AM P21.00010 Non-linear optical nano-structured probe for photonic force microscopy , ASWINI KANNEGANTI, HARSHIT VALLABH, NINAD INGLE, UT Arlington, XIAO ZHANG, JING LI, Rutgers Univ., SAMARENDRA MOHANTY, UT Arlington — Use of second-harmonic (SH) optical probes for imaging of microscopic samples has distinct advantages over fluorescence, which suffers from photobleaching. Further, SH nanoparticles can be optically trapped for probing interaction forces and even for topographic imaging of nanostructures. Here, we report SH generation in $ZnS(pda)_{1/2}$ (pda = propanediamine), a new class of nanostructured crystals. $ZnS(pda)_{1/2}$ is an isostructure of $ZnTe(pda)_{1/2}$ as confirmed by PXRD pattern. The SHG imaging of the nanocrystals was carried out by an ultrafast (∼100fs) Ti: Sapphire laser beam (wavelength: 960 nm; repetition rate: 80 MHz) focused to a diffraction limited spot by use of a 100X microscope objective leading to very high peak power density. Dependence of SHG intensity as a function of laser power and axial position of the nanoparticle in the focused laser microbeam was quantitated for the purpose of photonic force microscopy. The suspended $ZnS(pda)_{1/2}$ nanocrystals could be trapped using the near-IR Ti: Sapphire laser microbeam. The SHG intensity was found to fall very rapidly as the nanocrystal is displaced from the focused spot, which led to highly sensitive height measurements. Non-linear optical characterization of the $ZnS(pda)_{1/2}$ nanocrystals and its use in photonic force microscopic imaging will be presented.

10:24AM P21.00011 Design of a scanning gate microscope in a cryogen-free dilution refrigerator , MATTHEW PELLICCIONE, ADAM SCIAMBI, DAVID GOLDHABER-GORDON, Stanford University — We report on our design of an ultra-low temperature scanning gate microscope housed in a system with no liquid helium bath. The recent increase in efficiency of pulse-tube cryocoolers and pending scarcity of liquid helium have made "cryogen-free" dewars popular in recent years. However, this new style of dewar presents challenges for performing scanning measurements, most notably the increased vibrations introduced by the cryocooler. We will highlight the tradeoffs made in choosing such a system to house a scanner, and describe our efforts to achieve a stability suitable for measurements on mesoscopic systems.

10:36AM P21.00012 Electronic characterization of 1-D defects using scanning gate spectroscopy , STEVEN R. HUNT, Department of Physics and Astronomy, Univ. of California at Irvine, Irvine, CA 92697-4576, BRAD L. CORSO, PHILIP G. COLLINS — Scanning gate microscopy (SGM) is a technique particularly useful for characterizing transport in electronic devices. We have extended the SGM technique into a spectroscopy by measuring the entire bias dependence of conductance at every position on a surface. Much as in current imaging tunneling spectroscopy (CITS), the resulting data set is a multidimensional, detailed map of the electronic behavior of a surface. We apply this scanning gate spectroscopy (SGS) technique to scattering in one-dimensional, carbon nanotube circuits. Transport in one-dimensional systems depends critically on inhomogeneities, including isolated point defects. The SGS technique enables straightforward investigation of low-dimensional transport physics at such sites. In our experiments, metallic single-walled carbon nanotubes are investigated before and after the electrochemical introduction of a point defect, in order to clearly establish the contribution of different defect types. SGS directly images the energy dependence of a defect's scattering, providing a way to distinguish between different defect chemistries and quantitatively model its energy levels and transmission. This research is partly supported by the NSF (DMR-0801271).

10:48AM P21.00013 Scanning gate transconductance microscopy and spectroscopy of a mesoscopic ring , BENOIT HACKENS, FREDERICO MARTINS, SEBASTIEN FANIEL, VINCENT BAYOT, Universite catholique de Louvain, Louvain-la-Neuve 1348, Belgium, MARCO PALA, MINATEC, Grenoble, France, HERMANN SELLIER, SERGE HUANT, CNRS and Institut Neel, Grenoble, France, LUDOVIC DESPLANQUE, XAVIER WALLART, IEMN, Villeneuve d'Ascq, France — In scanning gate microscopy (SGM), a dc voltage is applied to a sharp tip moving in the vicinity of a device. This alters the electrostatic potential seen by electrons inside the device, and consequently changes the device conductance [1]. Here, we superimpose a small ac voltage to the dc bias applied on the tip, and record the change of device conductance at the tip bias modulation frequency, i.e. the local transconductance. We first image the low temperature transconductance of a mesoscopic ring patterned in a two-dimensional electron system (2DES) hosted in an InGaAs/InAlAs heterostructure. The tranconductance images are decorated by concentric features that we associate with charging of electron traps located close to the 2DES. We perform spectroscopy of these traps by positioning the tip close to them, and recording the ring transconductance as a function of the tip dc voltage and the bias accross the quantum ring. We observe Coulomb diamonds in our spectroscopic data, which confirms that Coulomb blockade is at play. [1] B. Hackens et al., Nature Physics 2, 826 (2006).

Wednesday, March 23, 2011 8:00AM - 11:00AM –
Session P22 DCMP: Metal-Insulator Phase Transitions I D163

8:00AM P22.00001 Revisiting the Anderson Model with Power-Law Correlated Disorder in 1D and 2D[1] , GREG PETERSEN, NANCY SANDLER, The Ohio University — The dimensionality of a disordered system directly affects the critical energy where a localization/delocalization transition occurs. In non-interacting systems with uncorrelated disorder, it is widely known that all states in one-dimension are localized. However, for some correlations there exist transition energies similar to mobility edges or small subsets of extended states that are robust against disorder. In this talk, we will present results on the diffusion of a wavepacket in a power-law correlated random potential of the form $\langle V(r)V(0)\rangle = \frac{1}{(a+r)^\alpha}$. We also report results for the participation ratio $P_r = \frac{1}{N}\frac{\langle|a_i|^2\rangle^2}{\langle|a_i|^4\rangle}$. Preliminary results for 1D chains support the existence of a mobility edge near the band center. Square and graphene lattices will also be discussed.

[1]This work has been supported by the NSF-PIRE mwn/ciam and NSF Grant DMR-0710581.

8:12AM P22.00002 Higher order correction to the RG β-function for the 3-d Anderson localization transition at unitary symmetry , TOMOYUKI NAKAYAMA, KHANDKER MUTTALIB, University of Florida, PETER WÖLFLE, Karlsruhe Institute of Technology — We have recently calculated the β-function of the conductance for Anderson Metal-Insulator transition including contributions from the ballistic regime. In three dimensional unitary case, the result of two-loop order diagrams is β(g)=1-a/g, where a is a constant and g is the dimensionless conductance. However, this result is valid only if there is no diagram with extra diffusons which contributes to the order of 1/g. We show that diagrams with extra diffuson propagators only have higher order contributions in the ballistic regime, which confirms our previous result.

8:24AM P22.00003 Singular Behavior of Electronic Eigenstates in the Anderson Model of Localization[1] , SONIKA JOHRI, Department of Electrical Engineering, Princeton University, Princeton, NJ 08544, R.N. BHATT, Department of Electrical Engineering and Princeton Center for Theoretical Science, Princeton University, Princeton, NJ 08544 — We report the observation of a singularity in the electronic properties of the Anderson Model of Localization with diagonal disorder[2] which is clearly distinct from the well- established mobility edge (localization-delocalization transition)[3,4] that occurs in dimensions $d > 2$. We present results of numerical calculations for various disorder distributions in dimensions $d = 1$, 2 and 3, of different properties of the electronic wavefunctions to establish this, and to understand its evolution with disorder distribution, dimension and lattice type. Our data suggest that the model is richer than has been originally believed.

[1]This work was supported by Department of Energy Grant No. DE-SC20002140.

[2]P. W. Anderson, Physical Review **109**, 1492 (1958).

[3]E. Abrahams, P. W. Anderson, D. C. Licciardello and T. V. Ramakrishnan, Physical Review Letters **42**, 673 (1979).

[4]For a recent review on Anderson Localization, see Ferdinand Evers and Alexander D. Mirlin, Reviews of Modern Physics **80**, 1355 (2008).

8:36AM P22.00004 Temperature dependence of the zero-bias anomaly in the two-site Anderson-Hubbard model[1] , R. WORTIS, W.A. ATKINSON, Trent University — Experiments on disordered strongly correlated electron systems show zero-bias anomalies which are not consistent with either of the two prevailing pictures, by Altshuler and Aronov and by Efros and Shklovskii. Numerical work on the two-dimensional Anderson-Hubbard model shows a zero-bias anomaly with a number of unique features. It has recently been shown that a zero-bias anomaly with many of the same features occurs in an ensemble of two-site Anderson-Hubbard systems. The simplicity of this system allows direct understanding of the mechanism of the anomaly. Here, the temperature dependence of this anomaly is explored. A novel feature is the existence of a temperature driven zero-bias anomaly which appears even in the atomic limit and augments the kinetic energy driven one in the presence of hopping.

[1]Research supported by the National Science and Engineering Research Council (NSERC) of Canada.

8:48AM P22.00005 Theoretical perspective on nearly frozen coulomb liquids , HANNA TERLETSKA, YOHANES PRAMUDYA, SERGEY PANKOV, EFSTRATIOS MANOUSAKIS, VLADIMIR DOBROSAVLJEVIC, Department of Physics and NHMFL, Florida State University — Various studies on systems with charge ordered states, such as Wigner crystal, show their extreme fragility resulting from strong frustrations caused by long-range Colulomb-like interactions. Here, a so-called nearly-frozen Coulomb liquid regime is identified featuring a soft Coulomb pseudo-gap with unconventional insulating-like transport. Despite intensive studies, such pseudo-gap regime is still poorly understood. By employing extended dynamical mean field theory (EDMFT) [1] to study a semi-classical lattice gas model of spinless electrons, we successfully demonstrate the existence of such an intermediate liquid regime, and show that the pseudo-gap is, in fact, a general feature for models with long-range interactions. Our analytical results are well supported by exact Monte Carlo calculations. Moreover, we show that standard theories, like self-consistent Gaussian approximation ("spherical model") and RPA, are ill-suited to describe this interesting regime. The spherical model approach provides the same as EDMFT freezing temperature Tc, but fails to capture the pseudo-gap feature. RPA, however, not only overestimates Tc, but also completely misses the pseudo-gap regime.
[1] S. Pankov and V. Dobrosavljevic, Phys. Rev. Lett. **94**, 046402 (2005).

9:00AM P22.00006 Bound states in the continuum in a multi-electron system[1] , RAHUL HARDIKAR, GONZALO ORDONEZ, Butler University — Bound states in a continuum (BIC) occur due to quantum interference of two identical adatoms in a one-dimensional (1D) band. In the past such states have been studied for a one- electron system using several analytical and theoretical methods. We extend the idea of BIC to a multi-electron system. To study this numerically we use the pure Hubbard hamiltoninan and add impurity sites at specific locations. Using this variant of the Hubbard model and an exact diagonalization method we prove that BIC can exist for multi-electron systems. We will also show theoretical proof of such states using the Bethe-Ansatz method

[1]Holcomb Awards Committee - Butler University

9:12AM P22.00007 Spectral functions across the Metal-Insulator transition in the disordered 2D Hubbard model[1] , KARIM BOUADIM, NGANBA MEETEI, YEN LEE LOH, NANDINI TRIVEDI, Ohio State University — We study the metal-insulator transition in the repulsive disordered 2D Hubbard model [1,2] using Determinant Quantum Monte Carlo (DQMC). We calculate the spin-spin and current-current correlations to learn about the nature of the conducting and insulating phases. We also obtain local spin-dependent spectroscopic properties, using the maximum entropy method, to understand the role of disorder on the transition in this highly correlated fermion system. We discuss implications of our results for scanning tunneling spectroscopy and dynamical conductivity experiments [3].

[1]. P.J.H Denteneer, R.T. Scalettar and N. Trivedi, Phys. Rev. Lett.83, 4610 (1999).
[2]. D. Heidarian and N. Trivedi, Phys. Rev. Lett. 93, 126401 (2004).
[3]. M.M. Qazilbash et. al., Science 318, 1750 (2007).

[1]Supported by DOE Grant No. DE-FG02-07ER46423 and NSF Grant No. DMR-0907275. We acknowledge computational support from Ohio Supercomputing Center.

9:24AM P22.00008 Time-Correlated Soliton Tunneling in Density Waves , JOHN H. MILLER, ASANGA IROSHAN WIJESINGHE, ZHONGJIA TANG, ARNOLD M. GULOY, University of Houston — In the quantum sine-Gordon model of a pinned charge or spin density wave, the electrostatic energy generated by charged soliton domain walls leads to a Coulomb blockade threshold electric field for quantum soliton-antisoliton pair creation. This field can be much smaller than the classical depinning field, since the quantum instability occurs as soon as the formerly lowest energy potential well rises to become a metastable well, or "false vacuum." The analogy to time-correlated single electron tunneling and comparison to recent experimental results, as well as broader implications of the proposed tunneling process, are briefly discussed. This work was supported by the State of Texas though the Texas Center for Superconductivity at the University of Houston and the Norman Hackerman Advanced Research Program, and by NIH R21CA133153 and ARRA supplement 3R21CA133153-03S, and by the Robert A. Welch Foundation, and DoE Basic Energy Sciences.

9:36AM P22.00009 Level spacing statistics for quantum k-core percolation , L. CAO, J.M. SCHWARZ, Syracuse University — Quantum percolation is the study of hopping transport of a quantum particle on randomly diluted percolation clusters. Quantum k-core percolation is the study of quantum transport on k- core percolation clusters where each occupied bond must have at least k occupied neighboring bonds. Within the random phase approximation, we found a random first-order phase transition for the k-core conduction transition on the Bethe lattice, and p_q, the quantum percolation critical probability, is equal to p_c, the geometric percolation critical probability [Phys. Rev. B **82**,104211 (2010)]. To further test this result, we numerically compute the level spacing distribution as a function of occupation probability p and system size. The simulation results provide confirmation for the existence of a discontinuous onset of quantum conduction at $p_q = p_c$.

9:48AM P22.00010 The onset of superfluidity of hardcore bosons in disordered ladders , JUAN CARRASQUILLA, FEDERICO BECCA, MICHELE FABRIZIO, International School for Advanced Studies, Trieste — The effect of disorder on the zero-temperature phase diagram of a two-leg ladder of hardcore bosons is investigated using quantum Monte Carlo simulations. We first review some aspects of the clean system which are relevant for the understanding of the disordered case. In the disordered case, an intervening Bose-glass phase between the frozen Mott insulator with zero (or one) bosons per site and the superfluid phase is found. We also investigate the effect of disorder exactly at half filling, where for small values of disorder, there is a commensurate phase with a gap to all excitations, which is eventually destroyed for larger values of disorder. We argue that this phase is always surrounded by the so-called Bose glass and a direct transition from the superfluid is found only in the clean system. Finally, a phase diagram based on our numerical evidence is suggested.

10:00AM P22.00011 Global phase diagram of the spinless Falicov-Kimball model in $d = 3$: renormalization-group theory[1] , OZAN S. SARIYER, Koç University, MICHAEL HINCZEWSKI, University of Maryland, A. NIHAT BERKER, Sabanci University — The global phase diagram of the spinless Falicov-Kimball model in $d = 3$ spatial dimensions is obtained by renormalization-group theory [1]. This global phase diagram exhibits five distinct phases. Four of these phases are charge-ordered (CO) phases, in which the system forms two sublattices with different electron densities. The phase boundaries are second order, except for an intermediate interaction regime, where a first-order phase boundary between two CO phases occurs. The first-order phase boundary is delimited by special bicritical points. The cross-sections of the global phase diagram with respect to the chemical potentials of the localized and mobile electrons, at all representative interaction and hopping strengths, are calculated and exhibit three distinct topologies. The phase diagrams with respect to electron densities are also calculated.

[1] O.S. Sarıyer, M. Hinczewski, and A.N. Berker, arXiv:1002.1821v1 (2010).

[1]This research was supported by the Alexander von Humboldt Foundation, the Scientific and Technological Research Council of Turkey (TÜBITAK), and the Academy of Sciences of Turkey.

10:12AM P22.00012 Improved determination of the self-energy and vertex function in Strong-Coupling Continuous-time Quantum Monte Carlo , HARTMUT HAFERMANN, Centre de Physique Théorique, École Polytechnique, 91128 Palaiseau Cedex, France, KELLY R. PATTON, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803, PHILIPP WERNER, Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland — The continuous-time quantum Monte Carlo method based on the strong coupling expansion is an efficient and flexible tool for the solution of multiorbital Anderson impurity models. However it is known that it is difficult to accurately compute the intermediate and high-frequency behavior of measured quantities. This leads to large errors, in particular for the self-energy when computed from Dyson's equation. A similar problem occurs for the vertex function when computed directly from the two-particle Green function. We propose an improved way of measuring these quantities, based on higher-order impurity correlation functions. The method yields very accurate estimates for the self-energy and vertex function over the full frequency range. In the segment representation, the improved estimators can be accumulated at essentially no additional computational cost.

10:24AM P22.00013 Surface effects in doping a Mott insulator , REZA NOURAFKAN, FRANK MARSIGLIO, Department of Physics, University of Alberta, Edmonton, Alberta, Canada T6G 2G7 — The physics of doping a Mott insulator is investigated in the presence of a solid-vacuum interface. Using the embedding approach for dynamical mean field theory we show that approaching a Mott insulating phase from the metallic side, a dead layer forms at the surface of the solid, where quasiparticle amplitudes are exponentially suppressed. In particular, we have demonstrated that the reduction of the quasiparticle weight detected by surface sensitive photoemission experiments of a doped Mott insulator are caused by both charge transfer and enhanced correlation effects at the surface. The expected modification of the intra-layer hopping at the surface and inter-layer hopping between the surface and the subsurface layer amplifies the surface effects.

10:36AM P22.00014 The Role of the Van Hove Singularity in the Quantum Criticality of the Hubbard Model , SANDEEP PATHAK, K.-S. CHEN, SHUXIANG YANG, MARK JARRELL, JUANA MORENO, Louisiana State University — A quantum critical point, separating a non-Fermi liquid region from a Fermi liquid, exists in the phase diagram of the Hubbard model [Vidhyadhiraja *et. al*, Phys. Rev. Lett. **102**, 206407 (2009)]. This quantum critical point is characterized by a vanishing spectral weight and a van Hove singularity (vHS) in the dispersion that crosses the Fermi level. The real part of the critical particle-particle susceptibility exhibits a algebraic decay with temperature, which results in the imaginary part showing scaling at large frequencies. This algebraic decay leads to higher superconducting transition temperatures as compared to the BCS theory, where the pairing susceptibility decays only logarithmically. In this talk, we examine the role of the van Hove singularity in determining this critical behavior. We calculate the bare particle-particle susceptibility of a d-wave pair field for the standard two-dimensional tight binding dispersion and for a hypothetical quartic dispersion having "flatter" or "extended" singularities. We find that the standard logarithmic vHS cannot correctly describe the critical algebraic behavior and it is essential to have an extended vHS that displays an algebraic singularity. Thus, our results emphasize the possible role of the extended vHS in the unexpectedly higher T_c of cuprates.

10:48AM P22.00015 Numerical study of real-time quantum dynamics in spin-electron coupled system , WATARU KOSHIBAE, CMRG, RIKEN, Japan, NAOTO NAGAOSA, Dept. of Appl. Phys., Univ. of Tokyo, CMRG, RIKEN, CERG, RIKEN, Japan, NOBUO FURUKAWA, ERATO-MF, Aoyama-Gakuin Univ., Japan — The photo-induced metal-insulator transition is studied by the numerical simulation of real-time quantum dynamics of a double- exchange model. The spatial and temporal evolutions of the system during the transition have been revealed including (i) the threshold behavior with respect to the intensity and energy of light, (ii) multiplication of particle-hole (p-h) pairs by a p-h pair of high energy, and (iii) the space-time pattern formation such as (a) the stripe controlled by the polarization of light, (b) coexistence of metallic and insulating domains, and (c) dynamical spontaneous symmetry-breaking associated with the spin spiral formation imposed by the conservation of total spin for small energy-dissipation rates.

Wednesday, March 23, 2011 8:00AM - 10:36AM –
Session P23 DCMP: Superconductivity: Josephson Effects I D165

8:00AM P23.00001 Tunable terahertz emission from Bi2Sr2CaCu2O8 mesa devices[1] , TIMOTHY BENSEMAN, ULRICH WELP, WAI-KWONG KWOK, ALEXEI KOSHELEV, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, CIHAN KURTER, University of Maryland, LUTFI OZYUZER, Izmir Institute of Technology, Turkey, KAZUO KADOWAKI, TAKASHI YAMAMOTO, University of Tsukuba, Japan — The so-called "terahertz gap," covering frequencies from approximately 0.3 to 1.5 THz, is of particular interest for a number of scientific and security applications, although no bright sources of coherent radiation presently exist in this range. However, stacks of high-temperature superconducting intrinsic Josephson junctions are a promising candidate. [1] Here we discuss recent progress in improving the performance of these devices. In particular, we demonstrate that via control of bias voltage and operating temperature, the emission from an 80-μm wide $Bi_2Sr_2CaCu_2O_8$ mesa can be tuned continuously over a frequency range in excess of 10% in the vicinity of 0.5 THz. We find that as the emission frequency increases from 0.420 to 0.492 THz, the linewidth increases from $<$2.25 GHz (limited by instrument resolution) to $\sim$9 GHz.

[1] L. Ozyuzer et al., Science 318 (2007) 1291-1293.

[1]This work was supported by DOE-BES under Contract No. DE-AC02-06CH11357.

8:12AM P23.00002 The relationship between oscillation modes and single crystalline Bi2212 mesa structures[1] , T. KASHIWAGI, K. DEGUCHI, M. TSUJIMOTO, N. ORITA, T. KOIKE, R. NAKAYAMA, K. DELFANAZARI, H. MINAMI, T. YAMAMOTO, K. KADOWAKI, University of Tsukuba, CREST-JST, WPI-MANA — Continuous electromagnetic (EM) radiation in terahertz region has been observed from a rectangular mesa structure of $Bi_2Sr_2CaCu_2O_{8+\delta}$(Bi2212) single crystals.[2] It has been established that the radiation frequency is determined by both ac Josephson effect and geometrical cavity resonance condition.[3] The observed radiation frequencies in the many rectangular mesas studied were inversely proportional to the width of the mesa and the fundamental modes equal to twice the mesa width. Recently, several mesas show different radiation characteristics which suggest the existence of the higher excitation modes such as one wave length excitation mode. The observed frequencies from above mesas are almost explained by the geometrical cavity model. In order to clarify the detail of the excitation modes, we also measured the radiation pattern of EM waves.

[1]This work was supported by CREST-JST and WPI-MANA project (NIMS). This work is in part performed in collaboration with Dr. Wai Kwok and his group in Argonne National Lab.

[2]L. Ozyuzer *et al.*, Science **318** (2007) 1291.

[3]K. Kadowaki *et al.*, J. Phys. Soc. Jpn. **79** (2010) 023703

8:24AM P23.00003 Coherent THz-wave emission from voltage- and number-controlled intrinsic Josephson junctions in $Bi_2Sr_2CaCu_2O_{8+\delta}$[1] , MANABU TSUJIMOTO, RYO NAKAYAMA, NAOKI ORITA, TAKASHI KOIKE, KOTA DEGUCHI, KAVEH DELFANAZARI, TAKASHI YAMAMOTO, TAKANARI KASHIWAGI, HIDETOSHI MINAMI, MASASHI TACHIKI, KAZUO KADOWAKI, University of Tsukuba — Intense and coherent terahertz electromagnetic wave (THz-wave) emission from the intrinsic Josephson junctions (IJJs) in single crystalline high-T_c superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi-2212) was reported in 2007 [L. Ozyuzer *et al.*, Science **318**, (2007) 1291.]. In the present work, we demonstrate the relationship between the bias condition and the resonance state by controlling both the applied voltage, V, and the number of resistive junctions, N. We directly observed that if N junctions are in resistive state, the resonance frequency, f_J, varies in accordance with the ac-Josephson relation; $f_J = (2|e|/h)V/N$, although frequency f_J has previously been thought to be uniquely determined by the geometrical condition due to the cavity resonance effect [M. Tsujimoto *et al.*, Phys. Rev. Lett. **105**, (2010) 037005.]. We also found that the emission intensity varies as a function of both f_J and N.

[1]CREST-JST, WPI-MANA, Strategic Initiative A (University of Tsukuba)

8:36AM P23.00004 Angular distribution and Josephson plasma modes of THz radiation emitted from Bi2212 mesas with various shapes[1] , KAZUO KADOWAKI, TAKANARI KASHIWAGI, MANABU TSUJIMOTO, TAKASHI YAMAMOTO, HIDEHIRO ASAI, HIDETOSHI MINAMI, Institute of Materials Science, University of tsukuba, RICHARD A. KLEMM COLLABORATION[2] — So far, we have measured angular dependence of the intensity of the THz emission from mesas of high-T_c superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ with various shapes such as rectangulars, squares, cylinders, triangulars, etc. and various dimensions larger or smaller than the penetration depth λ_c. The results have been analized by a model developed by Klemm and Kadowaki[3], which assumes coherent generation of the standing of wave cavity modes in a mesa due to the ac-Josephson effect. The higher harmonic modes are observed in some cases as expected in the model. However, it is often observed that the emission frequency does not obey the simple cavity mode, indicating that the cavity resonance may not be a stringent condition for the emission of the THz radiation. The implication is argued in terms of the emission dynamics from the Bi2212 mesa structure.

[1]CREST-JST, WPI-MANA, Special project (A) in Univ. of Tsukuba

[2]Univ. Central Florida

[3]Richard A. Klemm and K. Kadowaki, J. Phys. Condens. Matter **22** (2010) 375701.

8:48AM P23.00005 Superconductivity induced by current injection into non-superconducting $Bi_2Sr_2CaCu_2O_8$, Y. SIMSEK, Y. KOVAL, X.Y. JIN, S. PROBST, P. MÜLLER, Department of Physics, Universität Erlangen-Nürnberg, Germany — The carrier-doping induced transition from the antiferromagnetic state to the superconducting phase is still one of the most fascinating properties of high-Tc materials. Usually hole doping is achieved by non-stoichiometry. However, we already have shown that we can change the carrier concentration of $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystals by current injection along the c-axis. This effect is persistent up to annealing temperatures of approximately 270 K. Now, the interesting question is if "chemical" doping by oxygen excess is necessary at all. For this purpose we performed current-injection experiments on fully oxygen depleted $Bi_2Sr_2CaCu_2O_8$ which was not superconducting above 4.2 K. In order to eliminate the contact resistance of the highly resistive depleted material, we realized a "true" 4-point geometry by fabricating double cross-bar crystal stacks. C-axis resistivity, critical current, and critical temperature were measured by c-axis transport. We have observed that by carrier injection the conductivity can be increased until superconductivity above 4.2 K is reached. Continuing the doping by current injection, optimum-doped and even overdoped states were obtained. Using current injection at higher bias, we were able to reduce the hole concentration again.

9:00AM P23.00006 Magnetic-field-driven phase transitions in Josephson arrays , JOSHUA PARAMANANDAM, MATTHEW BELL, ALEKSANDR VEREVKIN, LEV IOFFE, MICHAEL GERSHENSON, Rutgers University — We have studied the phase transitions induced by the magnetic field B in arrays of small Josephson junctions. The number of nearest-neighbor junctions connected to a single superconducting island varied between 4 and 11 for different arrays. When frustrated by the magnetic field, the arrays demonstrated several quantum phase transitions at different critical values of the resistance between R=3-10 k, which is in line with earlier observations. In particular, with increasing B we observed transitions between three states: a) the superconducting state with zero R, b) the "metallic" state with a weak R dependence on T in the range 40mK<T<200mK, and c) the "insulating" state with an activation dependent $R(T)$. The activation energy, extracted from the current-voltage characteristics and the Arrhenius fitting of $R(T)$ in the "insulating" regime, has been studied in detail as a function of the temperature and the magnetic field. The data indicate the possible development of a strongly inhomogeneous state when approaching the superconducting-to-insulating transition.

9:12AM P23.00007 Series-parallel two dimensional arrays of $YBa_2Cu_3O_{7-\delta}$ thin film ion damage Josephson junctions[1] , JASPER DRISKO, SHANE CYBART, STEVEN ANTON, STEPHEN WU, JAMES PARKER, ROBERT DYNES, University of California, Berkeley — We have fabricated a number of series-parallel two dimensional arrays of $YBa_2Cu_3O_{7-\delta}$ thin film ion damage Josephson junctions. The arrays contain 1,000 to 15,000 Superconducting QUantum Interference Devices (SQUIDs) in different dimensional configurations and different SQUID area distributions. We have measured the electrical transport characteristics of each array and compare it to computer simulations based on the resistively shunted junction model to investigate the effect of mutual inductance between the SQUIDS within the array. We find there is good agreement between our simulation model and our experimental device when the parallel dimension of the device is less than 15 SQUIDs.

[1]This work was supported by AFOSR.

9:24AM P23.00008 Properties of linear arrays of Josephson junctions capacitively coupled to a diffusive metal[1] , ALEJANDRO LOBOS, THIERRY GIAMARCHI, DPMC-MaNEP, University of Geneva, Switzerland — Josephson junctions arrays (JJAs) are strongly-correlated quantum systems showing a rich and complex behavior at low-temperatures.[2] Besides their potential uses in applications, JJAs allow to investigate (under controlled conditions) many aspects of low-dimensional superconductivity which remain to be understood. In this work we study the phase diagram and the low-energy properties of a one-dimensional (1D) JJA capacitively coupled to a diffusive two-dimensional electron gas (2DEG) placed at a distance d, which provides dissipation.[3] We derive an effective field-theoretical model for the 1D JJA coupled to the 2DEG, and predict a superconductor-insulator transition (SIT) at $T = 0$, in agreement with former theoretical predictions. We discuss implications for transport experiments and for the observed SIT in 1DJJAs. Both in the superconducting and insulating phases, the coupling to the 2DEG produces deviations with respect to the resistivity as a function of T predicted for an isolated array.

[1]This work was supported in part by the Swiss SNF under MaNEP and division II.
[2]R. Fazio and H. van der Zant, Physics Reports **355**, 235 (2001)
[3]A. M. Lobos and T. Giamarchi, Phys. Rev. B **82**, 104517 (2010)

9:36AM P23.00009 Measurement of Aharonov-Casher effect in a Josephson junction chain[1] , IOAN MIHAI POP, CNRS, Institute NEEL, Grenoble, FLORENT LECOCQ, BERNARD PANNETIER, OLIVIER BUISSON, WIEBKE GUICHARD, CNRS, Institut NEEL, Grenoble — We have recently measured the effect of superconducting phase-slips on the ground state of a Josephson junction chain[2] and a rhombi chain.[3] Here we report clear evidence of Aharonov-Casher effect in a chain of Josephson junctions. This phenomenon is the dual of the well known Aharonov-Bohm interference. Using a capacitively coupled gate to the islands of the chain, we induce oscillations of the supercurrent by tuning the polarization charges on the islands. We observe complex interference patterns for different quantum phase slip amplitudes, that we understand quantitatively as Aharonov-Casher vortex interferences.

[1]European STREP MIDAS
[2]I. M. Pop et al. Nature Physics 6, 589–592 (2010)
[3]I. M. Pop et al. PRB, 78, 104504 (2008)

9:48AM P23.00010 Josephson Junction as a Magnetic Switch , LIUFEI CAI, CUNY-Lehman College and Graduate Center, EUGENE CHUDNOVSKY, CUNY Lehman College — We study electromagnetic interaction of a nanomagnet with a weak superconducting link. Equations that govern coupled dynamics of the two systems are derived and investigated numerically. We show that despite very weak magnetic field generated by the weak link, a time-dependent bias voltage applied to the link can initiate a non-linear dynamics of the nanomagnet that leads to the reversal of its magnetic moment. We also consider quantum problem in which a nanomagnet interacting with a weak link is treated as a two-state spin system due to quantum tunneling between spin-up and spin-down states. L. Cai and E. M. Chudnovsky, Phys. Rev B **82**, 104429 (2010).

10:00AM P23.00011 Switching Experiments on a Current-Biased MgB_2 Josephson Junction[1] , ROBERTO RAMOS, JEROME MLACK, JOSEPH LAMBERT, STEVEN CARABELLO, Department of Physics, Drexel University — As the current through a Josephson junction is increased, the voltage across the junction switches from zero to a finite voltage. This is analogous to the escape of a phase particle originally oscillating with a plasma frequency ω in a washboard potential well, to the running state. We report results of our switching experiments on current-biased MgB_2/I/Pb thin film junctions through a broad range of sub-Kelvin temperatures. Our results exhibit features in the escape rate Γ suggestive of substructure within the pi gap of MgB_2, which is consistent with our recent work demonstrating sub- structure within the pi and sigma superconducting energy gaps of MgB_2. Upon irradiation of microwaves with frequencies resonant with the plasma frequency, we observe enhancement of escape rates, which is a clear demonstration of microwave resonant activation in these devices. By manipulating frequency and power, we demonstrate good control over the escape of the phase particle.

[1]We wish to thank Profs. Xiaoxing Xi and Ke Chen for providing high-quality MgB_2 Josephson junctions.

10:12AM P23.00012 ABSTRACT WITHDRAWN –

10:24AM P23.00013 Cavity mode waves during terahertz radiation from rectangular $Bi_2Sr_2CaCu_2O_{8+\delta}$ mesas , RICHARD KLEMM, ERICA LABERGE, DUSTIN MORLEY, University of Central Florida, TAKANARI KASHIWAGI, MANABU TSUJIMOTO, KAZUO KADOWAKI, University of Tsukuba, Tsukuba, Japan — We re-examined the angular dependence of the radiation from the intrinsic Josephson junctions in rectangular mesas of $Bi_2Sr_2CaCu_2O_{8+\delta}$, in order to determine if the cavity mode part of the radiation arises from waves across the width w or along the length ℓ of the mesas, associated with "hot spots" [Wang *et al.*, Phys. Rev. Lett. **105**, 057002 (2010)]. Fits to the data of Kadowaki *et al.* [J. Phys. Soc. Jpn. **79**, 02373 (2010)] using both a uniform ac Josephson current source and a non-uniform cavity mode (or magnetic surface current) source suggest that both scenarios are equally probable. However, when $n\ell/2w$ is integral, where n is the index of the rectangular $TM^z(n,0)$ mode, standing cavity wave modes along the length of the mesa do not radiate in the xz plane perpendicular to the length of the mesa, suggesting experiments on such mesas could help to resolve the question.

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P24 DCOMP: Focus Session: What is Computational Physics? II followed by Computational Methods: Numerical Methods for Strongly Correlated Systems II D167

8:00AM P24.00001 US-Japan Workshops on Computational Physics - International Liaison Activities - , YUKO OKAMOTO, Nagoya University — In this talk, I will report on US-Japan workshops on computational physics. I will summarize what was done in the past workshops that were held in Hawaii and talk about future plans.

8:12AM P24.00002 Opportunities for Computational Discovery in Basic Energy Sciences , MARK PEDERSON, Department of Energy, Office of Basic Energy Sciences, Washington DC, 20585-1290 — An overview of the broad-ranging support of computational physics and computational science within the Department of Energy Office of Science will be provided. Computation as the third branch of physics is supported by all six offices (Advanced Scientific Computing, Basic Energy, Biological and Environmental, Fusion Energy, High-Energy Physics, and Nuclear Physics). Support focuses on hardware, software and applications. Most opportunities within the fields of condensed-matter physics, chemical-physics and materials sciences are supported by the Officeof Basic Energy Science (BES) or through partnerships between BES and the Office for Advanced Scientific Computing. Activities include radiation sciences, catalysis, combustion, materials in extreme environments, energy-storage materials, light-harvesting and photovoltaics, solid-state lighting and superconductivity. A summary of two recent reports by the computational materials and chemical communities on the role of computation during the next decade will be provided. In addition to materials and chemistry challenges specific to energy sciences, issues identified include a focus on the role of the domain scientist in integrating, expanding and sustaining applications-oriented capabilities on evolving high-performance computing platforms and on the role of computation in accelerating the development of innovative technologies.

8:24AM P24.00003 Discussion of Opportunities in Computational Physics[1] , BERND BERG, Florida State University, MARK PEDERSON, Department of Energy — A discussion of the points raised in the previous talk by Mark Pederson (DOE) will be encouraged, including: (1) Identifying models and strategies for effectively organizing and availing complex computational simulation capabilities to a broader scientific and technical community. (2) Identifying cross-discipline communication of capabilities to ensure sharing of algorithms. (3) Opinions on evolution of overlap between the basic energy scientific mission and the fields that are typically represented by the March-Meeting participants. (4) Interactions between the domains of computational physics, computer science, and applied mathematics. (5) The proper balance between individual and group achievement. (6) What role could DCOMP have in this?

[1]In part supported by the DOE grant DE-FG02-97ER41022.

8:36AM P24.00004 Enabling Computational Discovery and Design , DARYL HESS, Division of Materials Research, National Science Foundation, USA — Advanced cyberinfrastructure(CI), increases in computing power, and increasing use of data volumes are revolutionizing how science is done, changing the nature of the questions we ask, and opening new frontiers. From discovering new phenomena and states of matter to the challenge of designing new materials and matter, the focus on problems with many complex interacting degrees of freedom through computational investigation often leads to large amounts of data that require analysis, preservation, curation, and sharing across the community. Data from many sources plays an increasingly important role as a driver of discovery. I will discuss opportunities in computational and data enabled science and in building the CI of the 21^{st} century. Sustainable, maintained, and reliable shared software is an important component of a National CI framework that will empower computational scientists to engage the scientific frontiers and the pressing problems around us. The success of computational data enabled science requires innovation that leads to paradigms in attacking difficult problems. Education will play an important role in realizing the full potential of computation and data enabled science for discovery and design. Participation of the computational science community is an important ingredient to create a CI that will propel science forward; some self-assembly is required. NSF provides funding opportunities to help.

8:48AM P24.00005 Building Foundations for Future Advances in Computational Physics , BARRY SCHNEIDER, DARYL HESS, National Science Foundation — We continue the discussion on laying the cyberinfrastructure foundations to support future advances in computational science. We will focus on how NSF can help and encourage communication with the community in achieving this goal.

9:00AM P24.00006 Quo Vadis Computational Physics?[1] , RICHARD SCALETTAR, University of California, Davis — In this Focus Session, and in the preceding DCOMP Invited Symposium, "Great Advances of Computational Physics: Past, Present and Future," we have heard about the vision for our field, reviewed (and previewed) cutting-edge numerical work, and considered where the resources might come to support our endeavors. In this talk I will summarize some of the common themes of this discussion, as well as open up the floor for further thoughts on where our APS Division is heading.

[1]Research supported by the DOE SCIDAC program, DOE-DE-FC0206ER25793, and under ARO Award W911NF0710576 with funds from the DARPA OLE Program.

9:36AM P24.00007 Magnetic impurities in real lattices: A DMRG and ECA study , CARLOS BUSSER, University of Wyoming, WY, GEORGE MARTINS, Oakland University, MI, KHALED AL-HASSANIEH, Los Alamos National Laboratory, NM, ADRIAN FEIGUIN, University of Wyoming, WY — Magnetic interactions between strongly correlated impurities coupled to a sea of conduction electrons is a subject of great interest from both, experimental and theoretical studies. When many magnetic impurities are attached to the same conduction band a rich phase diagram can arise. By one hand the magnetic impurities can be strongly coupled to the spin of the electrons of the conduction band forming a Kondo singlet. By the other, through electron of the conduction band, a spin-spin interaction between the impurities can appears as a consequence the RKKY interaction. A competition between this two singles is expected. For these two effects is important to have a good description of the electrons with energy close to the Fermi level. Systems like the square lattice, with a van-Hove singularity at the middle of the band, or Graphene, with Dirac electrons, or Carbon nanotubes with multiple bands and multiples van Hove singularities need a proper description of the electrons in the lattice Hamiltonian. In this work we present, through a canonical transformation, a numerical method to study problems with several magnetic impurities coupled to arbitrary lattices using DMRG or ECA techniques.

9:48AM P24.00008 Quantum Monte Carlo simulations with tensor-network states[1] , JEONG PIL SONG, R.T. CLAY, Mississippi State University — Matrix-product states, generated by the density-matrix renormalization group method, are among the most powerful methods for simulation of quasi-one dimensional quantum systems. Direct application of a matrix-product state representation fails for two dimensional systems, although a number of tensor-network states have been proposed to generalize the concept for two dimensions. We introduce a useful approximate method replacing a 4-index tensor by two matrices in order to contract tensors in two dimensions. We use this formalism as a basis for variational quantum Monte Carlo, optimizing the matrix elements stochastically. We present results on a two dimensional spinless fermion model including nearest- neighbor Coulomb interactions, and determine the critical Coulomb interaction for the charge density wave state by finite size scaling.

[1]This work was supported by the Department of Energy grant DE-FG02-06ER46315.

10:00AM P24.00009 Diagonalization with matrix-product states[1] , CHEN LIU, ANDERS SANDVIK, Boston University — We consider matrix-product states (MPSs) combined with diagonalization as a method to study correlated quantum many-body systems. The Hamiltonian matrix is constructed in a non-orthogonal basis of MPSs. Diagonalizing this matrix (a generalized eigenvalue problem) gives the ground state as well as excitations. The accuracy is significantly improved compared to individual optimized MPSs. We discuss several ways to generate the MPS basis states in a suitable way and present results for one- and two-dimensional quantum spin systems.

[1]NSF DMR-0803510

10:12AM P24.00010 Multi-scale entanglement renormalization for critical systems , BELA BAUER, Theoretische Physik, ETH Zurich, LIZA HUIJSE, Department of Physics, Harvard University, KARELJAN SCHOUTENS, Institute for Theoretical Physics, University of Amsterdam, GUIFRE VIDAL, The University of Queensland, Department of Physics, Brisbane, MATTHIAS TROYER, Theoretische Physik, ETH Zurich — Determining information about the underlying conformal field theory of a critical system in one dimension, such as the central charge and scaling dimensions, is a notoriously difficult problem for numerical methods. Using a suitable tensor network state, the multi-scale entanglement renormalization ansatz [1], this information is directly accessible [2]. We apply this method to several critical systems in one dimension, including a supersymmetric model for lattice fermions and Yang-Lee chains.

[1] G. Vidal, Phys. Rev. Lett. 99, 220405 (2007)
[2] R.N.C. Pfeifer et al, Phys. Rev. A 79(4), 040301(R) (2009)

10:24AM P24.00011 Simulation of fermionic and frustrated lattice models in two dimensions with tensor network algorithms , PHILIPPE CORBOZ, Theoretische Physik, ETH Zurich, Switzerland/Institute for theoretical Physics, EPF Lausanne, Switzerland, GLEN EVENBLY, JACOB JORDAN, ROMAN ORUS, GUIFRE VIDAL, School of Mathematics and Physics, The University of Queensland, Australia, BELA BAUER, MATTHIAS TROYER, Theoretische Physik, ETH Zurich, Switzerland, FREDERIC MILA, Institute for theoretical Physics, EPF Lausanne, Switzerland, FRANK VERSTRAETE, Faculty of Physics, University of Vienna, Austria — The simulation of strongly correlated fermionic and frustrated systems in two dimensions is one of the biggest challenges in computational physics. Borrowing ideas and tools from quantum information and condensed matter physics, a new generation of simulation techniques for many-body systems, the so-called tensor network algorithms (e.g. PEPS, MERA), have been proposed in the last few years. These algorithms have been generalized to fermionic systems recently. We present a particularly simple formalism to account for the statistics of fermionic degrees of freedom in a tensor network. Benchmark results confirm the validity of this approach, and show that the computational cost of simulations does not depend a priori on the particle statistics, but on the amount of entanglement in the system.

10:36AM P24.00012 Dynamical simulation of integrable and non-integrable models in the Heisenberg picture[1] , DOMINIK MUTH, RAZMIK UNANYAN, MICHAEL FLEISCHHAUER, Fachbereich Physik und Forschungszentrum OPTIMAS, Technische Universitaet Kaiserslautern, D-67663 Kaiserslautern, Germany — The numerical simulation of quantum many-body dynamics is typically limited by the linear growth of entanglement with time. Recently numerical studies have shown, however, that for 1D Bethe-integrable models the simulation of local operators in the Heisenberg picture can be efficient as the corresponding operator-space entanglement grows only logarithmically. Using the spin-1/2 XX chain as generic example of an integrable model that can be mapped to free particles, we here provide a simple explanation for this. We show furthermore that the same reduction of complexity applies to operators that have a high-temperature auto correlation function which decays slower than exponential, i.e., with a power law. This is amongst others the case for models where the Blombergen-De Gennes conjecture of high-temperature diffusive dynamics holds. Thus efficient simulability may already be implied by a single conservation law (like that of total magnetization), as we will illustrate numerically for the spin-1 XXZ model.

[1]We acknowledge support through the SFB TRR49 of the DFG and the graduate school of excellence MAINZ/MATCOR.

10:48AM P24.00013 ABSTRACT WITHDRAWN –

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P25 DCMP: Superconductivity: Devices and Applications D166

8:00AM P25.00001 Microwave amplifier based on an inline dc SQUID , DAVID HOVER, YUNG-FU CHEN, LEON MAHER, GUILHEM RIBEILL, SHAO-JIANG ZHU, STEVE SENDELBACH, ROBERT MCDERMOTT, University of Wisconsin — The dc SQUID can be used as a sensitive, low-noise microwave amplifier if the signal to be amplified is suitably coupled to the SQUID. We have designed and fabricated microwave amplifiers based on inline dc SQUIDs, where the SQUID loop is formed from a thin ($\sim$ 100 nm) dielectric layer separating the base and counterelectrode wiring traces. The SQUID is embedded in a microstrip transmission line resonator at a current anti-node, and signal current is injected directly into the SQUID loop. With this design we have achieved gain greater than 20 dB at a frequency of 8.5 GHz. We provide a theoretical analysis of amplifier noise temperature, bandwidth, and gain, and describe measurements of amplifier noise temperature. We discuss application of these devices to the readout of superconducting quantum circuits.

8:12AM P25.00002 Spatial correlations of magnetic fluctuations in DC SQUIDS , STEVEN SENDELBACH, UMESHKUMAR PATEL, ROBERT MCDERMOTT, UW-Madison Department of Physics — Recent experiments indicate that there is a high density of unpaired spins residing on the surfaces of superconducting thin films used to implement SQUIDs and superconducting qubits. Fluctuations of these spins give rise to low frequency flux noise and dephasing of the qubit state. Realization of phase and flux qubits with improved dephasing times will require a deeper understanding of the microscopic physics that governs fluctuations of the surface spins. Here we describe experiments to probe the spatial correlation of magnetic fluctuators in a SQUID circuit. The SQUID loop incorporates multiple current taps, enabling one to locally address magnetic fluctuators. Preliminary data reveal correlated fluctuations on a length scale of order 10 μm. We discuss implications for qubit dephasing.

8:24AM P25.00003 Simulations of dependence of low frequency flux noise on SQUID geometry[1] , STEVEN ANTON, KEENAN PEPPER, JOHN CLARKE, UC Berkeley, IDA SOGNNAES, NTNU Norway, UC BERKELEY TEAM, NTNU NORWAY TEAM — It is generally accepted that the 1/f magnetic flux noise observed in dc SQUIDs and superconducting qubits originates in the random flipping of a uniform distribution of electron spins localized at the superconductor-insulator interface. Computer simulations and analytical calculations based on this model confirm the experimental result that the noise power at 1 Hz varies only slowly with SQUID dimensions. In particular, analytical calculations for a circular loop with radius R much greater than the loop linewidth W predict that the noise power scales as R/W. We present numerical computations that are valid for arbitrary geometry, including that of the square washer SQUID for which W approaches R. Making use of the reciprocity theorem, we solve the London equations numerically to find the current distribution in the superconductor, evaluate the Biot-Savart integral to find the corresponding magnetic field at any point and integrate over all spins, including those at the edges of the films, to find the total flux noise. We compare our results with our recent experimental measurements.

[1]Work supported by ARO and IARPA

8:36AM P25.00004 Dependence of low frequency flux noise on SQUID-washer dimensions[1] , J. BIRENBAUM, S.M. ANTON, A.D. FEFFERMAN, S.R. O'KELLEY, J. CLARKE, UC Berkeley, H-M CHO, G.C. HILTON, K.D. IRWIN, NIST Boulder, F.C. WELLSTOOD, Univ. of Maryland — The 1/f spectral density of low frequency magnetic flux noise at 1 Hz in dc SQUIDs and qubits varies slowly with the dimensions of the superconducting loop, in reasonably good agreement with predictions. Previous measurements on SQUIDs fabricated from a variety of superconductors under different conditions and in a variety of geometries, however, showed that the slope of the power spectrum varied considerably. We report flux noise measurements on six resistively-shunted dc SQUIDs fabricated simultaneously on a single Si chip using a Nb-trilayer process. The noise spectra of all six devices were measured using a SQUID in a single cool-down of our dilution refrigerator. The linewidths of the SQUID loops were varied systematically by a factor of more than 30. The variation in noise power at 1 Hz was small compared with the variation in line width, while the slope varied significantly, from approximately -0.5 to -1. Furthermore, for a given SQUID, the slope depended on temperature.

[1]Work supported by ARO and IARPA.

8:48AM P25.00005 A Novel System for Accurate Cryogenic S-Parameter Measurements , LEONARDO RANZANI, LAFE SPIETZ, JOSE AUMENTADO, NIST, Boulder — In order to study microwave devices operating at cryogenic temperatures (4K and below), an accurate characterization of their full scattering parameters is needed. Simple response calibration using a single through standard is usually performed at cryogenic temperatures due to its simplicity, but it is inaccurate since it only determines 4 of the 10 unknowns present in a general two port network environment. In this talk we will discuss a fully automated through-reflect-line (TRL) calibration system suitable for accurately characterizing 2-port S parameters for devices such as SQUID amplifiers and other cryogenic microwave circuits. Data for some typical devices up to 8GHz will be presented.

9:00AM P25.00006 Josephson Junction Circuits for Passive Non-Reciprocal Microwave Devices , LAFE SPIETZ, NORM BERGREN, JOSE AUMENTADO, NIST — We propose a method for using Josephson junction circuits to build non-reciprocal passive microwave components. We show that strong analogies can be made between the physics of ferrites used in traditional passive non-reciprocal microwave devices (that of the gyroscope) and certain classes of Josephson junction circuits. We describe a simple circuit which demonstrates these physical principles, and present both theoretical experimental results on this circuit.

9:12AM P25.00007 Probing the origin of 1/f critical-current noise in nanoscale Al/AlOx/Al Josephson junctions[1] , CHRISTOPHER NUGROHO, VLADIMIR ORLYANCHIK, ALLISON DOVE, GUSTAF OLSON, ZACHARY YOSCOVITS, JAMES ECKSTEIN, DALE VAN HARLINGEN, Department of Physics, University of Illinois at Urbana-Champaign — We present measurements of the low frequency noise in nanoscale Al/AlOx/Al Josephson junctions made by the shadow/angle evaporation technique. We investigate the differences in the nature of the charge trap fluctuations when the junction electrodes are in the normal state vs. in the superconducting state, as a test of some recent theoretical models. To do that, we compare the magnitude, temperature dependence, and magnetic field dependence of junction resistance fluctuations in the normal state above the Al transition temperature to that of the resistance and critical current fluctuations measured in the superconducting state. We also explore whether the observed fluctuators are thermally-activated or tunneling as a function of temperature.

[1]Supported by the IARPA Advanced Materials and Fabrication for Coherent Superconducting Qubits Program

9:24AM P25.00008 Decoherence and energy shift in phase qubits due to nonequilibrium quasiparticles , M. LENANDER, R.C. BIALCZAK, E. LUCERO, M. MARIANTONI, A. O'CONNELL, M. NEELEY, D. SANK, H. WANG, M. WEIDES, J. WENNER, T. YAMAMOTO, Y. YIN, J. ZHAO, A.N. CLELAND, J.M. MARTINIS — Nonequilibrium quasiparticle excitations are thought to be an important source of decoherence in Josephson qubits. We present a model analogous to the Mattis-Bardeen theory wherein the effects of quasiparticles introduce a complex environmental impedance to the junction. The real part causes energy relaxation in the qubit while the imaginary part causes a frequency shift. We present experimental data comparing these effects while injecting nonequilibrium quasiparticles into the system. The theory is used to qualitatively check the injection process. Then by comparing the decay rate and frequency shift, we quantitatively verify the theory without the need to directly measure the quasiparticle density. Agreement between theory and experiment is observed to within experimental uncertainty, about 10%. We examine infrared radiation as a source of nonequilibrium quasiparticles. Using these new tools, we hope to develop methods for improving qubit performance and to bound the contribution to energy decay from quasiparticles.

9:36AM P25.00009 Effect of an Ohmic environment on an optimally controlled flux-biased phase qubit , AMRIT POUDEL, MAXIM VAVILOV, University of Wisconsin-Madison — We analyze the effect of environment on the gate operation of flux-biased phase qubits. We employ the master equation for a reduced density matrix of the qubit system coupled to an Ohmic environment, described by the Caldeira-Leggett model. Numerically solving this equation, we evaluate the gate error as a function of gate time, temperature and environmental coupling strength for experimentally determined qubit parameters. Here we present the analysis for single-quadrature microwave (control) pulses as well as for two-quadrature pulses, which lower the gate error significantly for idealized systems in the absence of environment. Our results indicate that two-quadrature pulses with fixed and variable driving frequency have similar performance, which outweighs the performance of single-quadrature pulses, in the presence of environment.

9:48AM P25.00010 Quasiparticle relaxation of superconducting qubits in the presence of flux , GIANLUIGI CATELANI, Yale University, JENS KOCH, Northwestern University, LUIGI FRUNZIO, ROBERT SCHOELKOPF, MICHEL DEVORET, LEONID GLAZMAN, Yale University — Quasiparticle tunneling across a Josephson junction sets a limit for the lifetime of a superconducting qubit state. We develop a general theory of the corresponding decay rate in a qubit controlled by a magnetic flux. The flux affects quasiparticles tunneling amplitudes, thus making the decay rate flux-dependent. The theory is applicable for an arbitrary quasiparticle distribution. It provides estimates for the rates in practically important quantum circuits and also offers a new way of measuring the phase-dependent admittance of a Josephson junction.

10:00AM P25.00011 ABSTRACT WITHDRAWN –

10:12AM P25.00012 High count-rate superconducting transition edge sensors for near-IR single photon detection , FAUSTIN CARTER, DANIEL SANTAVICCA, LUIGI FRUNZIO, Yale University, ANTHONY ANNUNZIATA, IBM, Yale University, DANIEL PROBER, Yale University — Detection of individual near-IR photons with GHz count rates, good timing resolution, and high quantum efficiency is important in a number of applications. These include quantum key distribution, single-photon classical communication, and CMOS imaging for defect analysis. We propose a nano-scale superconducting niobium transition edge sensor (TES). The extremely small detector volume allows for single-photon sensitivity at 4 K, with a much faster response time (nsec) than conventional TES detectors operating below 0.4 K. Efficient photon coupling is achieved with a resonant near-IR planar antenna. The proposed device is intrinsically photon number resolving, unlike a niobium-nitride nanowire detector or an avalanche photodiode. We present preliminary results for device performance.

10:24AM P25.00013 Nano-structuring on the surface of high Tc-superconductors by STM&AFM , KAZUTO HIRATA, National Institute for Materials Science, TADASHI MACHIDA, SHUUICHI OOI, MINORU TACHIKI, National Institute for Materials Science, TAKASHI MOCHIKU — We demonstrate local insulation on a cleaved surface of Bi- 2212 single crystals using a local anodic oxidation by a atomic force microscope (AFM) and a scanning tunneling microscope (STM) for the first time. We have investigated the electrical properties of the modified region by using an STM-assisted near- field microwave microscope. From the experimental observations, we conclude that the modified region becomes an insulator with an associated dielectric loss locally. Varying the applied bias- voltage and the scanning speed can control the protrusion height and the line width of the regions. This provides a potential technique for reproducibly fabricating high temperature superconducting devices with stable electronic characteristics.

10:36AM P25.00014 An Integrated Balanced Superconductor-Insulator-Superconductor Heterodyne Mixer on a Silicon Membrane , M.P. WESTIG, K. JACOBS, M. SCHULTZ, M. JUSTEN, J. STUTZKI, C.E. HONINGH, I. Physikalisches Institut, Universitaet zu Koeln, Zuelpicher Straße 77, 50937 Koeln, Germany — We have designed and fabricated a 380-520 GHz integrated balanced Nb\Al\AlOx\Nb superconductor-insulator-superconductor (SIS) heterodyne waveguide mixer for submillimeter astrophysics. The response of the mixer measured with a Fourier transform spectrometer shows excellent agreement with the design. The novelty of our device is that we deposit the complete superconducting mixer circuit (tapered slotline antennas, hybrid coupler, MIM capacitors, SIS junctions, tuning circuits and blocking filters) on top of a 9 μm silicon membrane. The membrane is held suspended in a waveguide by 2.5 μm thick gold plated beamleads. We will show that silicon membrane technology and a thorough device design render the integration of SIS devices with larger circuits feasible. This is an important step towards large arrays of mixers. When using an appropriate superconductor technology, these devices are scalable to higher frequencies. We will present the design, fabrication results and first results of heterodyne measurements.

10:48AM P25.00015 c-Axis current flow arises in helically wound wire , YING JIA, U. WELP, G.W. CRABTREE, W.K. KWOK, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA, M. RUPICH, S. FLESHLER, A.P. MALOZEMOFF, American Superconductor Corp., 64 Jackson Road, Devens, MA 01434-4020, USA — c-Axis critical current density of second-generation YBCO wires in HTS cables due to the interaction of current flow with the induced magnetic field. However, the importance of c-axis critical current density (J_c^c) on the overall transport critical current is not clearly understood. We measured the temperature and field dependence of J_c^c using a mesa structure patterned into the YBCO layer of 2^{nd}-generation HTS tapes. We found, J_c^c –values of $\sim$ 4 kA/cm^2 at 77 K in self-field, corresponding to an unexpectedly high anisotropy of the critical current density $\gamma = J_c^{ab}\big/J_c^c$ = 500$\sim$600. We also investigated the effect of pinning microstructures on J_c^c and γ. Our result shows a direct correlation of J_c^c (77 K, sf) and γ to the density of stacking faults. An estimation reveals that the fraction of tape width associated with c-axis current flow grows linearly from 5% to 20% with increasing γ for a typical geometry and could affect the performance of power transmission in HTS cables.

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P26 DMP DCOMP: Focus Session: Iron Based Superconductors – Spin Dynamics D162/164

8:00AM P26.00001 High Energy Spin Excitations in Optimal doped Superconducting $BaFe_{1.9}Ni_{0.1}As_2$, MENGSHU LIU, Department of Physics and Astronomy, The University of Tennessee, Knoxville, Tennessee 37996-1200, USA, HUIQIAN LUO, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, RUSSELL EWINGS, TATIANA GUIDI, ISIS Facility, Rutherford Appleton Laboratory, STFC, Chilton, Didcot, Oxon, OX11 0QX, United Kingdom, PENGCHENG DAI, Department of Physics and Astronomy, The University of Tennessee, Knoxville, Tennessee 37996-1200, USA — The recent discovered iron pnictide superconductor which shows a transition temperature up to 50K has drawn much attention in the community. There are indications that superconductivity in the iron arsenides family may be driven by a magnetic pairing mechanism, the nature of which remains poorly understood. In our recent inelastic neutron scattering experiment on optimal doped $BaFe_{1.9}Ni_{0.1}As_2$ sample, spin excitation data are collected throughout the Brillouin zone and up to energy transfer of 400meV which was not probed before. We found that the scattering persists as high as 300 meV in the superconducting sample, and a spectra transfer similar to the parent compound with a spin nematicity was also observed

8:12AM P26.00002 Spin-phonon coupling in iron arsenide superconductors[1] , JENNIFER NIEDZIELA, DANIEL PARSHALL, KONSTANTIN LOKSHIN, U. of Tennessee - Knoxville, TN, ATHENA SEFAT, ORNL, Oak Ridge, TN, AHMET ALATAS, APS, Argonne National Laboratory, Darien, IL, TAKESHI EGAMI, U. of Tennessee - Knoxville, TN USA — In this work we present the results of an inelastic x-ray scattering experiment measuring the softening of the TA[110] phonon in $BaFe_2As_2$ as a function of temperature. Cooling through the structural transition temperature yields a softening of the phonon energy of the transverse acoustic mode nearly 1 meV from the value at room temperature at $\mathbf{q} = 0.1$. This phonon controls the structural phase transition, changing the symmetry from tetragonal to orthorhombic at the same temperature as the transition to long range antiferromanetic order. Even though the lattice distortion is minor, the anisotropy in the magnetic exchange constants is very large. We posit that this phonon mode couples to the orbital moment, and softening of this mode is required for the onset of long range antiferromagnetic ordering and the dramatic change in the exchange constants. This observation is suggestive that a mechanism of spin-phonon coupling is present in the pnictide systems, and is a possible contributor to the superconducting mechanism.

[1]The work was supported by Department of Energy Office of Basic Energy Sciences.

8:24AM P26.00003 Collapse of the spin resonance spectral weight in overdoped $Ba_{1-x}K_xFe_2As_2$[1] , RAY OSBORN, STEPHAN ROSENKRANZ, JOHN-PAUL CASTELLAN, EUGENE GOREMYCHKIN, DUCK-YOUNG CHUNG, HELMUT CLAUS, Argonne National Laboratory, MERCOURI KANATZIDIS, Northwestern University, TATIANA GUIDI, Rutherford Appleton Laboratory, UK — We report inelastic neutron scattering measurements of magnetic excitations in $Ba_{1-x}K_xFe_2As_2$ over a broad range of electron band filling within the superconducting phase. In an itinerant model, these excitations are resonantly enhanced when the superconducting energy gap changes sign on different parts of the electron Fermi surface. They are therefore sensitive both to the superconducting gap symmetry and to the Fermi surface geometry. Our results show that, in addition to becoming incommensurate because of the growing mismatch in the hole and electron Fermi surface volumes, the resonant spectral weight decreases proportionally to the resonance binding energy, vanishing at $x \sim 0.72$. A tight-binding model including $s_\pm$-symmetry pairing is able to reproduce these observations confirming that the resonance arises from the pairing of band electrons.

[1]Supported by U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under contract No. DE-AC02-06CH11357.

8:36AM P26.00004 Spin Correlations in Superconducting $Ba(Fe_{1-x}Co_x)_2As_2$[1] , STEPHEN HAYDEN, University of Bristol — Elastic and inelastic neutron scattering are used to study the spin correlations in superconducting $Ba(Fe_{1-x}Co_x)_2As_2$. Measurements on the antiferromagnetically ordered parents of this system [1] show a strongly anisotropic spin-wave velocity. Here we report [2] measurements of the magnetic excitations in a the superconducting composition, x=0.065, up to 80 meV and show that a similar anisotropy persists for superconducting compositions. The dispersive mode measured here connects directly with the spin resonance previously observed in this compound. When placed on an absolute scale, our measurements show that the local- or wavevector- integrated susceptibility is larger in magnitude than that of the ordered parents over the energy range probed. I will discuss the interpretation of our results in terms of the electronic structure and possible fluctuating nematic order.

[1] S. O. Diallo, *et al.* Phys. Rev. Lett. **102**, 187206 (2009); J. Zhao , *et al.* Nat. Phys. **5**, 555 (2009).
[2] Lester *et al.* Phys. Rev. B **81**, 064505 (2010); unpublished.

[1]Work preformed in collaboration with C. Lester, Jiun-Haw Chu, J. G. Analytis, T. G. Perring, S. Capelli, A. Stunault, I. R. Fisher.

9:12AM P26.00005 Multiband effect on the magnetic resonance spectrum of pnictide superconductors , TANMOY DAS, A.V. BALATSKY, LANL — The magnetic resonance behavior which is directly probed by the inelastic neutron scattering (INS) spectroscopy gives valuable information about the pairing mechanism of the unconventional superconductors. In high-T_c cuprate superconductors, INS exhibits a clear signature of a magnetic resonance mode in addition to its characteristic dispersive feature (known as "hour-glass" behavior) which are enhanced dramatically below T_c and the mode energy scales universally with the SC gap amplitude. In a multiband unconventional superconductors, the situation is more complex due to the presence of multi-orbital band structure, multiple-SC gaps as well as possibilities of having multiple pairing symmetries. We calculate magnetic susceptibility to show how does the magnetic resonance mode and its dispersion evolve both in energy as well as in momentum as a function of doping in both electron and holed doped pnictide superconductors. The inputs in our calculations are the Fermi surface information from ARPES or LDA and experimental values of superconducting gaps. We find that the magnetic resonance behavior is dramatically different in pnictide than in cuprates. The effects of multiple orbitals, gaps and different pairing symmetry play an important role. We argue that doping dependence of the resonance spectra can be understood from the topological change of the Fermi surface and the gap magnitudes, in good accord with experiments.

9:24AM P26.00006 Spin-orbit coupling in Fe-based superconductors[1] , M.M. KORSHUNOV, Department of Physics, University of Florida, Gainesville, Florida 32611, USA, I. EREMIN, Institut fuer Theoretische Physik III, Ruhr-Universitaet Bochum, D-44801 Bochum, Germany, P.J. HIRSCHFELD, Department of Physics, University of Florida, Gainesville, Florida 32611, USA — The recently discovered iron-based superconductors have attracted considerable attention mainly for their unconventional pairing state. In connection with the determination of pairing symmetry, the resonance peak observed in neutron scattering experiments [1] agrees well with predicted results for the extended s-wave ($s_\pm$) gap symmetry [2]. However, recent neutron measurements shows that there is anisotropy in the spin resonance [3]. In particular, S^zS^z component is different from S^+S^- component of the dynamical spin susceptibility. Such breaking of the spin-rotational invariance in the spin-liquid phase without long-range order can occur due to spin-orbit (SO) coupling. We study the role of the SO coupling in the multiorbital model for Fe-pnictides, and discuss how it influences spin resonance feature and the relation to SC pairing.

[1]. A.D. Christianson *et al.*, Nature **456**, 930 (2008). [2]. M.M. Korshunov and I. Eremin, Phys. Rev. B **78**, 140509(R) (2008); T.A. Maier and D.J. Scalapino, *ibid*, 020514(R) (2008). [3]. O.J. Lipscombe *et al.*, Phys. Rev. B **82**, 064515 (2010).

[1]Partial support was provided by DOE DE-FG02-05ER46236 (PJH)

9:36AM P26.00007 A LDA+DMFT+Vertex function study of dynamical magnetic susceptibility in iron based superconductors , HYOWON PARK, KRISTJAN HAULE, GABRIEL KOTLIAR, Rutgers University — We developed a method for computing dynamical magnetic susceptibility in complex correlated materials based on LDA+DMFT+Vertex function calculation. The dressed Greens function was obtained from the charge self-consistent LDA+DMFT calculation and the local Vertex function was computed from the quantum impurity model using a CTQMC impurity solver. We applied this method to compute the normal state magnetic susceptibility in iron pnictides and iron chalcogenides. Our result shows good agreement with inelastic neutron scattering data. At a low energy, the dynamical structure factor S(Q,w) is peaked at (π,0) momentum in $BaFe_2As_2$ and at ($\pi/2$,$\pi/2$) in FeTe, as expected for the distinct ordering of these compounds. At higher energy, the peak positions shifts to the (π,π) wave vector, in agreement with recent neutron experiments. We argue that this (π,π) magnetic response at high energy and the full spin dispersion above Neel temperature is captured by our realistic band structure method, LDA+DMFT.

9:48AM P26.00008 Neutron scattering study of spin fluctuations on hole-overdoped KFe_2As_2 , C.H. LEE, K. KIHOU, A. IYO, H. EISAKI, AIST, Jpn, H. K.-FURUKAWA, Ocha. Univ., H. USUI, K. KUROKI, The Univ. of Electro-Commun., T. SAITO, H. FUKAZAWA, Y. KOHORI, Chiba Univ., K. YAMADA, WPI, Tohoku Univ. — Spin fluctuations in Fe-based superconductors have attracted great attention since they can be a key factor of the formation of superconducting states. The inelastic neutron scattering technique is a powerful method to examine spin fluctuations, whereas measurements using a single crystal were restricted to Fe(Te,Se) or electron-doped AFe_2As_2 (A=Ba, Ca, or Sr) due to difficulty of growing a large single crystal. To overcome this problem, we have improved growth procedure and succeeded to grow single crystals of heavily hole-overdoped superconducting KFe_2As_2 ($T_c = 3.4$ K). It was believed that no spin fluctuation can be observed in KFe_2As_2, since the nesting of the Fermi surface disappears. To confirm the hypothesis, we have studied spin fluctuations of KFe_2As_2 by neutron scattering using single crystals at JRR-3 reactor of JAERI in Tokai. As results, a well-defined low-energy incommensurate spin fluctuation has been observed at ($\pi(1 \pm 2\delta)$,0) with $\delta = 0.16$. The direction of the peak splitting is perpendicular to that observed in Fe(Te,Se) or in $Ba(Fe,Co)_2As_2$ at high energies. The results suggest that spin fluctuation is more robust in hole-doped than in electron-doped Fe-based superconductors, or a new type of spin fluctuation emerges by heavily hole doping.

10:00AM P26.00009 Neutron Scattering Experiment on Magnetic Field Effect in Under-doped Superconducting $BaFe_{1.915}Ni_{0.085}As_2$, MIAOYIN WANG, PENGCHENG DAI, Department of Physics and Astronomy, University of Tennessee, Knoxville, MENG WANG, HUIQIAN LUO, Institute of Physics, Chinese Academy of Sciences, JEFFREY LYNN, SUNG CHANG, SONGXUE CHI, DEEPAK SINGH, JOSE RODRIGUEZ, NIST Center for Neutron Research, National Institute of Standards and Technology — In under-doped $BaFe_{2-X}(Ni,Co)_XAs_2$, superconductivity coexist with the anti-ferromagnetic (AFM) order. By applying a ~10 Tesla magnetic field parallel to a-b plan, we performed a series of elastic and inelastic neutron scattering measurement on BT-7 instrument in NCNR, NIST. We measured how magnetic bragg-peaks and spin excitation in $BaFe_{1.915}Ni_{0.085}As_2$ will change upon the change of the field.

10:12AM P26.00010 Spin excitations as in hole-doped $Ba_{0.67}K_{0.33}Fe_2As_2$ superconductor , CHENGLIN ZHANG, MENG WANG, MIAOYING WANG, JUN ZHAO, University of Tennessee, Physics Dept, MARTY KAROL, MARK LUMSDEN, Oak Ridge National Laboratory, SONGXUE CHI, SUNG CHANG, JEFFREY LYNN, National Institute of Standards and Technology, HUIQIAN LUO, TAO XIANG, Institute of Physics, Chinese Academy of Sciences, JIANGPING HU, Department of Physics, Purdue University, PENGCHENG DAI, University of Tennessee, Physics Dept, UNIV OF TENNESSEE, PHYSICS DEPT TEAM, OAK RIDGE NATIONAL LABORATORY TEAM, NIST TEAM, INSTITUTE OF PHYSICS, CHINESE ACADEMY OF SCIENCES TEAM — We used inelastic neutron scattering to study the optimally doped $Ba_{0.67}K_{0.33}Fe_2As_2$ (Tc=38K). In contrast to electron doped counterpart, we found that resonance is almost none-L dependence as shown in Fig.1 (b), but the spin gaps are. It is gaped along (0.5,0.5,0), however essentially gapless along (0.5,0.5,1). Meanwhile, the spin correlation is strongly temperature dependence which has not been observed in electron-doped 122 materials at all. The above findings clearly suggest that hole-doped region is indeed different from electron-doped region.

10:24AM P26.00011 ABSTRACT WITHDRAWN –

10:36AM P26.00012 Finite temperature spin dynamics of a square lattice $J_1 - J_2$ antiferromagnet and its implications for iron arsenides[1] , ELIHU ABRAHAMS, University of California Los Angeles, PALLAB GOSWAMI, RONG YU, QIMIAO SI, Rice University — Motivated by recent inelastic neutron scattering measurements in the paramagnetic phase of iron arsenides, we have studied the finite temperature spin dynamics of a square lattice $J_1 - J_2$ antiferromagnet in the parameter regime that gives rise to a collinear $(\pi, 0)$ ground state at zero temperature. We have calculated the dynamical structure factor $S(\mathbf{q}, \omega)$ in the paramagnetic state at finite temperatures using a modified spin wave theory. We have shown that short range antiferromagnetic correlations below the mean-field Ising transition temperature give rise to elliptic features for $S(\mathbf{q}, \omega)$ in momentum space. Employing an effective nonlinear sigma model analysis for the low energy and wave vector limit, we also account for fermion damping and circumvent the shortcoming of modified spin wave theory. Finally, considering a matrix $J_1 - J_2$ model, we point out the connection between the Ising transition and the putative orbital ordering in iron arsenides.

[1]NSF

10:48AM P26.00013 Neutron and ARPES constraints on the couplings of the multiorbital Hubbard model for the iron pnictides[1] , QINLONG LUO, ADRIANA MOREO, ELBIO DAGOTTO, Univ. of Tennessee/ORNL, GEORGE MARTINS, Oakland Univ., DAO-XIN YAO, Sun Yat-Sen Univ., MARIA DAGHOFER, IFW Dresden, RONG YU, Rice Univ. — The results of neutron-scattering and angle-resolved photoemission experiments for the Fe-pnictide parent compounds are shown to impose severe constraints on the range of values that can be considered "realistic" for the intraorbital Hubbard repulsion U and Hund coupling J in multiorbital Hubbard models treated in the mean-field approximation. Phase diagrams for undoped three- and five-orbital models are discussed, and the physically realistic regime of couplings is highlighted [1].

[1] Q. Luo *et al.*, Phys. Rev. B **82**, 104508 (2010), and references therein.

[1]This work was supported in part by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

Wednesday, March 23, 2011 8:00AM - 10:36AM –

Session P27 GQI: Focus Session: Semiconductor Qubits - Spin Readout, Backaction, and Valley Physics in Silicon C155

8:00AM P27.00001 Development of a Si/SiO_2based double quantum dot charge qubit with dispersive microwave readout[1] , M.G. HOUSE, University of California, Los Angeles, E. HENRY, A. SCHMIDT, University of California, Berkeley, O. NAAMAN, University of Calfornia, Berkeley, I. SIDDIQI, University of California, Berkeley, H. PAN, M. XIAO, H.W. JIANG, University of California, Los Angeles — Coupling of a high-Q microwave resonator to superconducting qubits has been successfully used to prepare, manipulate, and read out the state of a single qubit, and to mediate interactions between qubits. Our work is geared toward implementing this architecture in a semiconductor qubit. We present the design and development of a lateral quantum dot in which a superconducting microwave resonator is capacitively coupled to a double dot charge qubit. The device is a silicon MOSFET structure with a global gate which is used to accumulate electrons at a Si/SiO_2 interface. A set of smaller gates are used to deplete these electrons to define a double quantum dot and adjacent conduction channels. Two of these depletion gates connect directly to the conductors of a 6 GHz co-planar stripline resonator. We present measurements of transport and conventional charge sensing used to characterize the double quantum dot, and demonstrate that it is possible to reach the few-electron regime in this system.

[1]This work is supported by the DARPA-QuEST program.

8:12AM P27.00002 Dispersive microwave readout of a double quantum dot charge qubit in silicon , EDWARD HENRY, ANDREW SCHMIDT, QNL, UC Berkeley, MATHEW HOUSE, UCLA, OFER NAAMAN, H. PAN, MING XIAO, HONG-WEN JIANG, UCLA, IRFAN SIDDIQI, QNL, UC Berkeley, QNL, UC BERKELEY TEAM, JIANG GROUP, UCLA TEAM — Microwave resonators coupled to quantum systems have been used for fast dispersive measurement in many different architectures in solid state and atomic physics. The electronic states of a semiconductor quantum dot represent a promising candidate for quantum information processing. Our work is geared toward developing a fast, non-demolition readout of semiconductor qubit by coupling to a superconducting resonant circuit. We report on microwave measurements of a lateral quantum dot, realized using a silicon MOSFET structure, where the charge degree of freedom is capacitively coupled to a shorted quarter wave 6 GHz resonator. We characterize the sensitivity of this charge detection scheme and its implications for qubit readout fidelity.

8:24AM P27.00003 Radio Frequency Single Electron Transistors on Si/SiGe[1] , MINGYUN YUAN, ZHEN YANG, A.J. RIMBERG, Department of Physics and Astronomy, Dartmouth College, M.A. ERIKSSON, Department of Physics, University of Wisconsin, D.E. SAVAGE, Material Science Center, University of Wisconsin — Superconducting single electron transistors (S-SETs) are ideal for charge state readout due to their high sensitivity and low back-action. Upon successful formation of quantum dots(QDs) on Si/SiGe, aluminum S-SETs are added in the vicinity of the QDs. Coupling of the S-SET to the QD is confirmed by using the S-SET to perform sensing of the QD charge state at 0.3 K. We have formed a matching network for an SET with an off-chip inductor. The reflection coefficient of the radio frequency(RF) signal is shown to be modulated by the SET resistance. Efforts to develop an on-chip matching network and perform charge sensing with the RF-SETs are in progress. Recent experimental results will be discussed.

[1]This research was supported by the NSA, LPS and ARO.

8:36AM P27.00004 Two-detector two-qubit correlated continuous measurements and their implications for quantum computing , RUSKO RUSKOV, Laboratory for Physical Sciences,College Park, MD 20740, CHARLES TAHAN, Laboratory for Physical Sciences, College Park, MD 20740 — We calculate the full counting statistics for a system of two interacting qubits which are simultaneously measured by weakly coupled linear detectors. Two approaches are considered based on rate equations for the full system-detectors density matrix and on quantum filtering equations. Implications for the assessment of quantumness in physical devices based on charge qubits are considered. In addition we consider applications of such systems to practical quantum computing in silicon and/or GaAs quantum dots.

8:48AM P27.00005 Backaction due to Resonant Phonon Absorption in Quantum Dots Measured by a Quantum Point Contact , CAROLYN YOUNG, AASHISH CLERK, McGill University — Recent experiments have observed unexplained periodic resonances in the charging diagrams of both double [1] and triple [2] quantum dots (DQDs and TQDs). These resonances correspond to the generation of inelastic transitions, driven by energy transfer from a biased quantum point contact (QPC) charge detector used for measurement. In this talk, we present theoretical results describing how quantum backaction due to hot phonons, generated by the out-of-equilibrium QPC, can lead to excited state occupation under certain "blocking" conditions that result in slow ground state filling. We propose that recent experiments can be understood in terms of resonant phonon absorption in DQDs and TQDs; a process complementary to resonant phonon emission [3]. Our results shed light on an important contribution to the backaction of the QPC readout scheme widely used for QD-based quantum computation.

[1] D. Harbusch et al., Phys. Rev. Lett., 104, 196801 (2010).
[2] L. Gaudreau et al., App. Phys. Lett., 99, 193101 (2009).
[3] U. Gasser et al., Phys. Rev. B, 79, 035303 (2009).

9:00AM P27.00006 Measurement fidelity in the presence of coherent dynamics or dissipation , JIAN-QIANG YOU, Fudan University & RIKEN, S. ASHHAB, FRANCO NORI, RIKEN & University of Michigan — We analyze the problem of a charge qubit probed by a quantum point contact when the measurement is concurrent with Hamiltonian-induced coherent dynamics or dissipation. This additional dynamics changes the state of the qubit before the measurement is completed. As a result, the measurement fidelity is reduced. We calculate the reduction in measurement fidelity in these cases. References: S. Ashhab, J. Q. You, and F. Nori, New J. Phys. 11, 083017 (2009); Phys. Scr. T137, 014005 (2009).

9:12AM P27.00007 Probing coherent tunneling in semiconductor quantum dots using electromechanical backaction , JAMIE GARDNER, AASHISH CLERK, Department of Physics, McGill University — Self-assembled quantum dots have been studied intensely because of their possible applications to quantum information processing. While such dots are difficult to characterize using direct electrical transport measurements, it has recently been shown both theoretically [1] and experimentally [2] that a capacitively coupled AFM cantilever can serve as a sensitive probe of dot charge dynamics and electronic level structure. This sensitivity is based on the fact that the dot, which is tunnel-coupled to electrons in a reservoir, acts as a dissipative bath for the cantilever. Here, we extend previous theoretical work to describe an AFM cantilever coupled to a double quantum dot. Unlike a single-dot, the double-dot system exhibits both incoherent tunneling to the leads and coherent tunneling between the dots. We find that the cantilever's motion is affected by both kinds of tunneling and can yield significant information even in regimes where the total double-dot charge does not fluctuate. Cantilever dynamics can also be used to learn about the strength of dephasing processes in the double-dot. After presenting the theoretical approach to this problem, we will discuss the results in the context of current experimental efforts using InAs dots. These effects should also be accessible in a variety of other quantum dot setups. [1] S. D. Bennett, et al., Phys. Rev. Lett. **104**, 017203 (2010). [2] L. Cockins, et al., Proc. Nat. Acad. Sci. **107**, 9496 (2010).

9:24AM P27.00008 Few-electron states in SiGe double quantum dot structures with non-planar interfaces[1] , A.A. KISELEV, R.S. ROSS, M.F. GYURE, HRL Laboratories LLC, 3011 Malibu Canyon Road, Malibu CA 90265 — Valley-orbit effects of planar, non-planar, and imperfect heterointerfaces (both on the intra- and inter-dot scale) are directly captured in numerical simulations and analyzed theoretically for electrostatically defined accumulation mode (001) SiGe multi-dot structures. Our modeling is facilitated by explicitly allowing for an arbitrary and spatially inhomogeneous stacking of heterolayers in the active area of the device. Here we focus on results obtained for a double quantum dot (DQD) system, establishing the detailed structure of few-electron states, and, for two electrons, their spin- and valley-selective dynamics when the system is driven by pulse-modulating dot gate potentials. We identify valley-related avoided crossings and evaluate their strength affecting adiabaticity of applied bias sweeps. We consider a number of experimentally relevant scenarios stemming from (i) macroscopic interface imperfections, e.g., interface steps, and (ii) randomness of the substitutional solid solution in the SiGe barrier layers. Our findings are critically compared with results available for single valley III-V DQDs.

[1]Sponsored by the United States Department of Defense. Approved for Public Release, Distribution Unlimited.

9:36AM P27.00009 Extended interface states enhance valley splitting in Si/SiO2[1] , ANDRE SARAIVA, BELITA KOILLER, U. F. Rio de Janeiro, MARK FRIESEN, U. of Wisconsin — Interface disorder and its effect on valley degeneracy in the conduction band present an important theoretical challenge for operating spin qubit in silicon. Here, we demonstrate and investigate a counterintuitive effect occurring at Si/SiO2 interfaces. By applying tight binding methods, we show that intrinsic interface states can hybridize with conventional valley states to produce an anomalously large ground state energy gap. Such hybridization effects have not previously been explored in detail for valley splitting. We find that the splitting can be enhanced by disorder in the chemical bonds at the interface, in agreement with recent experiments.

[1]This work was supported in part by ARO and LPS, by NSF and CAPES. BK thanks CNPq, FUJB, INCT on Quantum Information and FAPERJ.

9:48AM P27.00010 Interface-mediated intervalley coupling in Si[1] , BELITA KOILLER, A.L. SARAIVA, Instit. de Fisica, UFRJ, Rio de Janeiro, Brazil, M.J. CALDERON, Instit. de Ciencia de Materiales de Madrid (CSIC), Spain, XUEDONG HU, Dep. of Physics, University at Buffalo-SUNY, S. DAS SARMA, Dep. of Physics, Condensed Matter Theory Center, University of Maryland, College Park, Maryland — The conduction band degeneracy in Si is detrimental to spin qubits, for which a nondegenerate ground orbital state is desirable. The Si valley degeneracy is reduced to 2 near an interface with an insulator, and it may be lifted by the spatially abrupt change in the crystal potential. Basic physical mechanisms for Si/barrier mediated valley coupling in different situations are addressed here. Theoretical studies of the interface-induced valley splitting in Si are presented. Abrupt and smooth interface profiles are considered, and the full plane wave expansions of the Bloch functions at the conduction band minima are included. Simple criteria are suggested for optimal fabrication parameters affecting the valley splitting, emphasizing the relevance of different interface-related properties. Refs: A.L.Saraiva et al, PRB 80, 081305 R (2009); arXiv:1006.3338

[1]Support: BK and ALS thank CNPq, FUJB, INCT on Quantum Information, and FAPERJ. M.J.C. acknowledges Ministerio de Ciencia e Innovación (Spain). XH amd SDS thank NSA and L PS. S.D.S. also thanks CMTC.

10:00AM P27.00011 Atomistic simulations of multi-valley silicon double quantum dots in the presence of disorder in the few electron regime[1] , RAJIB RAHMAN, ERIK NIELSEN, RICHARD MULLER, MALCOLM CARROLL, Sandia National Laboratories, Albuquerque, NM 87185 — The singlet-triplet based silicon double quantum dot (DQD) is a promising system for implementing a long-lived and controllable quantum bit. The multiple valleys present in silicon, however, may complicate the operation of such a qubit if the valley splitting is small. The valley splitting is affected by a large number of factors including interface roughness, lattice miscuts, electric and magnetic fields, barrier material, and alloy disorder. We employ an atomistic tight-binding (TB) method and a full configuration interaction (CI) to investigate few electron states of a multi-valley Si DQD. This unprecedented approach involving few million atoms allows us to investigate the role of atomic scale disorder (i.e., random alloy effects or interface roughness) on the energy levels and spin configurations of many electron DQDs.

[1]Sandia is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. DOE's NNSA under contract DE-AC04-94AL85000.

10:12AM P27.00012 Engineering anisotropic exchange interactions between quantum dot spin qubits , YUN-PIL SHIM, MARK FRIESEN, Department of Physics, Unviersity of Wisconsin-Madison, Madison WI 53706 — We present a method for engineering anisotropic exchange interactions between quantum dot spin qubits using a Heisenberg antiferromagnetic spin chain as a spin bus. An external magnetic field is applied to create XXZ interactions between spin qubits that are weakly connected to a spin bus whose ground state is non-degenerate. We analyze the dependence of the anisotropy of the effective interaction on the external field and on the length of the spin bus. We show that the tunable XXZ interaction mediated by the spin bus can be used to generate multi-qubit entanglement and to efficiently implement universal gates based on encoded qubits. We also show that the operation of the spin bus is qualitatively different when the spin bus is near one of its magnetic field-induced quantum phase transitions. In this case, the qubits interact with a bus pseudo-spin and the resulting entanglement between pairs of qubits is enhanced.

10:24AM P27.00013 Asymmetric Quantum Pd Films for Enhanced Hydrogen Separation[1] , GUANGFEN WU, Southeast U, U of Tennessee-Knoxville, Oak Ridge National Laboratory, WENGUANG ZHU, U of Tennessee-Knoxville, Oak Ridge National Laboratory, JINLAN WANG, Southeast U, ZHENYU ZHANG, Oak Ridge National Laboratory, U of Tennessee-Knoville,U of Science and Technology of China — Based on density functional theory calculations and numerical simulations, we have investigated the permeation of H2 through ultra-thin Pd quantum films. The H2 flux can be highly increased by the elevation of the chemisorption-well on the permeate side without significantly blocking the subsurface-surface penetration. We find that Cu-coated asymmetric Pd quantum films (with the Cu monolayer on the permeate side) will enhance the capability for H2 separation: the recombination barrier for H is reduced from 1.36 to 0.79 eV, while the subsurface-surface penetration barrier is only slightly increased from 0.04 to 0.10 eV. Numerical simulations show enhanced H2 flux by 5 orders of magnitude as an upper-limit for asymmetric Pd films over symmetric ones under similar conditions.

[1]Supported by DMSE of USDOE, USNSF, and NNSF of China.

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P28 DCMP: Carbon Nanotubes: Optical Properties C156

8:00AM P28.00001 Empirical Study of the π electron Plasmon Energy Dependence on the Bundling/De-bundling Effect in Single Wall Carbon Nanotubes , KIRAN LINGAM, RAMAKRISHNA PODILA, PENGYU CHEN, Clemson University, CODRUTA LOEBICK, NAN LI, LISA PREFFERLE, Yale University, APPARAO RAO, Clemson University — Many researchers have done detailed studies on optical, thermal and electronic properties of SWNTs. But, very few studies have been done on sub-nanometer SWNTs. Here we studied collective electron excitations in this quasi 1D system. At high excitation energies, broad absorption peak is observed which is attributed to the π plasmon (5-7 eV). We used UV-Vis NIR spectroscopy to determine the energy of the π plasmons in sub nanometer diameter SWNTs (0.4 nm to 0.9 nm). SWNTs form bundles due to van der Waal forces and this bundling influences their electronic structure. It is known that SWNTs wrapped with a surfactant can be isolated with long centrifugation. The hydrodynamic sizes of the dispersed SWNTs at different centrifugation times were determined by using the Dynamic Light Scattering technique. Systematic studies have been done on the dependence of the π plasmon energy on the nanotube bundle diameter. The energy of the π plasmon was found to vary with the bundle diameter and the energy to be given by the relation E= (-0.022 eV)*ln(d/1 nm)+5.34 eV. We have done similar studies on HiPCo and Carbolex SWNTs and the empirical relation obtained is consistent with the results above.

8:12AM P28.00002 Simultaneous measurement of length, concentration and brightness of single-walled carbon nanotubes with fluorescence correlation spectroscopy , DENIS PRISTINSKI, CONSTANTINE KHRIPIN, XIAOMIN TU, MING ZHENG, NIST — We report on the application of fluorescence correlation spectroscopy (FCS) to simultaneously measure the brightness, concentration, and length of single-walled carbon nanotubes (SWCNTs). The technique relies on the intrinsic bandgap luminescence of (6,5) chirality semiconducting SWCNTs in the near infra-red (NIR) range and does not require sample labeling. The nanotubes used in this study have been dispersed in solution of single stranded DNA and length fractionated via size exclusion chromatography. The SWCNT length measured by FCS was in excellent agreement with more traditional techniques - polarized dynamic light scattering (DLS) and atomic force microscopy (AFM). The apparent nanotube brightness is shown to grow linearly with the mean nanotube length, having a zero intensity cut-off at 110 nm, implying an exciton diffusion length of 55 nm for SWCNTs dispersed in sodium deoxycholate.

8:24AM P28.00003 Absolute Rayleigh Intensity and Uniform Optical Conductivity in Carbon Nanotubes , LIHONG HERMAN, Cornell Applied Physics, DANIEL JOH, JESSE KINDER, SANG-YONG JU, MICHAEL SEGAL, JEFFREYS JOHNSON, GARNET CHAN, JIWOONG PARK — We used a novel on-chip Rayleigh imaging technique to measure the absolute intensity of Rayleigh scattering of single-walled carbon nanotubes. The spatial distribution of the radiation scattered by the nanotubes is determined by their shape, but the intensity and spectrum of the scattered radiation are determined by exciton dynamics, quantum-dot-like optical resonances and other intrinsic properties. Moreover, the nanotubes display a uniform peak optical conductivity $\sim$8 e^2/ h, which we derive using an exciton model, suggesting universal behaviour similar to that observed in nanotube conductance. We further demonstrate a radiative coupling between two distant nanotubes, with potential applications in metamaterials and optical antennae. This is in contrast to the optical properties of metal nanostructures and show that nanotubes can form ideal optical wires.

8:36AM P28.00004 Dielectric screening dependence of excitonic transition energies in single-wall carbon nanotubes , PAULO ARAUJO, MILDRED DRESSELHAUS, Massachusetts Institute of Technology, ADO JORIO, Universidade Federal de Minas Gerais, KENTARO SATO, AHMAD NUGRAHA, RICHIIRO SAITO, Tohoku University — The measured optical transition energies E_{ii} of single-wall carbon nanotubes are compared with bright exciton energy calculations. The E_{ii} differences between experiment and theory are minimized by considering first, a diameter/chiral angle-dependent dielectric constant and second, a diameter/exciton size-dependent dielectric constant (k). In our description, k is composed of the screening contributions from the tube, represented by k_{tube}, and from the environment, represented by k_{env}. We discuss the main aspects of each approach and show that in the first case, different k dependencies are obtained for (E^S_{11}, E^S_{22}, E^M_{11}) relative to (E^S_{33}, E^S_{44}) which is understood as follows: A changing environment changes the k diameter dependence for (E^S_{11}, E^S_{22}, E^M_{11}), but for (E^S_{33}, E^S_{44}) the environmental effects are minimal. We show that in order to achieve a single dependence for all E_{ii}, the exciton's size should be taken into account, as considered in the second approach. The resulting calculated exciton energies reproduce experimental E_{ii} values within |50| meV for a diameter range (0.7< dt <3.8 nm) and 1.2 < Eii <2.7 eV, thus providing a theoretical justification for E_{ii} and important insights into the dielectric screening in one-dimensional structures.

8:48AM P28.00005 Temperature-Dependent Maximum Density of 1D Excitons in Carbon Nanotubes , THOMAS SEARLES, IAN WALSH, TAKAYUKI NOSAKA, WILLIAM RICE, JUNICHIRO KONO, Dept. of Electrical and Computer Engineering, Rice University — Previous studies have shown that an upper limit exists on the density of 1D excitons in single-walled carbon nanotubes (SWNTs) due to very efficient exciton-exciton annihilation (EEA). A recent theoretical study based on a dark-bright two-band exciton model predicts that there is a temperature at which the achievable exciton density will be maximized, surpassing the room-temperature upper limit. Therefore, we performed temperature-dependent (300 K to 11 K) photoluminescence (PL) on HiPco SWNTs embedded in an i-carrageenan matrix under high resonant excitation. To achieve high densities, we used pump fluences up to $\sim 10^{14}$ photons/cm^2, utilizing intense fs pulses from a wavelength-tunable optical parametric amplifier. We found that for each temperature the PL intensity saturates as a function of pump fluence and the saturation intensity increases from 300 K to a moderate temperature around 100-150 K. Below that critical temperature, the PL intensity decreases with decreasing temperature. Within the framework of diffusion-limited EEA, we successfully estimated the upper limit of the density of 1D excitons in SWNTs as a function of temperature and chirality

9:00AM P28.00006 Experimental Kataura Plot in Single-walled Carbon Nanotubes , KAIHUI LIU, FAJUN XIAO, RODRIGO CAPAZ, JACK DESLIPPE, Phys Dept. UC Berkeley, WENLONG WANG, IOP, CAS, Beijing, China, SHAUL ALONI, The Molecular Foundry, LBNL, Berkeley, STEVEN LOUIE, Phys Dept. UC Berkeley, ENGE WANG, ICQM, Peking University, Beijing, China, FENG WANG, Phys Dept. UC Berkeley, PHYS DEPT. UC BERKELEY TEAM, THE MOLECULAR FOUNDRY, LBNL, BERKELEY COLLABORATION, IOP, CAS, BEIJING, CHINA COLLABORATION, ICQM, SCHOOL OF PHYSICS, PEKING UNIVERSITY, BEIJING, CHINA COLLABORATION — Single-walled carbon nanotubes (SWNTs) comprise a family of more than 400 structures characterized by different chiral indices n-m, each having a distinct electronic structure that can be either metallic or semiconducting. An outstanding question is how the physical properties, such as optical transitions, vary with the exact nanotube structures. By combining TEM diffraction and Rayleigh scattering spectroscopy on the same individual nanotubes, we determine independently the chiral indices and optical transitions of over 170 single-walled nanotubes. These data permit us to create an experimental Kataura plot for single-walled carbon nanotubes.

9:12AM P28.00007 Optical Properties of Empty and Water-Filled Single-Wall Carbon Nanotubes , J.R. SIMPSON, Towson University, J.A. FAGAN, J.Y. HUH, A.R. HIGHT WALKER, National Institute of Standards and Technology, J.L. BLACKBURN, B.A. LARSEN, J. HOLT, National Renewable Energy Laboratory — The necessity for separation of single-wall carbon nanotube (SWCNT) populations to achieve desired properties presents a major technical barrier for the development of SWCNT-based applications, and has been the focus of significant academic and industrial research. Recent advances include the separation of SWCNT populations by diameter through buoyancy differences. Here we report on the optical spectroscopic properties of large diameter SWCNTs synthesized by laser ablation and electric arc methods and then separated by centrifugation to produced isolated bands of empty and water-filled nanotubes. This separation is consistent across multiple nanotube populations dispersed from different source material. Optical absorption, near-infrared fluorescence, and Raman spectroscopic measurements of the resulting empty and filled fractions reveal that water filling leads to systematic changes in the optical properties. Specifically, the peak locations in absorbance and fluorescence display red-shifts with the presence of water in the nanotube cavity and a hardening of the Raman radial breathing modes. The presence of water in the SWCNT interior is found to facilitate the subsequent separation into sub-populations of metallic and semiconducting SWCNTs.

9:24AM P28.00008 Rapid widefield Raman imaging of individual carbon nanotubes , ROBIN HAVENER, SANG-YONG JU, MICHAEL SEGAL, LIHONG HERMAN, JIWOONG PARK, Cornell University — Raman spectroscopy is a powerful tool for characterizing carbon nanotubes. Confocal micro-Raman imaging can provide detailed spatial and spectral information about individual nanotubes, but this technique is often time-consuming. We present a widefield Raman microscope capable of rapid and large-area imaging of carbon nanotube samples. Thanks to a widefield excitation geometry, a high-power excitation laser (3W in our experiment) can be used without causing thermal damage to nanotubes, which dramatically shortens image acquisition time ($\sim$20sec for G- band for a 60μm field of view). With a custom-built tunable bandpass filter, our widefield Raman images let us quantitatively compare the D, G and 2D-band intensities of many nanotubes with different known resonant energies, diameters, and metallicities, while providing the Raman scattering cross-section length for individual nanotubes. This technique allows Raman-based spatially resolved investigation of dynamic processes in nanotubes for the first time, which we demonstrate by real-time imaging of the oxidation of nanotubes at high temperatures.

9:36AM P28.00009 Absence of Broad G$^-$ Feature in Resonant Raman Spectra of Armchair Carbon Nanotubes , E.H. HAROZ, W.D. RICE, J. KONO, Department of Electrical & Computer Engineering, Rice University, J.G. DUQUE, C.G. DENSMORE, S.K. DOORN, Center for Integrated Nanotechnologies, Los Alamos National Laboratory — Unlike the radial breathing mode in carbon nanotubes (CNTs), the G-band Raman feature does not display a strong frequency dependence on nanotube structure. The appearance of a broad G$^-$ peak in CNT Raman spectra has been attributed to numerous phenomena including the presence of metallic nanotubes, although a consensus has yet to be achieved amongst researchers. Here, we present resonant Raman measurements on macroscopic ensembles enriched in armchair CNTs produced by density gradient ultracentrifugation. Our G-band data clearly show that the broad, lower-frequency G$^-$ mode is absent for armchair structures, in contrast with recent theoretical and experimental results, and only occurs with resonance of non- armchair metals. This forms a generalized correlation between G-band lineshape and nanotube structure due to the sampling of a large number of nanotubes of several armchair species.

9:48AM P28.00010 Infrared active vibrations in carbon nanotubes[1] , KATALIN KAMARAS, ARON PEKKER, Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, Budapest — The method of choice for the study of vibrational modes of carbon nanotubes has been almost exclusively Raman spectroscopy. Although calculations predict also infrared-active modes in nanotubes, so far only very few experimental results have been published. We conducted a systematic investigation of the infrared transmission of various types of single- and double-walled carbon nanotubes. Experiments were done on self-supporting transparent films in order to avoid perturbation from substrates. We find weak but reproducible vibrational peaks in the infrared spectrum. Their frequency scales with the diameter of the tubes, indicating their intrinsic character. Furthermore, on doping, some of the peaks change from Lorentzian to Fano-like character. This change can be explained by coupling of the tube vibrations to the conduction electrons introduced by doping. Finally, in double-walled nanotubes peaks typical of both outer and inner tubes can be distinguished. The vibrations of the inner tubes occur at the same frequency as those of single-walled tubes with the same diameter.

[1]Supported by NKTH under Project No. TECH-09-A2-2009-0134 (FIBERSC2).

10:00AM P28.00011 Far Infrared Optical Studies of Single and Double Walled Carbon Nanotubes , SHIN GRACE CHOU, NIST, AHMED ZEESHAN, GEORGY SAMSONIDZE, JING KONG, MILDRED DRESSELHAUS, JEFFREY FAGAN, DAVID PLUSQUELLIC — Variable temperature far infrared absorption measurements were carried out for single walled and double walled carbon nanotubes samples (SWCNT and DWCNT) encased in a polymer matrix to investigate the effects of temperature and surface interaction on the low frequency phonons associated with the circumferential vibrations. At a temperature where kBT is significantly lower than the phonon energy, the broad absorption features as observed at room temperature become well resolved phonon transitions. For a DWCNT sample whose inner tubes have a similar diameter distribution as the SWCNT sample studied, a series of sharp features were observed at room temperature at similar positions as for the SWCNT samples studied. The narrow linewidth is attributed to the fact that the inner tubes are isolated from the polymer matrix and from the weak inter-tubule interactions. First principles calculations are carried out to understand the pertinent interactions and the temperature-dependent effects.

10:12AM P28.00012 Influence of Defects and Doping on Optical Phonon Dynamics in Carbon Nanotubes , DANER ABDULA, KHOI NGUYEN, KWANGU KANG, SCOTT FONG, TANER OZEL, DAVID CAHILL, MOONSUB SHIM, University of Illinois Champaign- Urbana — The relaxation of electronic excitations induced by high bias or photoexcitation occurs primarily through optical phonon emission. Optical phonon relaxation may be affected by metallic/semiconducting character of carbon nanotubes, defect concentration, as well as doping. Changes in carbon nanotube G-band optical phonon population and pure dephasing lifetimes with doping and defects are described. Time-resolved incoherent anti-Stokes Raman spectroscopy is used to directly measure phonon decay lifetime, T_1, while total dephasing rate is inferred from static Raman linewidths. Defect concentration is varied by sample annealing and covalent functionalization showing increasing disorder reduces T_1 as well as overall dephasing time, T_2, with an even greater dependence. Samples with different metallic and semiconducting contribution have similar lifetimes, $T_1 \sim 1.2 \pm 0.1$ ps in the no defect limit. Doping is shown to increase G-band linewidth, and therefore overall dephasing rate, for semiconducting nanotubes while leaving T_1 unaffected.

10:24AM P28.00013 Ultrafast Terahertz Probes of Individualized, Chirality-Enriched Single-Walled Carbon Nanotubes , LIANG LUO, IOANNIS CHATZAKIS, JIGANG WANG, Department of Physics and Astronomy and Ames Laboratory, Iowa State University — Singled-walled carbon nanotubes (SWNTs) represent a model system to systematically investigate correlated charge excitation in 1-D limits. One of the most outstanding issues both in fundamental nanotube physics and for their technological development is to detect and understand optically-forbidden, dark collective states. Thus far supporting evidence of dark states has been demonstrated in static magneto-optics and light scattering. However, the unique internal transitions from dark excitonic ground states and their dynamic evolution remain highly elusive. We report our investigation of this problem using optical-pump, terahertz probe spectroscopy of individualized, (6,5) and (7,5) SWNTs. We measure transient THz conductivity from 1-15 meV at low temperature down to 4K with resonant and off-resonant excitation at the E_{22} transitions of (6,5) and (7,5) nanotubes. The intra-excitonic spectroscopy with THz pulses represents a fundamentally different spectroscopy tools to study dark excitons and shine new lights on the nature of excitonic ground states.

10:36AM P28.00014 Nonlinear Optical Response of Individual Carbon Nanotubes , TATYANA SHEPS, BRAD L. CORSO, ERIC O. POTMA, PHILIP G. COLLINS, Department of Physics and Astronomy and Department of Chemistry, Univ. of California at Irvine, Irvine, CA 92697 — Single walled carbon nanotubes (SWCNTs) are low dimensional conductors with unique nonlinear electro-optic properties. To investigate these properties we study the third-order, coherent anti-stokes (CAS) response of electrically connected individual SWCNTs on quartz substrates, using a four-wave-mixing (FWM) technique with femtosecond laser pulses. Because the CAS response is primarily electronic in nature [1], the signal from metallic SWCNTs is much stronger than from semiconducting ones. CAS easily distinguishes between the two types, as well as between semiconducting SWCNTs doped to be conductive or insulating. Furthermore, the CAS signal is sensitive to excitation resonances, the same effect that allows SWCNT fingerprinting by photoluminescence and Raman techniques. In addition to the strong electronic signal, we can also resolve a vibrational signal component at the G-band frequency, which suggests a method for studying chemical bond vibrations with this coherent technique. The good spatial resolution and high signal-to-noise achieved with femtosecond laser pulses provides opportunities for time-resolved optical measurements of SWCNT excitation dynamics. Funded by NSF Center for Chemistry at the Space-Time Limit at UCI (CHE-0847097).

[1] H. Kim et al, Nano Lett. 9 2991-2995 (2009)

10:48AM P28.00015 Second Harmonic Generation in Highly Aligned Carbon Nanotubes on GaAs , D.T. MORRIS, G.L. WOODS, J. KONO, ECE Dept., Rice University, C.L. PINT, R.H. HAUGE, Chemistry Dept., Rice University — Optical properties of carbon nanotubes (CNTs) have been extensively investigated during the last decade, and much basic knowledge has been accumulated on how light emission, scattering, and absorption occur in CNTs. However, their nonlinear optical properties remain largely unexplored, except for theoretical studies predicting highly chirality-selective nonlinear optical processes. In particular, all chiral nanotubes are expected to possess finite second-order nonlinear susceptibilities due to the lack of inversion symmetry. Here, we have observed second harmonic generation (SHG) from samples consisting of highly aligned CNTs on GaAs with linearly-polarized intense mid-infrared femtosecond radiation. SHG is expected from both the CNTs and the substrate, thus the contribution of the CNTs to the overall enhanced SHG signal will be obtained by factoring out contributions from the GaAs substrate, which include any anisotropic effects (absorption, polarization) from the CNTs on the fundamental light incident in the GaAs substrate. We performed detailed angular dependent measurements to separate the two contributions, based on the crystal symmetries of the two. The results will be shown as a function of laser power and wavelength, and discussed in light of CNT band structure.

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P29 GQI: Focus Session: Superconducting Qubits C148

8:00AM P29.00001 LeRoy Apker Award Talk: Parallel State Transfer and Efficient Quantum Routing on Quantum Networks[1] , CHRISTOPHER CHUDZICKI, MIT — We study the routing of quantum information in parallel on multi-dimensional networks of tunable qubits and oscillators. These theoretical models are inspired by recent experiments in superconducting circuits using Josephson junctions and resonators. We show that *perfect parallel state transfer* is possible for certain networks of harmonic oscillator modes. We further extend our model to analyze the distribution of entanglement between every pair of nodes in the network, and find that the routing efficiency of hypercube networks is both optimal and robust in the presence of dissipation and finite bandwidth.

[1]This research was supervised by Frederick W. Strauch; it was supported by Williams College and Research Corporation. A paper preprint based on this work is available online: (arXiv: 1008.1806).

8:36AM P29.00002 Towards long coherence superconducting qubits , MATTHIAS STEFFEN, IBM, ANTONIO CORCOLES, JERRY CHOW, CHAD RIGETTI, MARK KETCHEN, MARY BETH ROTHWELL, GEORGE KEEFE, JIM ROZEN, MARK BORSTELMANN, JACK ROHRS, DAVID DIVINCENZO — The capacitively shunted flux qubit (CSFQ) has recently been shown to have coherence times of 1-2 microseconds repeatedly over many devices at typical qubit operating frequencies. Experiments in our group strongly suggest that losses associated with the shunting capacitor limit the current coherence times. As a result we propose novel approaches towards decreasing capacitive losses by employing geometric and/or materials developments. We show experimental data and compare these with theoretical predictions

8:48AM P29.00003 Circuit QED without selection rules: the dispersive regime of the fluxonium qubit , GUANYU ZHU, JENS KOCH, Northwestern University — Manipulation and readout of superconducting qubits with microwave photons, as realized in circuit QED, commonly employ the dispersive regime. In this regime, the qubit-photon interaction strength is small compared to the relative detuning Δ, and manifests itself only in the dispersive energy shifts χ, crucial for dispersive readout and spectroscopy of the qubit. For Cooper Pair Box and transmon, these shifts are known to scale like $1/\Delta$ and $1/\Delta^2$, respectively, making readout at very large detuning challenging. We show that the relation between χ and Δ is mainly dictated by selection rules, and derive general expressions describing the dispersive regime of a multi-level qubit with arbitrary matrix elements. This generalization turns out essential for describing the dispersive regime of the fluxonium qubit, where no simple selection rules exist. We show that this lack of selection rules explains the suprising magnitude of disperse shifts, at detunings as large as $\sim$8GHz, and also causes peculiarities observed in the fluxonium spectroscopy.

9:00AM P29.00004 Tunable coupling in circuit quantum electrodynamics with a superconducting V-system , SRIKANTH SRINIVASAN, ANTHONY HOFFMAN, DEVIN UNDERWOOD, Princeton University, JAY GAMBETTA, Institute for Quantum Computing and Department of Applied Mathematics, University of Waterloo, ANDREW HOUCK, Princeton University — We demonstrate a new superconducting charge qubit that realizes a V-shaped energy level spectrum, enabling tunable coupling between the qubit and a superconducting cavity while retaining all of the advantages, including charge noise insensitivity, common to other charge qubits such as the transmon. Tunable coupling is achieved with quantum interference between the two excited states of the qubit. We report measurements of the vacuum Rabi splitting, showing that the coupling strength can be tuned from greater than 40 MHz to less than 200 kHz using fast flux bias lines. This dynamically tunable coupling is an intrinsic property of the qubit and requires no additional coupling circuit elements. This new qubit design shows great promise for future quantum information processing and quantum optics experiments.

9:12AM P29.00005 Inductive coupling of superconducting qubits to coplanar waveguide resonators[1] , J.D. STRAND, M.P. DEFEO, P. BHUPATHI, C. SONG, M. WARE, B. XIAO, B.L.T. PLOURDE, Syracuse University — Superconducting qubits coupled to microwave resonators provide a promising basis for a scalable quantum computing architecture and enable explorations of circuit quantum electrodynamics. One approach for achieving strong coupling between a qubit and resonator involves sharing the kinetic inductance of a narrow superconducting line. We are investigating different designs for inductively coupling qubits, including capacitively shunted flux qubits, to coplanar waveguide resonators. We are working to optimize the coupling while accommodating the space requirements of different qubit types and preserving the performance of the resonator. We present microwave measurements of these structures as well as modeling of the qubit-resonator coupling.

[1]Work supported by IARPA

9:24AM P29.00006 Transmon qubits coupled to compact resonators[1] , S. SHANKAR, K. GEERLINGS, E. EDWARDS, L. FRUNZIO, R.J. SCHOELKOPF, M.H. DEVORET, Applied Physics Dept., Yale University — Compact resonators comprising of a meander inductor and an interdigitated capacitor are desirable building blocks for a multi-qubit processor due to their small size. We present an experiment on a superconducting transmon qubit coupled capacitively to such a compact resonator. We have fabricated low-loss Nb based compact resonators with an area within 1 mm^2 on a sapphire substrate to operate between 5 and 8 GHz. The resonator geometry was optimized to achieve an intrinsic quality factor above 300,000 at single-photon microwave powers and temperatures below 100 mK. Transmon qubits were made using Al/AlOx/Al Josephson junctions shunted by an Al interdigitated capacitor with an identical width and gap as the resonator. We will present our experimental progress towards measuring relaxation times of these qubits.

[1]Work supported by IARPA, ARO and the NSF.

9:36AM P29.00007 Design of a dc SQUID Phase Qubit with Controlled Coupling to the Microwave Signal[1] , R.P. BUDOYO, A.J. PRZYBYSZ, B.K. COOPER, H. KWON, Z. KIM, B. CHENG, A.J. DRAGT, J.R. ANDERSON, C.J. LOBB, F.C. WELLSTOOD, University of Maryland, College Park, M. KHALIL, S. GLADCHENKO, M. STOUTIMORE, B.S. PALMER, K.D. OSBORN, Laboratory for Physical Sciences — We have designed an Al/AlO$_x$/Al dc SQUID phase qubit on a sapphire substrate with a qubit junction area of 0.3 μm^2 to minimize loss associated with two-level systems in the junction oxide barrier. The qubit junction is shunted with a 1.5 pF interdigitated capacitor, and is isolated from the bias leads by an LC filter and an inductive isolation network using a larger Josephson junction. A previous device we built with similar parameters had its relaxation time T_1 limited by coupling to the microwave line. To reduce this coupling, we adopted a transmission line design and verified the coupling strength using microwave simulations. The new design will also allow us to measure the coupling to the SQUID by throughput measurements. We will discuss our design, the microwave simulations, our estimates for the overall coherence time due to losses and noise from various sources, and our progress towards testing the device.

[1]Acknowledgement: DOD, JQI, and CNAM

9:48AM P29.00008 Two junction effects in dc SQUID phase qubit[1] , B.K. COOPER, H. KWON, A.J. PRZYBYSZ, R. BUDOYO, J.R. ANDERSON, C.J. LOBB, F.C. WELLSTOOD, JQI and CNAM, U. of Maryland — The dc SQUID phase qubit was designed to allow one isolation junction to filter bias current noise from a second junction operating as a single junction phase qubit. As junctions shrink to minimize dielectric loss, the Josephson inductances of each junction approach the coupling loop inductance and this single junction picture appears inadequate. We consider a two-junction model of the dc SQUID phase qubit, where the qubit now corresponds to one of the normal oscillatory modes of the full SQUID. We discuss applications of this model to sweet spots in various control parameters and unusual behavior in the tunneling state measurement.

[1]Funded by DOD, CNAM and JQI

10:00AM P29.00009 Two-Dimensional quantum dynamic in a dc SQUID[1] , FLORENT LECOCQ, Institut Neel, CNRS, Grenoble, France, I.M. POP, Z. PENG, I. MATEI, C. NAUD, F.W. HEKKING, W. GUICHARD, O. BUISSON, Institut Neel and LPMMC, CNRS, Grenoble, France, R. DOLATA, A.B. ZORIN, PTB, Braunschweig, Germany — The dynamics of a dc SQUID presents a large variety of quantum effects at very low temperature such as 2D MQT signature, multilevel and phase qubit dynamics. We have shown that along the zero current bias line, the quantum dynamics is protected from current fluctuations. Along this line, the potential is quadratic-quartic and enhanced phase qubit properties have been demonstrated[2] When the dc SQUID loop inductance is of the order of the Josephson inductance the dynamic becomes two dimensional. As a consequence, in addition to the oscillation mode producing the phase qubit, a second oscillation mode exists, called transverse mode. Here we report spectroscopic evidence and coherence properties of both oscillators as well as coherent oscillations between the quantum states of these two coupled oscillators.

[1]Supported by the EU project EuroSQIP and SOLID, and ANR QUANTJO.
[2]E. Hoskinson et al, Phys. Rev. Lett. 102, 097004 (2009)

10:12AM P29.00010 Stark effect and generalized Bloch-Siegert shift in a strongly driven two-level system , MATTI SILVERI, JANI TUORILA, University of Oulu, MIKA SILLANPÄÄ, Aalto University, School of Science, YURIY MAKHLIN, Landau Institute for Theoretical Physics, ERKKI THUNEBERG, University of Oulu, PERTTI HAKONEN, Aalto University, School of Science — A superconducting qubit was driven in an ultrastrong fashion by an oscillatory microwave field, which was created by coupling via the nonlinear Josephson energy. The observed Stark shifts of the "atomic" levels are so pronounced that one has to go beyond the rotating wave approximation to properly explain the measurements. The difference between the prediction of the rotating wave approximation and the full calculation including all higher orders constitutes the generalized Bloch-Siegert shift which was verified in the measurement. Based on the Floquet approach for the driven two-level system, we calculate the landscape of the quasienergy splitting and the matrix elements of the probe transition, which were probed by resonant absorption via a cavity. The calculation taking into account both the resonance condition and the magnitude of the probe absorption agrees well with the measurement results.

10:24AM P29.00011 Time-Reversal Symmetry and Temporal Coherent Back-Scattering in a Driven Two-Level System , SIMON GUSTAVSSON, Massachusetts Institute of Technology, MARK RUDNER, Harvard University, JONAS BYLANDER, LEONID LEVITOV, Massachusetts Institute of Technology, WILL OLIVER, MIT Lincoln Laboratory — Coherent backscattering, resulting from quantum interference of the paths related by time-reversal symmetry, is a phenomenon fundamental for quantum-chaotic dynamics. It manifests itself in diverse transport phenomena which were predicted and studied in mesoscopic electron systems in 1980's and 1990's: universal conductance fluctuations (UCF), weak localization and anti-localization, etc. Here we present first experimental realization of the essential physics of coherent backscattering in a driven quantum system, a two-level system repeatedly driven through an avoided level crossing. Our experiment is performed with a superconducting qubit driven through level crossing by a sequence of RF pulses. Each passage through the level crossing serves a Landau-Zener-type "scattering event," with the wave function splitting between the up and down qubit states in a coherent fashion and recombining at a subsequent passage through the level crossing. Time-reversal symmetry can be enforced in our system by the driving protocol, resulting in constructive interference in the up-down transition rates. We observe an enhancement of the speckle-like fringe contrast analogous to UCF, which is suppressed in the absence of time reversal symmetry.

10:36AM P29.00012 Dark states of cavity-coupled qubits , S. FILIPP, A.F. VAN LOO, A. WALLRAFF, ETH QUANTUM DEVICE TEAM — In circuit quantum electrodynamics (QED) the cavity-mediated dispersive interaction is the dominant inter-qubit coupling mechanism when the qubits are detuned from the resonator. This mechanism can be used to realize two-qubit gates. Here, we investigate the strength of this interaction explicitly considering the Fabry-Perot like multi-mode structure of the microwave frequency transmission line resonator. We observe the formation of dark states when the qubits are driven jointly by the same resonator microwave field and tuned into resonance with each other [1]. These dark states arise from the symmetry properties of the coupled quantum system at the avoided level crossing. Furthermore, we study the suppression of spontaneous emission of the coupled-qubit system by driving it into its dark state using microwave fields local to the individual qubits.

[1] S. Filipp *et al.*, arXiv:1011.3732 (2010).

10:48AM P29.00013 Entanglement between the charge and phase degrees of freedom in a superconducting qubit , MUN DAE KIM, Yonsei University — The charge and phase are conjugate variables with each other in superconducting qubits which are characterized by either the charge or the phase degree of freedom. In this study we propose a qubit scheme where the charge and phase degrees of freedom are entangled in the qubit. In our qubit the qubit states consists of the phase states of the qubit, while the qubit states can be measured through the charge state detection. The qubit operation can be performed at the optimal point with respect to both the external magnetic flux and gate voltage. We discuss the fidelity of the Rabi oscillation and the possible way of enhancement of fidelity.

Wednesday, March 23, 2011 8:00AM - 11:00AM –
Session P30 DCMP: Nanowires & Nanotubes: Growth & Absorption Kinetics C147/154

8:00AM P30.00001 Covalent functionalization of ZnO nanowires , ANDREIA LUISA DA ROSA, NEY MOREIRA, ADRIEL GARCIA, THOMAS FRAUENHEIM, University of Bremen — Understanding the interaction of organic species with inorganic nanostructures constitutes a step forward in the development of semiconductor based biosensors. In this work we have used density functional theory to investigate ZnO-(1010) nanowire surfaces modified with substituted methane molecules (Me-X, with X= OH, NH2, SH, COOH, and CN). We have found three relevant stabilization mechanisms acting on the surface stabilization: passivation of surface oxygen lone-pairs via dissociative chemisorption processes, electrostatic adsorbate-interations involving Zn surface sites and hydrogen bonding interactions involving oxygen surface sites. Covalent adsorbate-substrate interactions were found to play only a marginal role on the surface stabilization. Contradicting the usual chemical intuition, we have found no significant evidence for the formation of classical Lewis acid-base adducts on Zn surface sites. Finally we suggest that the functionalization with Me-COOH is also expected to be stable under ordinary laboratory conditions or in aqueous media.

8:12AM P30.00002 Growth and Characterization of Serrated GaN Nanowires , ZHENG MA, DILLON MCDOWELL, MOHAMED ABD ELMOULA, EUGEN PANAITESCU, DALMAU REIG, LATIKA MENON, Northeastern University — We describe our results on the growth of single crystalline GaN nanowires on catalyst-patterned substrates by means of chemical vapor deposition. The growth is carried out in a horizontal quartz tube inside a tube furnace wherein gallium oxide powder is used as reactor source and a mixture of ammonia and hydrogen gas is used as precursor. Growth of GaN nanowires are demonstrated on both Au and Ni-catalyst patterned substrates (either sapphire or silicon). The growth temperature is maintained at around 960 °C. We show that by controlling the deposition parameters, specifically the size of the catalyst and amount of gallium oxide GaN nanowires grow in a "serrated" pattern. The serrated nanowires maintain a stable, single crystalline state with very regular periodic serrations. The wires have been characterized by means of scanning electron microscopy, transmission electron microscopy and energy dispersive x–ray scattering measurements. Preliminary electrical transport measurements on single serrated GaN nanowires released onto a Si substrate show that the wires exhibit improved electron transport capabilities in comparison with regular GaN nanowires.

8:24AM P30.00003 GaAs nanowires and GaAs/AlGaAs core/shell nanowires synthesized by MOCVD[1] , BRIAN PETERS, NICHOLAS MINUTILLO, JOHN CARLIN, FENGYUAN YANG, The Ohio State University — Nanowires made by the "bottom-up" approach can be used in a variety of electrical and optoelectronic devices as well as in the study of low dimensional transport physics. We have grown GaAs nanowires using Au catalysts in a closed couple showerhead MOCVD system. A number of growth parameters, including the substrate temperature, growth rate, and Arsine/TMGa ratio, are explored to identify optimal conditions for growth of GaAs nanowires with large aspect ratio and minimal tapering. Higher substrate temperatures result in larger tapering and lower temperature leads to "kinks." Meanwhile, large V/III source ratio gives large tapering as well. We have found that our optimal conditions are at a substrate temperature of 420 °C and V/III ratio of ∼25, which gives a tapering of less than 1 nm increase in diameter per micron in length. In addition, GaAs/AlGaAs core/shell structured nanowires were also grown to minimize the surface states. Characterizations by SEM and photoluminescence will be presented.

[1]This work is supported by Department of Energy (DE-SC0001304).

8:36AM P30.00004 Fe doped ZnO nanotubes synthesized by low temperature electrochemical process , GOPAL SAPKOTA, KAROL GRYCZYNSKI, ARUP NEOGI, USHA PHILIPOSE, University Of North Texas, Denton,TX — We report the synthesis of Fe doped ZnO nanotubes (NTs) with tube diameter of about 60-100 nm and wall thickness of about 20nm. To the best of our knowledge, this is the first report on Fe doped ZnO NTs, that could possibly be ferromagnetic. Fe doping will enable us to tune the electrical, optical and magnetic properties of the NTs which are crucial for practical applications (spintronics and optoelectronics). The morphology of the NTs was found to be very sensitive to concentration and temperature of the electrolyte and growth time. Structural and compositional analysis revealed that Fe was incorporated into the ZnO lattice. High Resolution Transmission Electron Microscopy and X-ray diffraction shows good crystalline quality of the NTs with preferential growth along the wurtzite c-axis. Room temperature photoluminescence (PL) measurement of the NTs exhibit strong UV emission around 370nm whereas low temperature PL of the NTs exhibits the optical signature of Fe doping.

8:48AM P30.00005 Growth and Characterization of ZnMgO Nanowires by Thermal Chemical Vapor Deposition , GANG SHEN, SHAWN DAVID WILBERT, NICK HARRIS, NABIL DAWAHRE, WILLIAM BAUGHMAN, LEE BUTLER, JOSEPH BREWER, SEONGSIN MARGARET KIM, PATRICK KUNG — Zinc oxide (ZnO) nanowires are promising structures for nano-optoelectronic devices and applications ranging from solid-state lighting to photovoltaics because of the wide bandgap and large exciton binding energy of ZnO, in addition to serving as template matrices for nanoscale sensors. Alloying ZnO with MgO to achieve ternary ZnMgO compounds represents a potential approach for future optoelectronic heterostructure devices. Well-aligned ZnMgO nanowires (NWs) were grown on a sapphire substrate by thermal Chemical Vapor Deposition (CVD). The alignment of the ZnMgO NWs was confirmed by x-ray diffraction and electron microscopy along with elemental composition information through EDS analysis. The optical and vibrational properties of the ZnMgO NWs were studied by micro-Raman and micro-photoluminescence (PL) measurement. Through the combination of confocal laser scanning microscopy and the micro-Raman and micro-PL, the ZnMgO NWs were imaged at sub-micron resolution.

9:00AM P30.00006 Coating of Multi-walled Carbon Nanotubes with Inorganic - Organic Silicas , PURNATOSH SAHA, BRIAN GRADY, University of Oklahoma — Silica-coated multi-walled carbon nanotubes (MWCNTs) have been prepared by sol-gel techniques. An inorganic silica layer has been formed by hydrolyzation of tetraethoxy silane (TEOS) on surfactant-treated nanotubes. Additionally, a secondary layer has been deposited using organosilane precursors. Coating thicknesses have been measured by transmission electron microscopy (TEM) and thermogravimetric analysis (TGA) has also been used to determine the amount of silicates coating the nanotubes. The thickness of the final coating can be tailored by controlling reaction conditions and the number of layers. It is expected that carefully controlling the inorganic to organic ratio in the coatings will allow for the variation of its stiffness.

9:12AM P30.00007 Characterization of Co_2FeAl nanowires[1] , KESHAB R. SAPKOTA, I.L. PEGG, J. PHILIP, Catholic University of America — Heusler alloy, Co_2FeAl (CFA) is a potentially useful material in the field of spintronics due to its high spin polarization. The CFA nanowires are grown for the first time by the electrospinning method. The diameters of the wires formed are ranging from 80 – 100 nm. The structural characterization of the nanowires is done using X-Ray diffraction and Raman spectroscopy. The nanowires exhibit cubic structure with a lattice constant, $a =$ 2.44 Å. Parallel arrays of nanowires are grown for magnetic characterization using electric field applied at the collector plate. The nanowires exhibit ferromagnetic behavior with a Curie temperature higher than 400 K. Nanoscale devices are fabricated with single CFA nanowire to understand the magnetotransport properties.

[1]This work has been supported by funding from NSF under CAREER Grant No. ECCS-0845501 and NSF-MRI, DMR-0922997.

9:24AM P30.00008 A study of the effect of nitrogen doping in TiO_2 , LISA DEBEER-SCHMITT, NSSD, ORNL, XIAOFENG QIU, IBM TJ Watson Research Center, LARRY ANOVITZ, CSD, ORNL, WILLIAM HELLER, KEN LITTRELL, NSSD, ORNL, M. PARANS PARANTHAMAN, CSD, ORNL — TiO_2 nanotube arrays have great potential as photovoltaics due to its unique chemical and physical properties associated with highly ordered tubular geometry. Small-angle neutron scattering (SANS) can characterize the specific nitrogen doping impact to the nanotube array structures. N-doping holds the promise of overcoming the large intrinsic bandgap barrier, which prevent TiO_2 from utilizing larger portion of solar energy. Combining with nanotube structures, N-doping could further promote the energy conversion efficiency of TiO_2. The SANS data demonstrate that the nitrogen doping during the nanotube growth alters their structure. This stabilized structure is evident in the data via extra peaks in the nitrogen doped sample as compared to the pure. The results demonstrate that the nanotube array morphology can be manipulated by varying the growth conditions, making it possible to tailor the arrays to specific purposes.

9:36AM P30.00009 Spontaneous Formation of a Nanotube from a Square Ag Nanowire[1] , SONDAN DURUKANOGLU, Faculty of Engineering and Natural Sciences, Sabanci University, MINE KONUK, Department of Physics, Istanbul Technical University — The recently observed phenomenon of spontaneous formation of a tube from a regular, square Ag nanowire has been investigated through molecular static and dynamic simulations based on the interaction potentials obtained from the embedded atom method. With molecular static calculations, we investigate the effect of strain on this particular type of transformation by focusing specifically on square Ag nanowires. Our results demonstrate that the formation of hollow structures requires a combination of minimum basis size and high gradient stress. Using molecular dynamic simulation, we also discuss the effect of temperature on the evolution of silver nanowire during the elongation.

[1]This work is supported by TUBITAK under Grant No. 109T105.

9:48AM P30.00010 Effect of catalyst preparation on diameter of single-walled carbon nanotubes synthesized by alcohol CVD , THEERAPOL THURAKITSEREE, ERIK EINARSSON, The University of Tokyo, Tokyo 113-8656, Japan, RONG XIANG, Sun Yat-Sen University, Guangzhou 510275, China, SHINYA AIKAWA, SHOHEI CHIASHI, JUNICHIRO SHIOMI, SHIGEO MARUYAMA, The University of Tokyo, Tokyo 113-8656, Japan — We investigated the effect of various aspects of the catalyst preparation procedure on the diameters of SWNTs synthesized by the alcohol CVD method. Prior to nanotube growth, a Co/Mo binary catalyst was deposited by dip-coating, and then reduced under flowing Ar/H_2 at temperatures ranging from 300 to 800 °C. We found that the mean SWNT diameter depends on both reduction time and temperature, with lower reduction temperature or short reduction time resulting in smaller diameter SWNTs. The morphology of SWNTs changed from vertically aligned for reduction temperatures above 500 °C to randomly aligned when reduction occurred below 500 °C. Introducing small amount of water during heating, the mean diameter of the SWNTs was also reduced despite synthesis at 800 °C. Small diameter SWNTs were synthesized with this new cobalt/rhodium (Co/Rh) catalyst. The average diameter SWNT is similar to that from Co/Fe catalysts and slightly smaller than HiPco.

10:00AM P30.00011 Water monomer interaction with H-passivated Si nanowires from density functional theory , ABRAHAM HMIEL, YONGQIANG XUE, University at Albany-SUNY — A molecular-level understanding of the interaction between water and nanomaterials is essential for such important phenomena as corrosion, catalysis, electrochemistry and biology. In this talk we present density functional (DFT) study of the structure and energetics of water monomer binding to the surfaces of hydrogen terminated silicon nanowires (SiNWs), which represents the initial phase of interfacial water. We present results on the binding site and orientation of individual water molecules on the surfaces of [112] and [110] oriented SiNWs and analyze the energetics of water adsorption through potential energy surface scan along selected degrees of freedom.

10:12AM P30.00012 In-situ dynamical study of capillary absorption of molten silver nanodroplets by multiwall carbon nanotubes , YEN-SONG CHEN, YUAN-CHIH CHANG, TUNG HSU, CHIA-SENG CHANG, DEPT. OF PHYSICS, NATIONAL TAIWAN UNIVERSITY TEAM, INSTITUTE OF PHYSICS, ACADEMIA SINICA TEAM, DEPT. OF MATERIALS SCIENCE AND ENGINEERING, NATIONAL TSING-HUA UNIVERSITY COLLABORATION — Since the discovery of carbon nanotubes (CNTs), they have been widely investigated for their properties. Due to the large aspect ratio and the uniform diameters, the inner cavities of the CNTs are used as nano test tubes, siphons, catalyst carriers, and so on. Based on recent molecular dynamic simulations, a CNT with open end might act as a "capillary pipette" which can absorb nonwetting metal nanoparticles. In our study, the in-situ dynamical process of nonwetting Ag nanodroplets drawn into the hollow cores of multiwall carbon nanotubes (MWCNTs) was observed in an ultrahigh-vacuum transmission electron microscope equipped with a scanning tunneling microscopy probe. We discover this capillary absorption of melted Ag nanodroplets can occur only when the ratio of the Ag nanodroplet size to inner diameter of MWNTs is below a critical value, which is dependent on the inner diameter of MWCNTs. With continuous operations of capillary absorption for Ag nanodroplets, the one-dimensional Ag nanowires with a specific length could be fabricated inside the MWNTs for NEMS electronics or other applications.

10:24AM P30.00013 O_2 dissociation on nitrogen doped carbon nanotubes (10, 0) from first principles simulation , SHIZHONG YANG, Southern University/LONI Institute, GUANG-LIN ZHAO, EBRAHIM KHOSRAVI, Southern University — Reducing the amount of precious platinum (Pt) loading by identifying non-precious metal catalyst is essential for large-scale applications of fuel cells, which provide a cleaning energy technology. Recent experimental, theoretical, and simulation works accelerate the advance in the research area of doped carbon nanotubes acting as an alternate non-precious metal catalyst for dioxygen reduction in the fuel cells. First principles spin polarized density functional theory(DFT) simulations have been performed to understand O_2 dissociation on nitrogen doped carbon nanotubes. We have studied nitrogen substitutional doping of carbon nanotubes (CNTs) for dioxygen adsorption, reduction, and dissociation. The calculated results show that nitrogen prefers to stay at the open-edge of short CNTs. Two O_2 chemisorption sites are found, the carbon-nitrogen complex (Pauling site) and carbon-carbon long bridge (long bridge) sites. The spin polarized DFT calculations using the nudged elastic band (NEB) method show that O_2 dissociation at the Pauling site has a reaction energy barrier of about 0.55 eV. The unique open-edge structure and charge redistribution are crucial to the novel properties of nitrogen-doped CNTs as a new non-precious metal catalyst for fuel cells.

10:36AM P30.00014 Adsorption kinetics of polyatomic molecules on a heterogeneous surface , JARED T. BURDE, Southern Illinois University Carbondale, M. MERCEDES CALBI, University of Denver — We study the kinetics of adsorption of diatomic and triatomic molecules on the external surface of a carbon nanotube bundle. The Kinetic Monte Carlo algorithm is employed to track the number of particles adsorbed on the bundle and the orientation of those particles with respect to the surface at any given time. Our model is further complicated by the inclusion of a more complex surface geometry; a two dimensional, heterogeneous lattice better models the reality of groove between adjacent nanotubes on the outside of the bundle. This allows us to see interesting kinetic effects in the adsorption process, as the adsorbates have multiple transitional states through which they can pass as they evolve towards equilibrium.

10:48AM P30.00015 Simulations of adsorption on a single carbon nanotube , HYE-YOUNG KIM, Department of Chemistry and Physics, Southeastern Louisiana University, Hammond, LA 70402, SILVINA GATICA, Department of Physics and Astronomy, Howard University, Washington, DC 20059, MILTON COLE, Department of Physics, Pennsylvania State University, State College, PA 16802 — Using the grand canonical Monte Carlo method, we have evaluated the adsorption isotherms of simple gases (Ar, Kr, Xe) on a variety of carbon nanotubes. The adsorption potential is a sum of anisotropic atom-C interactions, dependent on the angle between the outward normal and the atom-C separation vector. For varying gas species and nanotube chirality, different commensurate phases are seen than on the surface of graphite. Comparison is made with recent experiments of Wang, et al, Science 327, 552 (2010).

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P31 DMP GSCCM DCOMP: Focus Session: Materials at High Pressure IV: Geophysical Materials and Magnetic Transitions C145

8:00AM P31.00001 Pressure-induced phase transitions in NaMgF3 post-perovskite[1] , KOICHIRO UMEMOTO, Department of Geophysics and Geology, University of Minnesota, RENATA WENTZCOVITCH, MSI and CEMS, University of Minnesota — Understanding the behavior of $MgSiO_3$ postperovskite(PPV) under extreme pressures is fundamental for modeling the interiors of solar giants and extrasolar planets. In 2006, $MgSiO_3$ post-perovskite was predicted to dissociate into MgO and SiO_2 at 1.1 TPa (Umemoto et al., Science 311, 983 (2006)). However, the predicted dissociation pressure is too high to be easily verified experimentally. Instead, a low-pressure analog, $NaMgF_3$ neighborite, has been studied to test for structural predictions in $MgSiO_3$. $NaMgF_3$ was predicted to dissociate at $\sim$40 GPa (Umemoto et al., Geophys. Res. Lett. 33, L15304 (2006)), but this has not been confirmed experimentally (Martin et al., Geophys. Res. Lett. 33, L11305 (2006); Grocholski et al. Geophys. Res. Lett. 37, L14204 (2010)) and the dissociation $MgSiO_3$ PPV is now being questioned. Here, we reexamine in detail the pressure dependence of crystal structures and phonon frequencies in $NaMgF_3$ and reveal the apparent reason why dissociation was not observed in this material.

[1]Work supported by NSF under ATM-0428774 (VLab), EAR-0757903, and EAR-1019853. Computations were performed at MSI and Laboratory for Computational Science and Engineering (LCSE).

8:12AM P31.00002 First-principles calculation of thermal conductivity of silicate perovskite at high pressures and high temperatures[1] , JIANJUN DONG, Auburn University, XIAOLI TANG, California Institute of Technology, ABBY KAVNER, UCLA, MOSES NTAM, Auburn University — The lattice thermal conductivity of silicate perovskite, the most abundant mineral in the Earth's lower mantle, is calculated by combining the first-principles electronic structure theory and Peierls-Boltzmann transport theory. The phonon scattering rate due to lattice anharmonicity and Mg/Fe mass disorder is evaluated for each mode at the extreme P-T conditions of the lower mantle. The predicted thermal conductivity of single crystal MgSiO3 perovskite at ambient condition, about 5.7 W/m/K, is in excellent agreement with experiment. Adding about 6% Fe will lower the thermal conductivity by nearly 40%. Our calculation also reveals an unique pressure dependence for the thermal conductivity of perovskite, and the calculated thermal conductivity of iron bearing perovskite is almost an order of magnitude lower than the previously estimates based on long extrapolation of single crystal data. Including a re-evaluation of radiative contribution, we discuss the implications of our results for the heat flow in deep Earth.

[1]Funded by NSF (EAR-0757847)

8:24AM P31.00003 Identification of post-pyrite transition in SiO2 by a genetic algorithm[1] , SHUNQING WU, Iowa state U and Xiamen U, KOICHIRO UMEMOTO, GEO, U of Minnesota, KAI-MING HO, MIN JI, CAI-ZHUANG WANG, Ames Lab, Iowa state U, RENATA WENTZCOVITCH, MSI and CEMS, U of Minnesota — Here we propose a new phase of SiO_2 beyond the pyrite-type phase. SiO_2 is one of the most important minerals in Earth and planetary sciences. So far, the pyrite-type phase has been identified experimentally as the highest-pressure form of SiO_2. In solar giants and extrasolar planets whose interior pressures are considerably higher than that on Earth, a post-pyrite transition in SiO_2 may occur at $\sim$ 1 TPa as a result of the dissociation of $MgSiO_3$ post-perovskite into MgO and SiO_2 [Umemtoto et al., Science 311, 983 (2006)]. Several dioxides considered to be low-pressure analogs of SiO_2 have a phase with cotunnite-type ($PbCl_2$-type) structure as the post-pyrite phase. However, a first-principles structural search using a genetic algorithm shows that SiO_2 should undergo a post-pyrite transition to a hexagonal phase, not to the cotunnite phase. The hexagonal phase is energetically very competitive with the cotunnite-type one.

[1]This work was supported by the U.S. Department of Energy, Office of Basic Energy Science, Division of Materials Sciences and Engineering and NSF under ATM-0428774 (VLab), EAR-0757903, and EAR-1019853.

8:36AM P31.00004 Spin crossover systems in the deep mantle , RENATA WENTZCOVITCH, Department of Chemical Engineering and Materials Science, Minnesota Supercomputing Institute, University of Minnesota — In recent years there has been much interest on spin crossovers found experimentally in the most abundant minerals of Earth's lower mantle ((Mg,Fe)O and (Mg,Fe)(Si,Fe)O_3-perovskite) under pressure. Spin crossovers are strongly dependent on thermodynamic conditions and a full understanding of this problem requires its investigation as function of pressure and temperature. There are several controversies, especially in the perovskite systems, and surprises are revealed by electronic structure calculations. The geophysical consequences of these crossovers are yet to be fully understood but could be fascinating. I will review progress we have made in understanding spin crossovers and give an overview of this phenomenon and its potential implications for the Earth.

Research carried out in collaboration with H. Hsu, K. Umemoto, P. Blaha, J. F. Justo, and C. R. S. da Silva. Research supported by the MRSEC Program of NSF under Award Number DMR-0212302 and DMR-0819885, and by NSF/ATM-0428774, EAR-0810212, and EAR-1047629.

9:12AM P31.00005 Insulator to Metal and Magnetic Transitions in FeO under High Pressure: DFT-DMFT Computations , R.E. COHEN, Geophysical Laboratory, Carnegie Institution, KRISTJAN HAULE, GABI KOTLIAR, Rutgers University — We have applied DFT+Dynamical Mean Field Theory (DMFT) to FeO under varying pressure and strain to understand possible transitions in FeO. We use an LAPW basis set, and the lattice terms are evaluated using the WIEN2K LAPW code. The impurity model is solved using continuous time quantum Monte Carlo (CTQMC). Temperature enters explicitly, so we made special efforts to understand high temperature behavior relevant to geophysics. The computations are fully self-consistent, including the impurity levels and crystal field splitting, and the total energy is evaluated using the full potential and charge density of the lattice plus impurity models. We find with increasing pressure in paramagnetic FeO in a cubic lattice and U=8 eV a high-spin low-spin transition, with a possible intermediate spin state (characterized by intermediate occupancies of the t2g and eg states) between. We find that at 300K cubic FeO remains insulating to a factor of two compression (over 600 GPa). However, high temperatures (e.g. 2000K) and rhombohedral lattice strain promote a metal insulator transition. We are delineating the phase boundaries. This work is supported by NSF.

9:24AM P31.00006 First-principles study of spin-state crossovers and hyperfine interactions of ferric iron in magnesium silicate perovskite[1] , HAN HSU, University of Minnesota, PETER BLAHA, TU Vienna, MATTEO COCOCCIONI, RENATA WENTZCOVITCH, University of Minnesota — The spin-state crossover in iron-bearing $MgSiO_3$ perovskite, the most abundant mineral in the Earth, may significantly affect the properties of Earth's lower mantle. However, details of this phenomenon have been very unclear, owing to the complicated nature of this mineral, mainly the coexistence of ferrous and ferric iron. Using the density functional theory plus Hubbard U (DFT+U) methods, we investigated the spin states and hyperfine interactions of ferric iron in this mineral. We show that a crossover from high-spin to low-spin state occurs within the lower-mantle pressure range, and it is accompanied by a noticeable volume reduction and an increase in iron nuclear quadrupole splitting (QS). These results are consistent with recent x-ray diffraction and Mössbauer spectroscopy measurements [K. Catalli *et al.*, Earth Planet. Sci. Lett. **289**, 68 (2010)].

[1]This work is primarily supported by the MRSEC Program of NSF under DMR-0212302 and DMR-0819885, and partially supported by EAR-0810212 and EAR-1047629. P.B. was supported by the Austrian Science Fund (P20271-N17). Calculations were performed at MSI.

9:36AM P31.00007 Ab initio melting curve of Fe and Fe-S alloys at extreme pressures: implications for Earth's and exoplanets' cores , JOHANN BOUCHET, CEA, GUILLAUME MORARD, Institut de Minéralogie et de Physique des Milieux Condensés, STEPHANE MAZEVET, CEA, FRANCOIS GUYOT, Institut de Minéralogie et de Physique des Milieux Condensés — Exoplanets with masses similar to that of Earth have recently been discovered in extrasolar systems [1]. A first order question for understanding their dynamics is to know whether they possess Earth like liquid metallic cores. However, the iron melting curve is unknown at conditions corresponding to planets of several times the Earth's mass (over 15 Mbar for planets with 10 times the Earth's mass [2]). In the density-temperature region of the cores of those super-Earths, we calculate the iron melting curve using first principle molecular dynamics simulations based on density functional theory. We also propose an equation of state for iron in this pressure range. Finally we show the melting curve of Fe_3S and discuss the effects of the addition of sulfur to the melting curve of pure iron.

[1] J. P. Beaulieu, D. P. Bennett, P. Fouque et al., Nature 439 (7075), 437 (2006).
[2] D. Valencia, R. J. O'Connell, and D. Sasselov, Icarus 181, 545 (2006).

9:48AM P31.00008 Elasticity of iron-bearing olivine polymorphs investigated by first principles , MARIBEL NÚÑEZ VALDEZ, School of Physics and Astronomy, University of Minnesota, YONGGANG YU, Dept. of Chemical Engineering and Material Sciences, University of Minnesota, RENATA WENTZCOVITCH, Dept. of Chemical Engineering and Material Sciences and Minnesota Supercomputing Institute, University of Minnesota — We calculate by first principles the effect of iron on the high pressure-temperature elasticity of olivine polymorphs: α-phase (olivine), β-phase (wadsleyite) and γ-phase (ringwoodite), the major constituents of the Earth's upper mantle and transition zone (TZ). We combine the LDA, the quasiharmonic approximation, and a model vibrational density of states for the solid solution to calculate the full elastic tensor C_{ij}, bulk (K) and shear (G) moduli of $(Mg_{0.875}Fe_{0.125})_2SiO_4$. Comparison with experimental data at ambient conditions validates our results. In the pressure and temperature range of the upper mantle and TZ we study single crystal wave propagation anisotropy and polarization anisotropy in aggregates with preferred orientation.

Research supported by NSF EAR-1019853 and EAR-0810272. Computations were performed at the Minnesota Supercomputing Institute.

10:00AM P31.00009 Polymerization of methane in the deep Earth[1] , LEONARDO SPANU, Department of Chemistry UC Davis, DAVIDE DONADIO, MPI for Polymer Research; Department of Chemistry UC Davis, DETLEF HOHL, Shell Global Solutions Inc. Houston, TX, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, Livermore CA, GIULIA GALLI, Department of Chemistry and Department of Physics, UC Davis — Determining physical and chemical properties of carbon fluids at high pressure and temperature is a key step towards understanding carbon reservoirs and fluxes in the deep Earth. The stability of carbon-hydrogen systems at depth greater than few thousands meters is poorly understood and the abiogenic hypothesis on the synthesis of higher hydrocarbon (HCs) in the Earth mantle remains controversial. We have used ab initio molecular dynamics simulations to investigate the formation of higher HCs from dissociation of pure methane, and of methane in contact with carbon surfaces and transition metals, in a range of pressure of $2-30$ GPa and temperature T=$800-4,000$ K [1]. We present results on the range of stability of pure methane and discuss how the interaction with transition metals or carbon deposits (graphite and diamond) affects the formation of higher HCs.

[1] Leonardo Spanu, Davide Donadio, Detlef Hohl, Eric Schwegler, Giulia Galli (*submitted)*

[1]Work supported by a grant from Stichting Shell Research (SSR).

10:12AM P31.00010 Solubility and erosion of icy cores in giant planets , HUGH WILSON, BURKHARD MILITZER, University of California Berkeley — The core-mantle boundary of a giant planet consists of an interface between dense rock/ice below and fluid hydrogen-helium above. Whether this phase boundary remains stable, however, or whether the core material is dissolved and redistributed throughout the interior, remains unknown, and has major consequences for planetary interior and formation models. In this work we use density functional theory molecular dynamics calculations to compute the free energy of solubility for the icy components of the core into fluid hydrogen, to investigate whether solubility is thermodynamically preferred at the extreme temperature and pressure conditions prevalent at the core-mantle boundaries of Jupiter and Saturn. The consequences for Jupiter and Saturn, as well as for giant exoplanets, will be discussed.

10:24AM P31.00011 Post-stishovite transition in AlOOH-incorporated SiO2[1] , KATSUYUKI KAWAMURA, Tokyo Institute of Technology, KOICHIRO UMEMOTO, RENATA WENTZCOVITCH, University of Minnesota, KEI HIROSE, Tokyo Institute of Technology — In 2007, Lakshtanov et al. [Proc. Nat. Acad. Sci. 104, 13588 (2007)] showed that the incorporation of AlOOH into SiO_2 significantly reduces the transition pressure between stishovite and $CaCl_2$-type phases. In the present paper, we investigate theoretically the effect of hydrogen and aluminum on this transition. First-principles calculations show that aluminum has no effect on the transition pressure. However, hydrogen bonds play a crucial role, suggesting that a cooperative redistribution of hydrogens aids the post-stishovite transition. Large-scale molecular dynamics simulations using model potentials confirm this effect and reveal the nature of the hydrogen motion. This effect produces a strong temperature dependence on the transition pressure and should make the latter sensitive to hydrogen content in the material.

[1]This work was supported by NSF under ATM-0428774 (VLab), EAR-0757903, and EAR-1019853. The computations were performed at the Minnesota Supercomputing Institute (MSI).

10:36AM P31.00012 Thermodynamic properties of $MgSiO_3$ majorite and phase transitions near 660-km depth in $MgSiO_3$ and Mg_2SiO_4: a first principles study[1] , YONGGANG YU, Virginia Tech, RENATA WENTZCOVITCH, U. Minnesota, VICTOR VINOGRAD, U. Frankfurt, ROSS ANGEL, Virginia Tech — Thermodynamic properties of $MgSiO_3$ tetragonal majorite have been calculated at high P-T within the quasiharmonic approximation based on DFT using both LDA and GGA. The LDA results compare exceptionally well with measured thermodynamic properties. A classical Monte Carlo simulation based on a cluster expansion method demonstrates that disorder between Mg and Si in the octahedral sites in majorite does not occur below 3600 K within 30 GPa. The calculated phase boundaries between majorite (mj), perovskite (pv), and ilmenite (il) $MgSiO_3$ agree much better with experiments by using GGA than by LDA. The Clapeyron slopes (CS) predicted by GGA and LDA are close to each other: 0.9 – 1.7 MPa/K for mj-pv, 6.9 – 7.9 MPa/K for mj-il, and -7 – -3 MPa/K for il-pv transition. The triple point predicted by GGA is at 21.8 ± 1 GPa and 1840 ± 200 K which is $\sim$400 K lower than most experiments. Our calculations also reveal that wadsleyite decomposes to an assemblage of majorite plus periclase above 2280 K with a large negative CS (-22 – -12 MPa/K) and that ringwoodite decomposes to ilmenite plus periclase below 1400 K (1.2 MPa/K). The geophysical implications to mantle convection and the composition of the Earth's transition zone will also be discussed.

[1]NSF: EAR-0738692, EAR-1047629, and ATM-0428774 (VLab)

10:48AM P31.00013 A first-principles investigation of hydrous defect and IR frequencies in forsterite: The case for Si vacancies[1] , MARC HIRSCHMANN, KOICHIRO UMEMOTO, RENATA WENTZCOVITCH, DAVID KOHLSTEDT, ANTHONY WITHERS, University of Minnesota — We investigate charge-balanced hydrous magnesium and silicon defects ($(2H)^X_{Mg}$, $(4H)^X_{Si}$) by first principles. Here we propose two new lowest-energy hydrogen configurations for $(4H)^X_{Si}$. With these new configurations, the distribution of OH-stretching phonon frequencies in Group I ($>$ 3450 cm-1) are better reproduced. Substitution of silicon with 4 hydrogens gives rise to significant elongation of distances between oxygen ions at the tetrahedron of the silicon vacancy. Our calculations indicate that the correlation between O-O distances and O-H-stretching phonon frequencies, which has been well established for hydrous minerals, does not apply directly to nominally anhydrous minerals and should not be used to determine the identity of the hydrous defects responsible for infrared absorption peaks.

[1]This work was supported by NSF under EAR-0757903 and EAR-1019853. The computations were performed at the Minnesota Supercomputing Institute (MSI).

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P32 DCMP: Optical Properties and Dynamics of Quantum Dots and Quantum Wells

C144

8:00AM P32.00001 Sub micron scale patterning of material optical response through focused ion beam induced InAs/GaAs quantum dot nucleation , TIMOTHY SAUCER, JIEUN LEE, ANDREW MARTIN, DEBORAH TIEN, JOANNA MIRECKI-MILLUNCHICK, VANESSA SIH, The University of Michigan — We report on the technique of using a focused ion beam to produce preferential sites for InAs/GaAs quantum dot nucleation. We mill an array of holes in the GaAs substrate and then deposit a thin layer of InAs below the critical thickness for dot formation in unpatterned areas. The array of holes on the substrate act as preferential nucleation sites and induce quantum dot formation only in the patterned regions. We conduct photoluminescence spectroscopy in a templated multilayer quantum dot sample at temperatures down to 10K and for various patterning conditions. We find that outside of our patterning regions we have no quantum dot luminescence, indicating that the patterning modifies the optical response of the material. We find that we can control this quantum dot formation down to array spacings of 250nm, showing excellent potential for this technique to be used for sub micron spatial control of a material's optical properties.

8:12AM P32.00002 Photoluminescence imaging of Focused-Ion-Beam induced individual quantum dots , JIEUN LEE, TIMOTHY SAUCER, Department of Physics, University of Michigan, ANDREW MARTIN, Department of Materials Science and Engineering, University of Michigan, DEBORAH TIEN, Department of Physics, University of Michigan, JOANNA MILLUNCHICK, Department of Materials Science and Engineering, University of Michigan, VANESSA SIH, Department of Physics, University of Michigan — Quantum dots are nanostructures that confine electrons in 3 spatial dimensions. Due to their discrete atom-like energy levels, a wide variety of applications related to the optical properties of dots are possible. One such application is to integrate quantum dots in optical nanocavities for the enhanced interaction between electrons and photons. However, self-assembled dots typically nucleate at random locations, hindering the accurate coupling between the dot and cavity. Therefore, spatial control on self-assembled dots at the fabrication level is highly desirable. Here, we report on optical measurements conducted on InAs quantum dots that are prepatterned in a square array by a focused-ion-beam. Using scanning confocal microscopy, we spatially map the photoluminescence of individual quantum dots. Single dot luminescence with 160 μeV linewidth is observed indicating good optical quality and statistical analysis over 16 array sites show reasonable placement accuracy and emission inhomogeneity.

8:24AM P32.00003 Strongly confined excitons in self-assembled InGaAs quantum dot clusters , MEGAN CREASEY, XIAOQIN LI, Department of Physics, University of Texas at Austin, JIHOON LEE, Department of Electrical Engineering, Kwangoon University, ZHIMING WANG, GREGORY SALAMO, Institute of Nanoscale Science and Technology, University of Arkansas — Quantum dot clusters (QDCs) consisting of regular geometric patterns of six InGaAs quantum dots (QD) are grown on a GaAs substrate using a hybrid growth method that combines droplet homoepitaxy and Stranski-Krastonov growth. These novel structures have potential applications as tunable single photon sources, entangled photon sources, or error corrected qubits - devices critical to the fields of secure optical communications and quantum computing We study the photoluminescence arising from a single cluster using both continuous wave and ultrafast spectroscopic techniques with variations in the sample temperature and excitation power. Our results suggest excitons (bound electron-hole pairs) are strongly confined within the individual QDs rather than loosely confined throughout the entire QDC. The work at Texas is supported financially by NSF, ARO, AFOSR, ONR, the Welch Foundation, and the Alfred Sloan Foundation. The work at Arkansas is supported by the NSF.

8:36AM P32.00004 Selective control of polarized luminescence from GaN/AlN self-assembled quantum dots , DANIEL RICH, OFER MOSHE, Ben-Gurion University, BENJAMIN DAMILANO, JEAN MASSIES, Centre National de la Recherche Scientifique — GaN/AlN self-assembled quantum dots (QDs) were grown by the Stranski-Krastanov method on Si(111) using molecular beam epitaxy. During the subsequent cooling from growth temperatures, the thermal expansion coefficient mismatch between the Si substrate and GaN/AlN film containing vertically stacked QDs leads to an additional biaxial tensile stress at the Si/III-Nitride interface. We have modified the thermal stress in the QD layers by etching stripes of varying widths using inductively coupled Cl/Ar plasma reactive ion etching. The results show that a suitable choice of stripe width and orientation can create regions of in-plane uniaxial stress ranging from 20-30 kbar which enables a selective and local control of polarized emission from the QDs. Localized cathodoluminescence (CL) spectroscopy of the QDs exhibits emissions from both the ground and excited states, whose relative contributions depend on the level of excitation and temperature. We have studied these emissions using time- and polarization-resolved CL for ensembles of QDs. The effects of screening of the polarization field in the QD, state-filling, changes in the polarization anisotropy and lifetime with varying excitation were studied experimentally and modeled with a self-consistent 6x6 k.p calculation method.

8:48AM P32.00005 Polarization states of charged excitons in coupled InAs/GaAs quantum dot molecules , RAMANA THOTA, SWATI RAMANATHAN, KUSHAL WIJESUNDARA, ERIC STINAFF, Department of Physics and Astronomy, and Nanoscale and Quantum Phenomena Institute, Ohio University, Athens, Ohio 45701-2979, USA, ALLAN BRACKER, DAN GAMMON, Naval Research Laboratory, Washington, DC 20375, USA — The polarization state of charged excitons in coupled InAs/GaAs dots can reveal useful information about the spin state of its charge carriers. In this study, we examine the complete polarization state through Stokes parameter measurements to relate the polarization parameters of the luminescence to the spin configurations of the various charged excitons they originate from. We demonstrate that this method is a useful tool to identify and possibly create spin states for quantum computation applications.

9:00AM P32.00006 Resonant Fluorescence from Quantum Dot Molecular Excitonic Transitions , MARK KERFOOT, University of California, Merced, ALLAN BRACKER, DANIEL GAMMON, Naval Research Laboratory, MICHAEL SCHEIBNER, University of California, Merced, UNIVERSITY OF CALIFORNIA, MERCED COLLABORATION, NAVAL RESEARCH LABORATORY COLLABORATION — Quantum dot molecules formed by two vertically stacked quantum dots are a rich testing ground for basic concepts regarding the measurement and control of quantum states. The well defined geometry is ideal for studying interaction mechanisms, such as the interaction of two dipoles each located in one of the quantum dots of the quantum dot molecule. A prerequisite for doing so is the ability to detect the interaction mediated changes in the properties of the individual, uncoupled quantum dots. Here we use resonant fluorescence to study exciton transitions in quantum dot molecules. We measure the photoluminescence of the same transition we optically excite with a narrow band laser. With this method, features on the scale of the homogeneous line width of the intradot exciton transition are well resolved. This enables us to study the fine-structure of different charge and spin configurations with high sensitivity.

9:12AM P32.00007 Exchange-controlled spin dynamics in coupled quantum dots , ERIC A. STINAFF, KUSHAL C. WIJESUNDARA, Department of Physics and Astronomy, and Nanoscale and Quantum Phenomena Institute, Ohio University, Athens, OH 45701, USA, ALLAN BRACKER, DAN GAMMON, Naval Research Laboratory, Washington, DC 20375, USA — We measure circular polarization memory of neutral exciton states with polarization dependent photoluminescence spectra. As a consequence of anisotropic exchange interaction a low degree of circular polarization memory was observed in the spatially direct and indirect excitons where they anticross. With applied electric field as we tune the excitonic emission from intra-dot to inter-dot the electron-hole wave function overlap reduces and we observe an increase in polarization memory due to reduced exchange interaction. We observe a sudden unexpected dip in circular polarization memory of the spatially indirect exciton state that is coincident with the applied field where the single hole level resonance is observed. Possible mechanisms for this loss of circular polarization memory will be presented.

9:24AM P32.00008 Two-body and three-body interactions in phonon-assisted exciton energy transfer between quantum dots , KAIJIE XU, CARLO PIERMAROCCHI, Department of Physics and Astronomy, Michigan State University — We theoretically study the dynamics of exciton energy transfer between semiconductor quantum dots. Phonons play a critical role in the exciton energy transfer process when the energy of the dots involved in the process is different. We find that the phonon-assisted energy transfer cannot be correctly described by two-body exciton-photon and exciton-phonon interactions if each dot is modeled as a single-level exciton system. Higher excited levels of the exciton state have to be included to properly describe the phonon-assisted process. However, excited states can be traced out by introducing a single-level exciton model with an effective three-body exciton-photon-phonon coupling term. The three-body term describes a change in the exciton-photon dipolar coupling due to phonon-induced deformations of the ground exciton wavefunction. The multi-level exciton model with two-body interactions and the single-level exciton model with three-body interaction reproduce the same exciton transfer rates to the leading order contributions of perturbation theory.

9:36AM P32.00009 ABSTRACT WITHDRAWN –

9:48AM P32.00010 Optical lattices for electrons in semiconductors , CARLO PIERMAROCCHI, MICHAEL G. MOORE, MARTIN J. A. SCHUETZ, Michigan State University, MONIQUE COMBESCOT, Instutute of Nanosciences, Pierre et Marie Curie University, Paris France — We theoretically investigate the trapping of electrons in a semiconductor using counter-propagating laser beams. We consider two different physical mechanisms that can lead to an efficient electron trapping: (a) Pauli blocking between the electron and a virtual exciton coupled to the laser field, and (b) the virtual excitation of a three-body Coulomb resonance corresponding to a bound charged exciton state (a trion). Both processes induce a momentum transfer between photon and electron, and lead to a sinusoidal trap for electrons with a period determined by the laser beam modulation. The depth of the potential is proportional to the laser intensity and inversely proportional to the exciton-photon detuning. Competing effects such as laser heating, phonons, and disorder are analyzed.

10:00AM P32.00011 Many-body two-quantum coherences in 2DFT spectra of semiconductors , DENIS KARAISKAJ, University of South Florida, A. BRISTOW, X. DAI, JILA, CU and NIST, L. YANG, S. MUKAMEL, University of California Irvine, R. MIRIN, NIST Boulder, S. CUNDIFF, JILA, CU and NIST — Investigating the correlations of multiple excitons in semiconductors is a challenging many-body problem that has drawn considerable experimental and theoretical attention over the last two decades. Nonlinear four-wave mixing (FWM) experiments have long been known to provide direct probes for the many-body effects in the ultrafast dynamics of excitons in quantum wells. However, it is very difficult to separate the different contributions such as excitation induced dephasing, excitation induced shift, local field effects, and multiple exciton correlations. With the advent of two-dimentional Fourier-transform (2DFT) spectroscopy, the biexcitonic contributions could be isolated and the many-body contributions could be identified. Phase-resolved 2DFT spectra for the negative delay FWM signal will be presented which show interesting diagonal and off-diagonal peaks. The energy positions, line shapes, and the complexity of the 2D peaks indicate significant many-body coherences and reinforce the ability of 2DFT to disentangle two-quantum transitions (D. Karaiskaj, *et al.*, Phys. Rev. Lett. **104**, 117401 (2010)).

10:12AM P32.00012 Electron transfer and relaxation dynamics in heterovalent ZnSe/GaAs quantum well structures , AMIT DONGOL, HANS PETER WAGNER, Department of Physics, University of Cincinnati, OH-45221, USA — We investigate the electron transfer and relaxation dynamics in heterovalent ZnMgSe/ZnSe quantum wells (QW's) grown on GaAs using the nonlinear optical method of three-beam degenerate four-wave-mixing (FWM). We use ultra-short (90 fs) laser pulses with non-collinear wave-vectors $\mathbf{k}_1$, $\mathbf{k}_2$ and $\mathbf{k}_3$ at a center wavelength of 441 nm ($\sim$2.81 eV) which is resonantly tuned to the heavy hole exciton transition energy at 25 K. In the experiment the time coincident strong pump pulses $\mathbf{k}_1$ and $\mathbf{k}_2$ creates both an exciton density grating in the QW and an electron-hole pair grating in the GaAs while the delayed weak pulse $\mathbf{k}_3$ simultaneously probes the exciton lifetime T_1 as well as the electron grating injection time T_t from the substrate into the QW. Intensity dependent experiments reveal that the diffraction efficiency due to the electron grating increases faster with increasing $\mathbf{k}_1$ and $\mathbf{k}_2$ pulse intensities than the FWM efficiency due to the generated exciton density grating. This behavior which is attributed to exciton bleaching at high intensities enables the discrimination of times T_1 and T_t, both being in the order of a few tens of picoseconds.

10:24AM P32.00013 Excitons in moving lattices , JASON LEONARD, ALEXANDER WINBOW, MIKAS REMEIKA, YULIYA KUZNETSOVA, ALEXANDER HIGH, AARON HAMMACK, LEONID BUTOV, University of California at San Diego, JOSEPH WILKES, ALRUN GUENTHER, ALEXANDER IVANOV, Cardiff University, MICAH HANSON, ARTHUR GOSSARD, University of California at Santa Barbara — We report on the study of indirect excitons in moving lattices–conveyers–created by a set of AC voltages applied to the electrodes on the sample surface. The wavelength of this moving lattice is set by the electrode periodicity, the amplitude is controlled by the applied voltage and the speed is controlled by the AC frequency. We probed the conveyer speeds from well below to well above the sound velocity. We observed the dynamical localization-delocalization transitions for excitons in the conveyers and measured its dependence on the exciton density and conveyer speed and amplitude. We also developed the theory of exciton transport via conveyers.

10:36AM P32.00014 Effect of growth kinetics on intersubband transitions in GaN/AlN multiple quantum wells[1] , J. YANG, S.D. CARNEVALE, T.F. KENT, Department of Materials Science and Engineering, The Ohio State University, Columbus, OH. 43210, M.R. BRENNER, Department of Electrical and Computer Engineering, The Ohio State University, Columbus, OH, 43210, R.C. MYERS, Department of Materials Science and Engineering, Department of Electrical and Computer Engineering, The Ohio State University, Columbus, OH. 43210 — The large conduction band offset of nearly 2 eV between GaN and AlN provides very large electron confinement that could be useful for ultrafast intersubband–based photonics operating at telecommunications wavelengths. However, it is difficult to control interface roughness and compositional profiles with monolayer precision, which is crucial for engineering sublevels for quantum cascaded intersubband photonics. Here we examine the effect of Ga-rich and N-rich growth conditions of highly-confined GaN/AlN multiple quantum wells prepared by plasma-assisted molecular beam epitaxy. Structural quality is examined through high-resolution x-ray diffraction and atomic force microscopy. The efficiency of intersubband and interband transitions in these heterostructures is measured using temperature dependent absorption and photoluminescence spectroscopy.

[1]Work supported by the Office of Naval Research.

10:48AM P32.00015 Trions and quatrons in Semiconductor Coupled Quantum Wells , ROMAN YA. KEZERASHVILI, OLEG L. BERMAN, New York City College of Thechnology, City University of New York — The three-body restricted problem for trions, when a spatially separated exciton and electron or hole are located in the parallel quantum wells (QW), is reduced to the 2D two body problem for the exciton and the projection of the electron or hole on the plane of the excitonic QW. In the limit of a large spatial separation of the QWs the eigenfunctions and energy spectrum for the trions are obtained analytically. It is shown that the Schrödinger equation for the trion can be reduced to the 2D two-body problem with Coulomb electron-hole interaction for the 2D direct exciton and the Schrödinger equation for the 2D harmonic oscillator for the relative motion of the exciton and the image of the projection of the electron or hole on the plane of the quantum well with the exciton. The 2D Wigner crystallization of the trions in the coupled QWs is discussed. The four-body restricted problem for spatially separated exciton and electron and hole, located in the in three parallel QWs, is reduced to the 2D three body problem for the exciton and the projection of the electron and hole on the plane of the excitonic QW. In the limit of a large spatial separation of the QWs the eigenfunctions and energy spectrum for quatron formed by the exciton and electron and a hole are obtained analytically. The 2D superfluidity and Kosterlitz-Thouless phase transition in the dilute Bose gas of quatrons is discussed.

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P33 DMP DCOMP: Focus Session: Dielectric, Ferroelectric, and Piezoelectric Oxides: BiFeO3 C143/149

8:00AM P33.00001 Manipulation of the domain structure in mixed-phase BiFeO3 epitaxial films , YI-CHUN CHEN, HSIN-HUA LEE, FENG-NAN CHU, WEN-CHUAN HSIEH, Department of Physics, National Cheng Kung University, Q. HE, Advanced Light Source, Lawrence Berkeley National Laboratory, WEN-I LIANG, YING-HAO CHU, Department of Materials Science and Engineering, National Chiao Tung University — Strain-induced phase transformation in epitaxial films is the newly advance in thin-film growth techniques. Under the compressive strain from the substrate, the stable phase of multiferroic BiFeO3 (BFO) films transformed from rhombohedrally- to tetragonally- distorted monoclinic perovskite, which simulated the material system near the morphotropic phase boundary. In this study, we used piezoresponse force microscopy (PFM) to investigate the intrinsic domain structures in the mixed-phase BFO epitaxial films. PFM taken along the principal crystallographic directions revealed the domain polarizations. The IP PFM images indicated the coexistence of at least two monoclinic phases with IP distortions along [100] and [110]. The domains were distributed in the way to minimize the local electrostatic energy, and the mixed phase pattern can be effectively controlled by external fields. The dynamic switching parameters for the domain and phase manipulation, such as switching speed, switching direction, and applying voltages, were systematically investigated. This study provides basic understanding and electrical control of this unique phase boundary.

8:12AM P33.00002 Oxygen ordering and electrochromism in Ca-doped $BiFeO_3$[1] , JAN SEIDEL, Lawrence Berkeley National Laboratory, Berkeley, CA, WEIDONG LUO, Vanderbilt University, Nashville, TN and ORNL, Oak Ridge, TN, PHI NGUYEN, Rutgers University, Piscataway, NJ, SURESHA SIRIYARA JAGANNATHA, ALAN LEE, SANG-YONG KIM, Lawrence Berkeley National Laboratory, Berkeley, CA, CHAN-HO YANG, KAIST, Daejeon, Republic of Korea, STEPHEN PENNYCOOK, SOKRATES PANTELIDES, Vanderbilt University, Nashville, TN and ORNL, Oak Ridge, TN, RAMAMOORTHY RAMESH, Lawrence Berkeley National Laboratory, Berkeley, CA — We show that calcium-doped bismuth ferrite thin films exhibit an electrochromic effect arising from an intrinsic mechanism due to redistribution of carriers, without the need for additional electrolytes that are needed in common electrochromic devices. The absorption change and coloration efficiency at the band edge are $4.8\times10^6 m^{-1}$and $190 cm^2 C^{-1}$, respectively, which are among the highest reported values for inorganic electrochromes. These experimental findings are supported by optical absorption calculations from first-principles theory, confirming the strong absorption change at the band edge.

[1]Supported by DOE under contract No. DE-AC02-05CH1123, and the National Research Foundation of Korea (NRF) (2010-0013528). J.S. acknowledges support from the Alexander von Humboldt Foundation.

8:24AM P33.00003 Polarity Control of Ferroelectric $BiFeO_3$/Metal Junctions for Switchable Diode and Photovoltaic Devices , TAE WON NOH, DAESU LEE, T.H. KIM, ReCFI, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Republic of Korea, S.H. BAEK, C.M. FOLKMAN, C.B. EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA, J.-G. YOON, Department of Physics, University of Suwon, Kyunggi-do 445-743, Republic of Korea — Ferroelectric materials possess spontaneous polarization which can be used to control numerous functionalities of the materials by switching the polarization or modifying domain structure with an electric field. One of emerging phenomena in ferroelectrics is the control of charge transport by switching the polarization. Although charge conduction ($i.e.$, leakage current) in ferroelectrics has been considered as a detrimental factor to practical applications, an interaction between conduction and ferroelectric polarization has recently attracted much attention as a route for novel functionalities. In this presentation, we will report on the ferroelectric control of charge conduction in $BiFeO_3$/metal junctions: the $BiFeO_3$/metal interfaces can have either blocking or non-blocking contacts according to the polarization direction of the $BiFeO_3$ films, allowing non-volatile control of diode-like conduction characteristics. The resulting rectifying and photovoltaic effects can be turned on and off, as well as be flipped in polarity, depending on the ferroelectric domain structures.

8:36AM P33.00004 ABSTRACT WITHDRAWN –

8:48AM P33.00005 Magnetic Order in single-crystal $BiFeO_3$, MEHMET RAMAZANOGLU, SANG-WOOK CHEONG, VALERY KIRYUKHIN, Rutgers Univ. Physics Dept., WILLIAM RATCLIFF, NCNR, NIST, S. LEE, KAERI — We report neutron scattering studies of the magnetic order in multiferroic Bismuth Ferrite ($BiFeO_3$). In ferroelectric monodomain single crystals, there are 3 equivalent magnetic cycloidal domains. The cycloid period slowly grows with increasing temperature, and the antiferromagnetic transition is 2nd order. The equivalent magnetic domain populations do not change with temperature, except in the close vicinity of the Neel temperature. No evidence for the spin-reorientation transitions proposed in previous Raman studies is found. The magnetic cycloid is slightly anharmonic for T=5 K. The anharmonicity is much smaller than previously reported in indirect NMR studies. At room temperature, a circular cycloid is observed. The observed anharmonicity provides important clues for understanding electromagnons in $BiFeO_3$.

9:00AM P33.00006 Chemical substitution induced ferroelectric polarization rotation in $BiFeO_3$ thin films[1] , ICHIRO TAKEUCHI, DAISUKE KAN, ANBUSATHAIAH VARATHARAJAN, University of Maryland — The direction of the polarization vector in ferroelectric materials is an important parameter critical to a number of applications. Polarization orientation in ferroelectric thin films can be controlled by various approaches such as electric- field induced rotation and strain engineering using exotic substrates. We have performed systematic chemical substitution of rare earth cationic dopants, in particular Sm in the $BiFeO_3$thin films, and found that the polarization vector rotates from the (111) to the (001) direction as a continuous function of the dopant concentration. This is accompanied by enhanced dielectric ϵ_{33} as well as piezoelectric coefficient d_{33}, and the maximum in d_{33} (110 pm/V) is achieved at 14% Sm. We will discuss the correlation between the polarization rotation, structural evolution and other properties as a function of chemical substitution.

[1]Work at Maryland was supported by UMD-NSF-MRSEC (DMR 0520471) and ARO W911NF-07-1-0410. The work was also supported by the W. M. Keck Foundation and NEDO.

9:12AM P33.00007 Strain-stabilized phases of BiFeO3 and the role of first-principles calculations , ALISON HATT, Lawrence Berkeley National Lab — After many years of focused attention from the scientific community, the ferroelectric material $BiFeO_3$ (BFO) continues to be one of the most intriguing and technologically promising of the multifunctional ferroelectrics. Here I will discuss some of the recent developments on BFO thin films, including the metastable "super-tetragonal" phase achievable in epitaxial thin films. This strain-stabilized phase has been observed to coexist with a bulk-like phase, and reversible switching between the two has been demonstrated by acting on their ferroelectric polarizations with an external electric field. [Zeches *et al.*, Science 326, 977 (2009).] Related work finds a phase transition path of rhombohedral-to-monoclinic-to-tetragonal for epitaxially strained BFO, suggesting comparison to a compositional morphotropic phase boundary. I will discuss these results with an emphasis on the contributions from first-principles calculations, and provide context for understanding the calculated behaviors.

9:48AM P33.00008 Experimental evidence of stress-induced R-M_A-M_C-T phase transition in $BiFeO_3$ films , HANS CHRISTEN, JOONG-HEE NAM, CHARLEE BENNETT, HYUN-SIK KIM, MICHAEL BIEGALSKI, Oak Ridge National Laboratory — Recent reports on epitaxial $BiFeO_3$ films show that the crystal structure changes from nearly rhombohedral ("R-like") to nearly tetragonal ("T-like") at strains exceeding ≈-4.5%, with the "T-like" structure being characterized by a highly-enhanced c/a ratio. While both the "R-like" and the "T-like" phases are monoclinic, our detailed x-ray diffraction results reveal a symmetry change from M_A and M_C type, respectively. Therefore, the ferroelectric polarization is confined to different (pseudocubic) planes in the two phases. By applying additional strain or by modifying the unit cell volume of the film by substituting Ba for Bi, the monoclinic distortion in the "T-like" M_C phase is reduced, i.e. the system approaches a true tetragonal symmetry. Therefore, in going from bulk to highly-strained films, a phase sequence of rhombohedral(R)-to-monoclinic("R-like" M_A)-to-monoclinic("T-like" M_C)-to-tetragonal(T) is observed. This sequence is otherwise seen only near morphotropic phase boundaries in lead-based solid-solution perovskites (i.e. near a compositionally induced phase instability), where it can be controlled by electric field, temperature, or composition. Our results now show that this evolution can occur in a lead-free, stoichiometric material and can be induced by stress alone.

10:00AM P33.00009 Strained $BiFeO_3$ Films: Rhombohedral-Orthorhombic and Rhombohedral-Tetragonal Phase Transitions. Part I: Phase-Field Simulations[1] , GUANG SHENG, JINGXIAN ZHANG, ZI-KUI LIU, LONG-QING CHEN, Department of Materials Science and Engineering, The Pennsylvania State University, YULAN LI, Pacific Northwest National Laboratory, THE PENNSYLVANIA STATE UNIVERSITY TEAM, PACIFIC NORTHWEST NATIONAL LABORATORY COLLABORATION — In this study, the strain-temperature phase stability diagrams of (001) $BiFeO_3$ thin film were constructed using both thermodynamic analysis and phase-field simulations. The predicted diagram reveals a tetragonal to distorted rhombohedral phase boundary around 4.3% compressive strain and rhombohedral to orthorhombic boundary at around 2% tensile strain, both at room temperature. The predicted transition temperatures for rhombohedral-orthorhombic and rhombohedral-tetragonal transitions are in reasonable agreement with experimental observations. We will also discuss domain structure evolutions of $BiFeO_3$ thin films during the above two transitions from phase-field simulations.

[1]This work was supported by the DOE Basic Science under the grant No. DOE DE-FG02-07ER46417

10:12AM P33.00010 Strained BiFeO3 Films: Rhombohedral-Orthorhombic and Rhombohedral-Tetragonal Phase Transitions. Part II: Film Growth by Molecular-Beam Epitaxy , CAROLINA ADAMO, Cornell University, R. MISRA, A. MELVILLE, C. HEIKES, Q. HE, Y. CHU, J. LEE, R. HAISLMAIER, S. DENEV, V. GOPALAN, R. RAMESH, P. SCHIFFER, D. SCHLOM — Recently, Zeches et al.[1] reported the strain-temperature phase stability diagram of (001) BiFeO3 thin films. Depending on the strain and temperature the stable polymorph of BiFeO3 is predicted to be (monoclinically distorted) rhombohedral, tetragonal, or orthorhombic. To test these predictions commensurate BiFeO3 thin films were grown by adsorption-controlled reactive molecular-beam epitaxy on (110) YAlO3, (110) NdGaO3, (100) LSAT, (001) SrTiO3, (110) DyScO3, (110) TbScO3, (110) GdScO3, (110) SmScO3, (110) NdScO3, and (110) PrScO3 single crystalline substrates. The films span a biaxial strain range from -6.7% to +1.4%. Four-circle x-ray diffraction was used to determine the in-plane and out-of-plane lattice parameters. The rocking curve full widths at half maximum in omega of the films were nominally identical to the substrates on which they are grown and ranged from 11 arc sec (0.003 degrees) on (110) PrScO3 to 49 arc sec (0.014degrees) on (110) YAlO3. Magnetic data and second harmonic generation results will be presented. [1] R. J. Zeches, M. D. Rossell, J. X. Zhang, A. J. Hatt, Q. He, C.-H. Yang, A. Kumar, C. H. Wang, A. Melville, C. Adamo, G. Sheng, Y.-H. Chu, J. F. Ihlefeld, R. Erni, C. Ederer, V. Gopalan, L. Q. Chen, D. G. Schlom, N. A. Spaldin, L. W. Martin, and R. Ramesh, Science 326, 977 (2009).

10:24AM P33.00011 Strained $BiFeO_3$ films: rhombohedral-orthorhombic and rhombohedral-tetragonal phase transitions. Part IV: ultraviolet Raman spectroscopy study[1] , DMITRI A. TENNE, A.K. FARRAR, G. MOLINO, Physics Dept., Boise State University, Boise, ID, C. HEIKES, C. ADAMO, J.H. LEE, A. MELVILLE, D.G. SCHLOM, Cornell University, Ithaca, NY, G. SHENG, L.Q. CHEN, Pennsylvania State University, University Park, PA, Y.-H. CHU, National Chiao Tung University, Hsinchu, Taiwan, Q. HE, R. RAMESH, University of California, Berkeley, CA — Epitaxial $BiFeO_3$ films grown by molecular-beam epitaxy on substrates inducing different lattice-mismatch strain ($YAlO_3$, $SrLaAlO_4$, $PrScO_3$) have been studied by variable- temperature ultraviolet Raman spectroscopy. Temperature evolution of Raman spectra from $BiFeO_3$ films indicates the phase transitions from rhombohedral to tetragonal phase in compressively strained films on $YAlO_3$ and $SrLaAlO_4$ substrates. The films grown on PrScO3 substrates are subject to ∼1.3% tensile strain, and undergo the transition from rhombohedral to orthorhombic phase at about 550-600 K. The temperature dependence of Raman intensities of certain characteristic peaks indicates the possibility of coexisting rhombohedral and orthorhombic phases in the temperature range 400-550 K. Raman results are consistent with the phase diagram calculated using the phase field model.

[1]Supported by NSF and Research Corporation for Science Advancement.

10:36AM P33.00012 Emergence of 90° Domain Walls in Multiferroic $BiFeO_3$ Thin Film , JAN-CHI YANG, YING-HAO CHU, National Chiao Tung University, CHUN-YEN PENG, HSIANG-JUNG CHEN, National Chiao Tung University, LI CHANG, QING HE, RAMAMOORTHY RAMESH, UC Berkeley, CHAO-HUI YEH, HENG-JUI LIU, SHENG-JIE LIAO, PO-WEN CHIU, CHIH-HUNG LAI, National Tsing Hua University — Multiferroics have been a fascinating area for condensed materials research since these materials offer the exciting potential applications that taking advantages of multiple orders. Multiferroic $BiFeO_3$ (BFO) has played a key role in rejuvenating the field after a report of large ferroelectric polarization. Inside this material, domain walls (DWs) of BFO are of great interests. In recent study, room-temperature conductivity at ferroelectric DWs has been observed. In this work, through epitaxial strain, BFO thin films are grown on $NdScO_3$, which provide tensile strain on BFO films, and thus results in orthorhombic-like phase and corresponding periodic 90° DWs. X-ray reciprocal mapping and piezoresponse force microscopy has confirmed the orthorhombic-like and 90° DW structure. The transport behaviors of these natural formed 90° DWs as a function of temperatures and magnetic fields have been probed to understand their fundamental properties. In addition, exchange bias studies and X-ray magnetic dichroism spectromicroscopy have further revealed the magnetic properties in these DWs. Our results show that 90° DW in orthorhombic-like BFO possesses unusual electronic and magnetic behaviors, which are different from that in bulk and might be used for modern electronic devices and nanoelectronic.

10:48AM P33.00013 ABSTRACT WITHDRAWN –

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P34 DMP: Focus Session: Interfaces in Complex Oxides - Transport and Optics C141

8:00AM P34.00001 Electrodynamics and electronic structure of LVO/SVO superlattices investigated by optical spectroscopy , DA WOON JEONG, Seoul National Univ., Korea, WOO SEOK CHOI, TAE DONG KANG, Seoul National Univ, DAVID ADRIAN, CNRS, France, YUN SANG LEE, Soongsil Univ., Korea, WILFRID PRELLIER, CNRS, TAE WON NOH, Seoul National Univ — Perovskite vanadium oxide has intriguing coupling between orbital, spin and lattice degrees of freedom that bears novel physical properties. For example, filling controlled insulator to metal transition could be observed in $(La_{1-x}Sr_x)VO_3$, and orbital ordering was predicted theoretically for the interface valence state ($V^{3.5+}$) between $LaVO_3$ and $SrVO_3$ [1]. Here, we investigated the charge dynamics and electronic structures of $(LaVO_3)_{6m}(SrVO_3)_m$ (m=1,2, and 4) superlattices using optical spectroscopy. We found a reduction of Drude spectral weight as the superlattice periodicity is decreased, consistent with the transport result [2]. Moreover, interband transition of $(LaVO_3)_6(SrVO_3)_1$ was quite different from other larger period superlattices. New peak structure at 3.5eV was developed possibly due to the correlation between the electronic structure and orbital confinement. Electrodynamics and electronic structure reconstruction will be discussed.

[1] G. Jackeli *et al.*, PRL, **101**, 216804 (2008)
[2] W. C. Sheets *et al.*, APL **91**, 192102 (2007)

8:12AM P34.00002 Geometrically confined doping in $LaVO_3/SrVO_3$ superlattices , U. LUEDERS, A. DAVID, PH. BOULLAY, R. FRÉSARD, W. PRELLIER, P.-E. JANOLIN, CRISMAT TEAM[1], SPMS TEAM[2] — A number of theoretical predictions show that in complex oxides the confinement of t_{2g} electrons to two dimensions can alter strongly the physical properties of these systems compared to their 3D counterpart. To approach experimentally the 2D limit we propose geometrically confined doped superlattices as $LaVO_3/SrVO_3$. Here, a one unit cell thick layer of $SrVO_3$ is introduced between insulating $LaVO_3$ layers to create conducting zones with a 2D character. We synthesized this kind of superlattices by PLD on $SrTiO_3$ (001) substrates. The 2D character of the doped charge carriers influences strongly the physical properties of the superlattices. While the bulk solid solution is an insulating antiferromagnet, in the superlattices, room-temperature magnetism is observed due to the reduction of the bandwidth and a transition from a high temperature weakly localized phase to a low temperature metallic phase is shown to be connected to a structural transition from a metrically tetragonal to monoclinic phase. With the help of theoretical calculations, we will show that these peculiar properties are due to a change of the orbital physics in the vicinity of the $SrVO_3$ doping layers.

[1]UMR CNRS-ENSICAEN, Caen, France
[2]UMR CNRS- Ecole Centrale, Châtenay-Malabry, France

8:24AM P34.00003 Theory of $LaVO_3/SrVO_3$ superlattices[1] , HUNG DANG, ANDREW MILLIS, Department of Physics, Columbia University, New York, NY 10027 — We present dynamical mean field theory calculation and compare to experimental data [1] of the magnetic, orbital order and metal-insulator phase diagrams of $LaVO_3/SrVO_3$ superlattices. The calculation is based on a three-orbital model system; semiclassical and quantum Monte Carlo impurity solvers are used.

[1] U. Luders, W. C. Sheets, A. David, W. Prellier, and R. Fresard, Phys. Rev. B 80, 241102(R) (2009).

[1]Supported by the Basic Energy Sciences Program of the US Department of Energy under grant DOE ER 046169.

8:36AM P34.00004 New Optical Absorption Bands in Atomic Layer Superlattices[1] , JAMES ECKSTEIN, Depertment of Physics, University of Illinois, Urbana, IL — Using atomic layer-by-layer molecular beam epitaxy, atomic layer superlattices can be constructed that exhibit new electronic, optical and lattice effects not present in the individual components. In particular, new optical transitions giving rise to sharp absorption peaks can be created by placing a layer of a material with occupied source states next to a layer of another material with unoccupied destination states. We combine atomic layers of $SrTiO_3$ and $LaMnO_3$ into superlattice structures with component layers as thin as single monolayer and find a new absorption band due to a transition from manganese- to titanium-derived states. The energy of the new transition depends on how the bands line up at the interface. Furthermore, a substantial shift of spectral weight occurs as well, while retaining a constant sum rule. This work was supported by the Department of Energy Basic Energy Sciences at the Fredrick Seitz Materials Research Laboratory, University of Illinois, Urbana. This work was done in collaboration with Xiaofang Zhai, Mao Zheng, Amish Shah, Chandra Mohapatra, and Jian-Min Zuo.

[1]This work was supported by the Department of Energy Basic Energy Sciences at the Fredrick Seitz Materials Research Laboratory, University of Illinois, Urbana.

9:12AM P34.00005 Colossal Magnetoresistance in thin films of the Mott metal $CaVO_3$[1] , JIWEI LU, University of Virginia — Bulk $CaVO_3$ (CVO) is a Pauli paramagnetic metal with a singe 3d electron. Some unusual drastic changes in the magneto-resistance, magnetic susceptibility and the Hall effect have been reported in single crystal CVO. We have simultaneously synthesized epitaxial CVO films grown on three differently oriented $SrTiO_3$ substrates. The temperature dependent conductivity of these CVO films demonstrated very strong Fermi metal behavior and the resistance ratio, defined as R(300 K)/R (2K) was more than 3000. Colossal magneto-resistance (MR) as well as large crystalline anisotropic was observed at low temperatures. The maximum MR, defined as (R(7 T)-R(0 T))/R(0 T)*100 %, was over 1500 % at 2 K and 7 Telsa on the CVO films deposited on a (110) SrTiO3 single crystal substrate, and didn't show any sign of saturation. An MR of over $\sim$ 500 % and $\sim$ 200 % were observed on (111) and (100) orientation films under the same condition, respectively. The MR ratio was much larger than that of single crystal CVO. We will discuss the peculiar MR in association with the magnetic ordering, oxygen stoichiometry and Fermi surface.

[1]The author is grateful to the financial support by the ARO.

9:24AM P34.00006 High frequency conductivity of few unit cell thick $LaNiO_3$ layers[1] , DANIEL OUELLETTE, Department of Physics, University of CA, Santa Barbara, JUNWOO SON, SUSANNE STEMMER, Materials Department, University of CA, Santa Barbara, S. JAMES ALLEN, Department of Physics, University of CA, Santa Barbara — We have measured the dc and optical conductivity of ultra-thin films of the correlated metal $LaNiO_3$ and of superlattices with alternating $LaNiO_3$ and insulating $SrTiO_3$ layers, all grown epitaxially on LSAT substrates with modest tensile strain in the $LaNiO_3$. In the superlattices, the $LaNiO_3$ layers are 4 unit cells (1.6 nm) thick and the $SrTiO_3$ is either 4 or 10 unit cells thick. Isolated films thinner than 4 nm are insulating; however, both the superlattices and thicker films consistently show a coherent peak in the optical conductivity. Furthermore, the optical conductivity at several hundred GHz is in excellent agreement with the dc electrical conductivity. We consider the possibility of a percolation threshold in ultra-thin LaNiO3 layers and discuss implications for the nature of the $LaNiO_3/SrTiO_3$ interface.

[1]Support from the Army Research Office through a MURI program is gratefully acknowledged.

9:36AM P34.00007 Quasi 2D correlated metals: Unusual transport properties in strained heteroepitaxial ultrathin films[1] , E.J. MOON, B.A. GRAY, J. LIU, M. KAREEV, Phys. Dep., Univ. of Arkansas, Fayetteville, B. DABROWSKI, Phys. Dep., Northern Illinois Univ., J.W. FREELAND, APS, Argonne National Lab., I-C. TUNG, M.J. BEDZYK, Mat. Sci. Eng., Northwestern Univ., L.H. TJENG, Max Planck Inst. for Chem. Phys. of Solids, Germany, S.G. ALTENDORF, F. STRIGARI, Physikalisches Inst., Univ. zu Köln, Germany, V.P. KUNETS, G.J. SALAMO, J. CHAKHALIAN, Phys. Dep., Univ. of Arkansas, Fayetteville — We explore the electrical transport and magnetoconductance in quasi 2D strongly correlated heteroepitaxial films of $LaNiO_3$ to investigate the effect of quantum confinement and strain on electron-electron and electron-lattice interactions over the whole temperature range (2-300K) including the effect of metal-insulator transition. The quantum corrections to the conductivity indicate that the combination of the weak localization and the electron-electron interaction in the quasi 2D limit gives rise to unusual T-dependent resistivity. Ultrathin films spanning tensile strain up to $\sim$4% are used to obtain the enhanced driving effects between the two corrections for the observed localization at low temperatures. Intrinsic transport properties of strained $LaNiO_3$ films with the characteristic multi-band structure will be discussed.

[1]supported by DOD-ARO and NSF

9:48AM P34.00008 Strain-modified thermopower of ultrathin $LaNiO_3$ films[1] , NARAYAN PRASAI, JOSHUA COHN, University of Miami, EUN JU MOON, JIAN LIU, MICHAEL KAREEV, BENJAMIN GRAY, JAK CHAKHALIAN, University of Arkansas, JAMES RONDINELLI, Advanced Photon Source, Argonne National Laboratory — The influence of epitaxial strain on electronic transport in the correlated metal $LaNiO_3$ is investigated through measurements of thermopower (TEP) in the temperature range $5\text{K} \leq \text{T} \leq 330\text{K}$ on a series of fully-strained, 10-unit-cell-thick films grown by pulsed-laser deposition on (100)-oriented $YAlO_3$, $LaAlO_3$, $SrTiO_3$, and $GaScO_3$ substrates. The TEP exhibits an electron-like, linear-T contribution for $T \geq 150$ K with a slope approximately independent of strain, but a magnitude that varies systematically with strain. A peak in the TEP at $T \approx 25$ K also correlates with strain and is unaffected by a 9-T magnetic field. The implications of these results for strain-modified charge-carrier diffusion and phonon drag contributions to the TEP will be discussed.

[1]Work at the Univ. Miami was supported by an award from the Research Corporation, and at Univ. Ark. by the DOD-ARO under Contract No. 0402-17291 and NSF Contract No. DMR-0747808.

10:00AM P34.00009 Strain control of the metal-insulator transition of NdNiO3 epitaxial ultrathin films , JIAN LIU, M. KAREEV, B. GRAY, University of Arkansas, P. RYAN, J.W. KIM, J.W. FREELAND, Argonne National Lab, J. CHAKHALIAN, University of Arkansas — Metal-insulator transition (MIT) is the hallmark of strongly correlated electron systems. It often couples with the multiple degrees of freedom of d electrons in complex oxides, resulting in diverse and intriguing properties. While MIT has been studied for decades, heteroepitaxy is emerging as a promising way to manipulate correlated electrons and stabilize unusual phases in nanostructures. Understanding its effect on the MIT in ultrathin structures is fundamentally and technologically critical. To this end, we have grown perfectly strained atomic layers of NdNiO3 by laser MBE on a series of substrates with large variation in lattice mismatch. The extensive measurements including electric and thermal transport, synchrotron based XRD and XAS show dramatic modifications of electronic properties with lattice mismatch. Possible microscopic mechanisms are discussed. J.C. was supported by DOD-ARO under the Contract No. 0402-17291 and NSF Contract No. DMR-0747808.

10:12AM P34.00010 Two-dimensional electron gas in $SrTiO_3$, BHARAT JALAN, Materials Department, UCSB, S. JAMES ALLEN, Department of Physics, UCSB, SUSANNE STEMMER, Materials Department, UCSB — We report on Shubnikov-de Haas (SdH) oscillations in a two-dimensional electron gas (2DEG) in delta-doped $SrTiO_3$ thin films. The existence of a 2DEG is confirmed by the angular dependence of the SdH oscillations. The observed SdH oscillation frequency corresponds to a carrier concentration of, which is only 4% of the total Hall carrier density. We show that the only electrons in one of the sub-bands confined by the delta-doping potential have sufficient mobility to exhibit quantum oscillations. Guided by the similarity of the confined d-band electron states in $SrTiO_3$ to the confined hole systems in conventional semiconductors, quantum oscillations are interpreted in terms of spin and Landau level splitting. Despite the inherent complexity of a sub-band that is derived from four d-band states near the conduction band minimum of $SrTiO_3$, we show that the quantum oscillations can be modeled quantitatively. Alternative routes to realize high mobility 2DEGs in $SrTiO_3$ will also be discussed.

10:24AM P34.00011 High Temperature Conductance Characteristics of Differently Modified $LaAlO_3/SrTiO_3$-Heterostructures , FELIX GUNKEL, SUSANNE HOFFMANN-EIFERT, FZ Juelich, PGI-7 and JARA-FIT, Juelich, Germany, JOSÉE E. KLEIBEUKER, PETER BRINKS, MARK HUIJBEN, GUUS RIJNDERS, GERTJAN KOSTER, Mesa+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands, REGINA DITTMANN, RAINER WASER, FZ Juelich, PGI-7 and JARA-FIT, Juelich, Germany — In order to understand the physical origin of the high charge carrier density at the conducting interface between $SrTiO_3$ (STO) and $LaAlO_3$ (LAO) the role of defects has to be clarified. In this study, LAO/STO-heterostructures modified in stacking sequence and growth conditions were investigated by means of high temperature conductance (HTC) measurements under changing oxygen ambience. Under measurement conditions the samples are in equilibrium with the surrounding oxygen atmosphere, which rules out the effect of mobile oxygen vacancies on the interface conductivity [Gunkel et al., APL 97(2010)]. The HTC characteristics show a significant dependency on the preparation procedure of STO and LAO close to the interface. Nevertheless, a common conduction and charge compensation mechanism can be identified. The results are discussed with respect to the defect chemistry model of perovskite oxides.

10:36AM P34.00012 Magnetotransport behavior of $LaAlO_3/SrTiO_3$ and Ar-irradiated $SrTiO_3$: implications on Rashba Spin-Orbit coupling and magnetism in quasi-2-dimensional electron gases[1] , J.H. NGAI, Y. SEGAL, F.J. WALKER, S. ISMAIL-BEIGI, K. LEHUR, C.H. AHN, Yale University, D. SU, Y. ZHU, Brookhaven National Laboratory — Quasi 2-dimensional electron gases (Q2DEG) in complex oxide heterostructures exhibit a wide range of tunable behavior that promises potentially new functionalities. In particular much interest has focused on the Q2DEG at the $LaAlO_3/SrTiO_3$ interface, where evidence for Rashba spin-orbit coupling and magnetic behavior has recently been found through magnetotransport measurements. At present it is unclear whether the spin-orbit and magnetic effects are unique to the $LaAlO_3/SrTiO_3$ interface, or if they arise from the properties of doped $SrTiO_3$. In order to shed light on this issue, we compare the magnetotransport properties of $LaAlO_3/SrTiO_3$ and Ar^+-irradiated $SrTiO_3$. Strikingly similar magnetotransport behavior is observed between $LaAlO_3/SrTiO_3$ and Ar^+-irradiated Q2DEGs. However, our analysis indicates changes in the confinement or thickness of the Q2DEG can account for the magnetotransport observed. Implications of our results on Rashba spin-orbit coupling and magnetism at the $LaAlO_3/SrTiO_3$ interface will be discussed.

[1]NSF MRSEC DMR-0520495 and DMR-1006256

10:48AM P34.00013 Can an oxygen vacancy form a Kondo center at the $LaAlO_3/SrTiO_3$ interface?[1] , MOHAMMAD SHERAFATI, BIRABAR NANDA, SASHI SATPATHY, University of Missouri — Recently a Kondo resistance minimum has been observed at the interface between $LaAlO_3$ and $SrTiO_3$[1]. It has been suggested that the effect is due to the scattering of interface electrons from magnetic centers just like in the original Kondo effect; however, the origin of such magnetic centers is not understood. In this work, we evaluate the idea of whether an oxygen vacancy in $SrTiO_3$ might produce a magnetic center. We focus on an isolated vacancy in bulk $SrTiO_3$ from density-functional calculations and provide evidence that of the two electrons released to the system by the oxygen vacancy, one becomes localized near the vacancy site, while the other forms a delocalized state. The results suggest that the localized electron could form a Kondo center resulting in a resistance minimum as observed in the experiments.

[1] A. Brinkman *et al.*, Nature Mater. **6** 493 (2007).

[1]Work supported by the US Department of Energy

Wednesday, March 23, 2011 8:00AM - 11:00AM –
Session P35 DCMP: Topological Insulators: Magnetotransport C140

8:00AM P35.00001 Transition from n-type to p-type topological insulator thin films of Bi_2Te_3 , JIN-FENG JIA, Key Lab for Atomic, Molecular and Nanoscience, Department of Physics, Tsinghua University, Beijing 100084, P. R. China, GUANG WANG, XIE-GANG ZHU, YAO-YI LI, TONG ZHANG, JING WEN, XI CHEN, KE HE, Institute of Physics, The Chinese Academy of Sciences, Beijing 100190, P. R. China, LI-LI WANG, XU-CUN MA, YI-YANG SUN, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, New York 12180, USA, SHENG-BAI ZHANG, QI-KUN XUE — By using angle-resolved photoemission spectroscopy, we have investigated the electronic structure of the Bi_2Te_3 films on Si(111) prepared by molecular beam epitaxy. It is found that the Bi_2Te_3 films change from n-type to p-type topological insulator when the growth mode changes layer-by-layer to step-flow, for a given beam flux ratio of $Te_{2(4)}/Bi$. In situ scanning tunneling microscopy/spectroscopy (STM/STS) measurements reveal formation of different defects, i. e., Te_{Bi} and Bi_{Te} antisite defects, which are responsible for the n- and p-type conductivity transition. A mechanism for the transition is proposed based on the STM experiment and first-principles calculations. The work suggests a simple way to regulating the chemical potential and Dirac fermion density on the surface of a topological insulator without external doping.

8:12AM P35.00002 Magneto-Transport in Epitaxial Thin Film Sb_2Te_3 , E.C. GINGRICH, N.O. BIRGE, Michigan State University, G. WANG, C. UHER, University of Michigan — We report magneto-transport measurements in epitaxially grown thin films of Sb_2Te_3. Sb_2Te_3 is a topological insulator candidate expected to possess a single Dirac cone on its surface.[1] Both semiconducting and metallic samples were measured, identified by the temperature response of their resistivities. Shubnikov-deHaas (SdH) oscillations were found in measurements with fields up to 9T in metallic samples at liquid helium temperature, but have yet to be observed in semiconducting samples. Measurements will be presented along with plans for further research.

[1]H. Zhang et al., Nat. Phys. 5, 438 (2009).

8:24AM P35.00003 Anomalous galvanomagnetism, cyclotron resonance and microwave spectroscopy of topological insulators[1] , EWELINA HANKIEWICZ, GRIGORY TKACHOV, Wuerzburg University — The surface quantum Hall state, magneto-electric phenomena and their connection to axion electrodynamics have been studied intensively for topological insulators. One of the obstacles for observing such effects comes from nonzero conductivity of the bulk. To overcome this obstacle we propose to use an external magnetic field to suppress the conductivity of the bulk carriers. The magnetic field dependence of galvanomagnetic and electromagnetic responses of the whole system shows anomalies due to broken time-reversal symmetry of the surface quantum Hall state, which can be used for its detection. In particular, we find [1] linear bulk dc magnetoresistivity and a quadratic field dependence of the Hall angle, shifted rf cyclotron resonance, nonanalytic microwave transmission coefficient and saturation of the Faraday rotation angle with increasing magnetic field or wave frequency.

[1] G. Tkachov and E. M. Hankiewicz arXiv:1011.2756 (2010)

[1]The work was supported by DFG grant HA5893/1-1.

8:36AM P35.00004 Experimental evidence on a diffusive metallic surface state by the magneto-resistance oscillation in the topological insulating Bi_2Te_3 , FENGQI SONG, YUYUAN QIN, ZHAOGUO LI, QIANGHUA WANG, JIANGUO WAN, GUANGHOU WANG, National Lab of Solid State Microstructures, Nanjing University, Nanjing, China, ZHE QU, High Magnetic Field Laboratory, Chinese Academy of Sciences, Hefei, China — The spin helicity seems bound to the generation of the surface state (SS) in a three-dimensional strong topological insulating system. Here we demonstrate a diffusive metallic SS by measuring the magneto-resistance oscillations in the Bi_2Te_3 nanoflakes. The products of the oscillating periods and the cross sections of the flakes result in the values of the flux quantum (h/e) and the half quantum (h/2e). The first observation of the h/2e oscillation shows the violence of the spin helicity of the SS The h/e oscillation persists during increasing the magnetic field, while the h/2e oscillation fails, indicating the diffusive origin of the SS and its weak antilocalization. The diffusive SS is found robust against the increases of the circumference till 10 micrometers and the temperatures till 64K, when the h/e oscillation disappears. The diffusive SS can be further activated by the spin-polarized scattering formed by the deposited Co islands. All the evidence agrees to recent simulations on a weak-localized SS upon the presence of strong disorder centers. This research was supported by the National Key Projects for Basic Research of China (Grant numbers: 2009CB930501, 2010CB923401).

8:48AM P35.00005 Two-dimensional surface state revealed in the quantum limit of a topological insulator[1] , R. MCDONAD, NHMFL/LANL, J. ANALYTIS, SLAC, J.-H. CHU, Standford, S. RIGGS, I. FISHER, Stanford, G. BOEBINGER, FSU/NHMFL — Topological insulators possess a metallic surface state of massless particles, known as Dirac fermions whose spin is coupled to their momentum. The realization of this in Bi2Se3 has sparked considerable interest owing both to the potential for spintronic devices and in the investigation of the fundamental nature of topologically non-trivial quantum matter. However, the conductivity of these compounds tends to be dominated by the bulk of the material owing to chemical imperfection, making the transport properties of the surface nearly impossible to measure. We have systematically reduced the number of bulk carriers in the material Bi2Se3 to the point where a magnetic field can collapse them to their lowest Landau level. Beyond this field, known as the three-dimensional (3D)'quantum limi', the signature of the 2D surface state can be seen. At still higher fields, we reach the 2D quantum limit of the surface Dirac fermions. In this limit we observe an altered phase of the oscillations, which is related to the peculiar nature of the Landau quantization of topological insulators at high field. Furthermore, we observe quantum oscillations corresponding to fractions of the Landau integers, suggesting that correlation effects can be observed in this new state of matter.

[1]Supported by NSF Division of Materials Research through DMR-0654118, US DOE, BES 'Science in 100 T' programme and by DOE BES contract 73 DE-AC02-76SF00515

9:00AM P35.00006 The surface-state of the topological insulator Bi2Se3 revealed by cyclotron resonance , OSCAR AYALA-VALENZUELA, NHMFL, Los Alamos National Laboratory, JAMES G. ANALYTIS, JIUN-HAW CHU, SLAC, Stanford University, MOAZ-M. ALTARAWNEH, NHMFL, Los Alamos National Laboratory, IAN R. FISHER, SLAC, Stanford University, ROSS D. MCDONALD, NHMFL, Los Alamos National Laboratory — Recently, a large number of surface-sensitive probes have reported the existence of Dirac quasiparticles, similar to those reported in graphene, on the surface of single crystals of Bi2Se3 and related compounds. To date transport measurements of TIs have been dominated by the conductivity of the bulk, leading to substantial difficulties in resolving the properties of the surface. To this end, we use high magnetic field, rf- and microwave-spectroscopy to selectively couple to the surface conductivity of Bi2Se3 at high frequency. In the frequency range of a few GHz we observe a crossover from quantum oscillations indicative of a small 3D Fermi surface, to cyclotron resonance indicative of a 2D surface state. The frequency-magnetic field scaling of this resonance is inconsistent with the bulk effective mass, but more consistent with the dispersion and band filling of a Dirac-like surface state as observed by ARPES, with substantial many-body renormalization. Measurements as a function sample thickness aid in separating bulk and surface contributions and indicate that the band filling of the Dirac cone varies from cleave to cleave.

9:12AM P35.00007 Surface Hall response of 3D topological insulators , DIMITRIE CULCER, Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei 230026, Anhui, China, SANKAR DAS SARMA, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742-4111, USA — We determine the Hall conductivity due to the surface states of 3D topological insulators in the presence of a weak perpendicular magnetic field and/or magnetization. We consider electron doping and calculate all known contributions to the Hall current, including the intrinsic, skew scattering and side jump terms. Skew scattering contributes to in the Born approximation, as well as giving the usual contribution of third order in the scattering potential. We identify a side-jump scattering term together with an intrinsic side-jump term, which give contributions of a similar magnitude. The dominant term by several orders of magnitude is of the order of the conductivity quantum, and includes a topological contribution and a renormalization due to scattering. The result is independent of the Rashba spin-orbit constant, as well as of the impurity concentration. It has different signs depending on whether the principal source of scattering is charged impurities or short-range interface roughness. We expect our results to help disentangle surface transport from bulk transport in these materials [1].
[1] D. Culcer, E. H. Hwang, T. D. Stanescu, and S. Das Sarma, Phys. Rev. B 82, 155457 (2010).

9:24AM P35.00008 In Search of the Quantum Anomalous Hall Effect in Ferromagnetic Cr-Bi_2Se_3 Topological Insulator Thin Films[1] , PASCAL P.J. HAAZEN, J.-B. LALOE, Francis Bitter Magnet Lab, MIT, D. HEIMAN, Dept. of Physics, Northeastern University, P. JARILLO-HERRERO, Dept. of Physics, MIT, J.S. MOODERA, Francis Bitter Magnet Lab, MIT — A recent prediction that the topological insulator Bi_2Se_3 can become magnetically ordered upon doping with Cr or Fe opens up the possibility of observing the quantum anomalous Hall effect, in the absence of an external magnetic field [1]. We report on molecular beam epitaxy-grown Cr-Bi_2Se_3 thin-films with a Cr content of $0 \sim 10$ at.%, and their properties. Our films show highly oriented crystallinity up to a Cr content of 8%, as required for ferromagnetic ordering. Films with Cr were ferromagnetic; the measured saturation magnetic moment per Cr atom is $1\mu_B$ for the crystalline films, with a T_C of up to $\sim 25K$. Currently we are investigating the transport characteristics. Varying the electro-chemical potential level in our quantum anomalous Hall insulators by gating should give rise to plateaus of Hall conductance as the Fermi level passes through the energy gap, due to the breaking of time-reversal symmetry caused by the magnetic ions.

[1] R. Yu et al. Science 329, 61 (2010)

[1]NSF DMR 0504158 and MIT Lincoln Laboratory contract number FA8721-05-C-0002.

9:36AM P35.00009 Quantum Oscillations in a topological insulator Bi_2SeTe_2 with large bulk resistivity[1] , JUN XIONG[2], DONGXIA QU, ROBERT CAVA, N. PHUAN ONG, Princeton University — To date, transport experiments on Topological Insulators are seriously hampered by bulk conductance G_b arising from impurity bands or band bending. Because of the large G_b, the surface currents carried by the massless Dirac surface states have been very difficult to resolve. We report measurements on the new topological insulator Bi_2SeTe_2 which has an unusually highly bulk resistivity ρ (6 Ωcm at 4 K, or 1,000 times higher than in Bi2Te3). Despite the large ρ, Shubnikov-de Haas (SdH) oscillations are clearly resolved in the Hall conductance up to 38 K, which implies a very high surface mobility. In a field B of 14 T, Landau Levels (LLs) n = 4-9 are well resolved. We will describe the value of the Onsager phase γ fixed by the index plot of the LLs.

[1]Supported by NSF DMR 0819860.
[2]presenter

9:48AM P35.00010 Thermoelectric Properties of Non-Metallic Topological Insulator Bi_2Te_3 at High Magnetic Fields[1]

, DONG-XIA QU, YEW SAN HOR, ROBERT J. CAVA, N. PHUAN ONG, PRINCETON UNIVERSITY TEAM

— Three-dimensional topological insulators are a new class of electronic systems characterized by a bulk insulating state and conducting surface states with Dirac-like energy-momentum dispersion [1, 2]. One of the interesting aspects of this material is how the surface states affect thermoelectric properties of the whole electronic system, given that the bismuth based topological insulators are also excellent thermoelectric materials. We studied the low-temperature thermoelectric transport properties of high-mobility bulk topological insulator Bi_2Te_3 at high magnetic fields up to 35 T. We found remarkably large quantum oscillations in the thermopower of the surface states over a field range of 14 to 35 T. The existence of a non-zero Berry's phase in surface electrons is confirmed from the magneto-oscillations of both thermopower and magnetoresistance.

[1] L. Fu, C. L. Kane, and E. J. Mele, Phys. Rev. Lett. **98**, 106803 (2007)
[2] Y. Xia *et al.*, Nat. Phys. **5**, 398 (2009).

[1]Supported by NSF-MRSEC under Grant DMR 08-19860.

10:00AM P35.00011 Large thermoelectric figure of merit for three-dimensional topological Anderson insulators via line dislocation engineering[1]

, OLEG TRETIAKOV, ARTEM ABANOV, Texas A&M University, SHUICHI MURAKAMI, Tokyo Institute of Technology, JAIRO SINOVA, Texas A&M University — We study the thermoelectric properties of three-dimensional topological Anderson insulators with line dislocations. We show that at high densities of dislocations the thermoelectric figure of merit ZT can be dominated by one-dimensional topologically protected conducting states channeled through the lattice screw dislocations in the topological insulator materials with a nonzero time-reversal-invariant momentum such as $Bi_{0.9}Sb_{0.1}$. When the chemical potential does not exceed much the mobility edge the ZT at room temperatures can reach large values, much higher than unity for reasonable parameters, hence making this system a strong candidate for applications in heat management of nanodevices.

[1]This work was supported by NSF under Grant Nos. DMR-0547875 and 0757992, by the Research Corporation Cottrell Scholar Award, and by the Welch Foundation (A-1678).

10:12AM P35.00012 Quantum Oscillations and Quantum Hall Effect in Topological Insulator Material Bi_2Se_3

, HELIN CAO, IRENEUSZ MIOTKOWSKI, TIAN SHEN, YONG CHEN, Department of Physics, Purdue University, West Lafayette, IN 47907 USA — Bi_2Se_3 has attracted strong attention recently as a prototype topological insulator material. We have measured magneto-transport in metallic Bi_2Se_3 crystals. At high magnetic field (B), the longitudinal resistance (R_{xx}) displays characteristic Shubnikov–de Haas (SdH) oscillations (periodic in 1/B). The measurements in tilted magnetic field show the SdH oscillations are only controlled by the perpendicular component of B, indicating 2D nature of charge carriers. We also observed quantized plateaus in Hall resistance (R_{xy}) concomitant with the minima in R_{xx}. From the temperature dependence of the SdH oscillations, we extract a Fermi velocity $\sim$5.9*10^5m/s, and an effective mass $\sim$0.14m_e (m_e is the electron mass). We discuss possible relations of our observations to topological surface states, as well as contributions from individual 2D quintuple layers of Bi_2Se_3.

10:24AM P35.00013 High field magnetotransport in high purity crystals of topological insulator Bi_2Se_3[1]

, NICHOLAS BUTCH, PAUL SYERS, JOHNPIERRE PAGLIONE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park — We have synthesized crystals of high purity undoped Bi_2Se_3 with carrier density less than 10^{17} cm^{-3} and high bulk mobility. Thorough characterizations of transport and optical properties in fields up to 14 T suggest a high surface scattering rate [1-3]. In a search for quantum oscillations from the surface carriers, we performed measurements of longitudinal and Hall resistance in pulsed magnetic fields of up to 60 T. Due to the as-yet poorly characterized environmental sensitivity of the Bi_2Se_3 surfaces, we performed on-site cleaving and application of leads under dry flowing nitrogen. The Hall measurements and temperature- and angle-dependence of the longitudinal magnetoresistance will be discussed.

[1] N. P. Butch, et al., Phys. Rev. B 81, 241301 (2010)
[2] A. B. Sushkov, et al., Phys. Rev. B 82, 125110 (2010)
[3] G. S. Jenkins, et al., Phys. Rev. B 82, 125120 (2010)

[1]This work was supported by the NSF-MRSEC at the University of Maryland, DMR # 0520471.

10:36AM P35.00014 Anomalous Aharonov-Bohm Conductance Oscillations from Topological Insulator Surface States[1]

, YI ZHANG, ASHVIN VISHWANATH, University of California, Berkeley — We study Aharonov-Bohm (AB) conductance oscillations arising from the surface states of a topological insulator nanowire, when a magnetic field is applied along its length. With strong surface disorder, these oscillations are predicted to have a component with anomalous period $\Phi_0 = hc/e$, twice the conventional period. The conductance maxima are achieved at odd multiples of $\Phi_0/2$, implying that a π AB phase for electrons strengthens the metallic nature of surface states. This effect is special to topological insulators, and serves as a defining transport property. A key ingredient, the surface curvature induced Berry phase, is emphasized here. We discuss similarities and differences from recent experiments on Bi_2Se_3 nanoribbons, and optimal conditions for observing this effect.

[1]We acknowledge insightful discussions with H. Mathur, D. Carpentier, J. Moore, and G. Paulin, and DOE Grant No. DE-AC02-05CH11231 for support.

10:48AM P35.00015 First-principles calculation of the full orbital magnetoelectric response

, ANDREI MALASHEVICH, UC Berkeley, IVO SOUZA, Centro de Fisica de Materiales, San Sebastian, SINISA COH, DAVID VANDERBILT, Rutgers University — The possibility of a quantized magnetoelectric (ME) effect in Z_2 topological insulators suggests that the orbital part of the ME response can, at least in principle, be comparable in magnitude to the total response of known ME materials.[1] A band theory of the orbital ME response of generic insulators was recently developed,[2] paving the way for first-principles calculations. Two types of terms contribute to the response. The Chern-Simons term, which only depends on the unperturbed valence Bloch states, was the subject of a recent Wannier-based calculation.[1] The Kubo terms require a knowledge of the Bloch states at first order in the electric field and can be calculated by finite differences from the change in orbital magnetization induced by small electric fields.[2] We present preliminary results of such a calculation for Cr_2O_3, using the Berry-phase approach to calculate the electronic structure under a finite electrical bias. By monitoring the field-induced changes in orbital and spin magnetization and comparing the results obtained with and without structural relaxation, all contributions to the ME coupling can be computed.

[1]S. Coh *et al.*, arXiv:1010.6071.
[2]A. Malashevich *et al.*, New J. Phys. **12**, 053032 (2010)

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P36 DMP: Focus Session: Graphene: Growth, Characterization, and Devices: Electronic Structure C142

8:00AM P36.00001 Electronic properties of the Graphene/SiC $(000\bar{1})$ interface: a First Principles study , THUSHARI JAYASEKERA, SHU XU, K.W. KIM, MARCO BUONGIORNO-NARDELLI, North Carolina State University — In this talk, we will discuss the electronic properties of epitaxial graphene on the SiC $(000\bar{1})$ surface (C-terminated face) using Density Functional Theory. In our calculations we focus on mono- and bi-layer graphene with AA, AB and turbostratic stacking sequences. Of the three, the turbostratic is the most observed during growth on SiC $(000\bar{1})$. However, no theoretical investigations are available to understand the effect of the substrate on this growth sequence. We will investigate the energetics of different stackings and explain their electronic properties. We will also discuss the role of the interfaces in the stabilization of the individual stacking sequences and indicate possible routes for chemical functionallizations at the heterojunction to facilitate the tuning of the electronic and transport properties of these systems.

8:12AM P36.00002 Local surface potential variations and charge puddling in graphene on SiC(0001)[1] , A.E. CURTIN, W.G. CULLEN, M.S. FUHRER, Materials Research Science and Engineering Center and Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, R.L. MYERS-WARD, L.O. NYAKITI, V.D. WHEELER, D.K. GASKILL, U.S. Naval Research Laboratory, Code 6800, Washington, DC 20375 — We performed Kelvin probe microscopy in ultra-high vacuum on epitaxial graphene grown on SiC(0001). In agreement with previous work, we see discrete surface potentials corresponding to interface layer and monolayer regions separated by steps of ∼100 mV. We used the step width to determine the spatial resolution of the probe to be approximately 20 nm. Within a monolayer area we see smaller fluctuations in surface potential of only a few mV. The data set limits on the scale of possible electron/hole puddles in monolayer graphene on SiC(0001).

[1]This work was supported by the University of Maryland MRSEC.

8:24AM P36.00003 Electric Field Effects on Electronic Structures of Epitaxial Graphene on SiC , HYUNGJUN LEE, Department of Physics and IPAP, Yonsei University, SEUNGCHUL KIM, JISOON IHM, Department of Physics and Astronomy, Seoul National University, YOUNG-WOO SON, Korea Institute for Advanced Study, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University — We report first-principles calculations of atomic and electronic structures of epitaxial single-layer graphene on Si-faced SiC(0001) surface under homogeneous transverse electric fields. We find that atomic positions are insensitive to applied electric fields, but the electronic band structures of the graphene layer are shifted in energy, depending strongly on the applied electric fields, while those of the buffer layer are almost unchanged. This effect finally results in field-induced closing of the energy gap at the Dirac energy point and recovery of the conic feature of the low-energy band structures of free-standing graphene, which are verified and analyzed further with a tight-binding model. The recovery of conical dispersion of the single-layer graphene and ambipolar field-effect behavior makes epitaxial single-layer graphene one of the promising alternatives to current state-of-the-art transistors for radiofrequency applications. This work was supported by the NRF of Korea (Grant No. 2009-0081204). Computational resources have been provided by KISTI Supercomputing Center (KSC-2008-S02-0004).

8:36AM P36.00004 Plasmarons in Quasi-freestanding Epitaxial Graphene , AARON BOSTWICK, Lawrence Berkeley National Laboratory — Graphene is a remarkable new electronic material with many unique properties. To realize its promise, it is essential to understand how its charge carriers interact. By measuring the spectral function of charge carriers in quasi-free-standing graphene, we show that at finite doping, the well-known linear Dirac spectrum does not provide a full description of the charge-carrying excitations. We find that there also exist composite "plasmaron" particles, consisting of holes coupled to density oscillatons of the graphene electron gas. The Dirac crossing point is resolved into three crossings: the first between pure charge bands, the second between pure plasmaron bands, and the third a ring-shaped crossing between charge and plasmaron bands.

9:12AM P36.00005 Effective screening and the plasmaron bands in Graphene , A. WALTER, FHI, Max-Planck-Gesellschaft and ALS, E. O. Lawrence Berkeley Laboratory, K.J. JEON, EETD, E. O. Lawrence Berkeley Laboratory, A. BOSTWICK, ALS, E. O. Lawrence Berkeley Laboratory, L. MORESCHINI, Y.S. KIM, ALS, E. O. Lawrence Berkeley Laboratory, Y.J. CHANG, FHI, Max-Planck-Gesellschaft and ALS, E. O. Lawrence Berkeley Laboratory, F. SPECK, M. OSTLER, T. SEYLLAR, U Erlangen-Nürnberg, K. HORN, FHI, Max-Planck-Gesellschaft, E. ROTENBERG, ALS, E. O. Lawrence Berkeley Laboratory — In the following we investigate the plasmaron bands in the presence of differing effective screening, by changing the interface layer between graphene and a SiC substrate. ARPES data is presented and the deviation of the band structure from the Dirac cone picture is attributed to electron, hole, plasmon interactions. Comparison to G_0W -RPA theory is used to determine the effective dielectric constant of the underlying layer and a range of values (ε_S ∼219 to ∼11.6) is found. This investigation indicates that, in addition to the long list of unique and interesting properties, graphene is an ideal candidate for investigating the effective screening in the context of electron-hole-plasmon interactions. It is also shown that plasmaronic and electronic properties of graphene can be manipulated semi-independently, a necessity if it is to be employed in future "plasmaronic" devices.

9:24AM P36.00006 Phonon-Induced Gaps in Graphite and Graphene Observed by Angle-Resolved Photoemission , YANG LIU, University of Illinois, Urbana-Champaign, LONGXIANG ZHANG, MATTHEW BRINKLEY, GUANG BIAN, TOM MILLER, TAI-CHANG CHIANG, UNIVERSITY OF ILLINOIS, URBANA-CHAMPAIGN TEAM — Graphene systems, made of sheets of carbon atomic layers, have unusual electronic structures known as Dirac cones. While strong interest in the electronic structure of these graphitic materials has driven extensive ARPES studies, prior work has mostly focused on the quasiparticle band dispersion relations associated with the Dirac cones. Largely unexplored are spectral regions far away from the quasiparticle bands, where direct emission from the quasiparticles is forbidden, but indirect emission through coupling to phonons is allowed. Our ARPES measurements of graphite and graphene layers at low temperatures reveal heretofore unreported gaps at normal emission, one at around 67 meV and another much weaker one at around 150 meV. The major gap features persist to room temperature and beyond, and diminish for increasing emission angles. We show that these gaps arise from electronic coupling to out-of-plane and in-plane vibrational modes at the K point in the surface Brillouin zone, respectively, in accordance with conservation laws and selection rules governed by quantum mechanics. Our study suggests a new approach for characterizing phonons and electron-phonon coupling in solids.

9:36AM P36.00007 Many-Body Interactions in Quasi-Freestanding Graphene , DAVID SIEGEL, University of California, Berkeley / Lawrence Berkeley National Lab, CHEOL-HWAN PARK, University of California, Berkeley, CHOONGYU HWANG, Lawrence Berkeley National Laboratory, JACK DESLIPPE, University of California, Berkeley / Lawrence Berkeley National Lab, ALEXEI FEDOROV, Advanced Light Source, Lawrence Berkeley National Laboratory, STEVEN LOUIE, ALESSANDRA LANZARA, University of California, Berkeley / Lawrence Berkeley National Lab — The Landau-Fermi liquid picture for quasiparticles assumes that charge carriers are dressed by many-body interactions, forming the basis of any theory of solids. Whether this picture still holds for a semimetal like graphene at the neutrality point, i.e. when the chemical potential coincides with the Dirac point energy, is one of the long-standing puzzles in this field. Here we present the first direct measurements of the self-energy in graphene near the neutrality point, by using high-resolution angle-resolved photoemission spectroscopy. These exciting findings set a new benchmark in our understanding of many-body physics in graphene and a variety of novel materials with Dirac fermions.

9:48AM P36.00008 Abnormal temperature-dependent self-energy in graphene , CHOONGYU HWANG, LBNL, DANIEL GARCIA, DAVID SIEGEL, PU YU, SWANEE SHIN, UC Berkeley, LBNL, XIAOZHU YU, LBNL, ALEXEI FEDOROV, ALS, LBNL, EUGENE HALLER, RAMAMOORTHY RAMESH, DUNG-HAI LEE, ALESSANDRA LANZARA, UC Berkeley, LBNL — Dynamics of charge carriers are determined by their self-energy associated with many-body interactions. By using angle-resolved photoemission spectroscopy, we study the origin of abnormal temperature-dependent self-energy in graphene, and discuss the results in terms of a quantum phase transition as a function of temperature. Our findings provide another example of novel electronic properties of graphene and deeper understanding of the ground state of charge carriers in graphene.

10:00AM P36.00009 Graphene/substrate charge transfer characterized by inverse photoelectron spectroscopy , LINGMEI KONG, Department of Physics, University of Nebraska-Lincoln, Lincoln, NE USA, CAMERON BJELKEVIG, SNEHA GADDAM, MI ZHOU, Department of Chemistry, University of North Texas, Denton, TX USA, YOUNGHEE LEE, GANGHEE HAN, Department of Physics, Department of Energy Science, Sungkyunkwan University, Suwon, Korea, HAEKYUNG JEONG, Department of Physics, Daegu University, Gyeongsan, Korea, NING WU, ZHENGZHENG ZHANG, JIE XIAO, PETER DOWBEN, Department of Physics, University of Nebraska-Lincoln, Lincoln, NE USA, JEFFRY KELBER, Department of Chemistry, University of North Texas, Denton, TX USA — Wave vector-resolved inverse photoelectron spectroscopy (IPES) measurements demonstrate that there is a large variation of interfacial charge transfer between graphene and various substrates. IPES measurements of CVD single layer graphene on BN(0001)/Ru(0001), Ru, Ni(poly), and Cu(poly) indicate a substrate-to-graphene charge transfer of approximately 0.07, 0.06, 0.03 e- per carbon atom respectively and a charge transfer of 0.02 e- from graphene to the MgO substrate per carbon atom. IPES and photoemission data also indicate that graphene/MgO(111) has a band gap. These data demonstrate that IPES is an effective method for precise measurement of substrate/graphene charge transfer due to the extreme surface sensitivity of IPES.

10:12AM P36.00010 Characterization of Image States in Graphene on Ir(111)[1] , JERRY I DADAP, Columbia University, New York, MARKO KRALJ, MARIN PETROVIC, Institut za fiziku, Zagreb, Croatia, KEVIN KNOX, NADER ZAKI, ROHAN BHANDARI, PO-CHUN YEH, RICHARD M. OSGOOD JR., Columbia University, New York — Two dimensional electron systems involving graphene and graphene/metallic interfaces are increasingly of interest in condensed matter physics. Here, we demonstrate two-photon photoemission to map the image states of highly perfect and weakly bonded graphene on an Ir(111) substrate to reveal the effects of interaction with the underlying metal substrate. We observe a monotonic decrease in the work function with increasing graphene coverage from 5.6±0.1 eV for clean Ir to 4.5±0.1 eV for full graphene ML. We observe n=1, 2, 3 image states with nearly free electron dispersion. Despite the minimal coupling between the graphene and Ir, the energy spacing of the image states is consistent with a single Rydberg series description, in contrast to the expected bifurcation of the image states into odd and even states for a pure graphene layer. At large $k_{||}$, we observe a weak state deviating from the n=1 dipersion. We explain this effect in terms of scattering from the Ir substrate.

[1]This work is supported by DOE Contract No. DEFG 02-04-ER-46157

10:24AM P36.00011 Electronic and chemical properties of epitaxial graphene intercalated with $FeCl_3$, KRISTIN SHEPPERD, FENG WANG, JEREMY HICKS, HOLLY TINKEY, EDWARD CONRAD, Georgia Institute of Technology — Epitaxial graphene has emerged as the platform for large-scale graphene-based electronics. To fully exploit the unique properties of graphene for electronic materials, a number of materials issues need to be resolved. One important challenge is being able to control the doping of graphene without altering its band structure and disrupting the sp2 graphene bonding. One approach to accomplish this is intercalation of atomic or molecular species between individual graphene layers. We report the intercalation of multilayers of epitaxial graphene (EG) with the electron-acceptor $FeCl_3$. We will present results on experiments focused on the intercalation of $FeCl_3$ into multilayers EG grown on the C-face of SiC(000-1). Intercalation with different staging was achieved by a standard two-zone vapor transport method. The chemical and electronic properties of the EG-$FeCl_3$ intercalation compounds were analyzed using Raman spectroscopy, X-ray photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED).

10:36AM P36.00012 Accessing high energy sub-bands in bilayer graphene - a transport study , DMITRI K. EFETOV, PATRICK MAHER, SIMAS GLINSKIS, PHILIP KIM, Columbia University — In contrast to single layer graphene sheets with its two distinct valence and conduction bands merging at the Dirac Point, multilayer graphene sheets are known to have additional sub-bands at higher energies. Whereas the low energy sub-bands in these systems are well studied, the higher energy sub-bands could so far not be accessed in a transport measurement of graphene samples sitting on typical SiO_2/Si back gates. Employing a poly(ethylene)oxide-$CsClO_4$ solid polymer electrolyte gate we demonstrate the filling up of the high energy sub-bands in bilayer graphene samples at carrier densities above $\sim$ 2.7x10^{13} cm^{-2} . The onset of these sub-bands is defined by a slight increase of the resistivity and the onset of Shubnikov de Haas (SdH) oscillations. Measurements of the magneto-resistance, the SdH oscillations and the Hall Effect enable us to deduce the carrier densities and mobilities for both, the high and low energy bands simultaneously. In addition, we find that the onset energy of these sub-bands can be tuned by varying the bilayer interlayer asymmetry.

10:48AM P36.00013 Magnetic-field induced Electron-K-Phonon Interaction in the optical response of multi-layer epitaxial graphene , GERARD MARTINEZ, MILAN ORLITA, MAREK POTEMSKI, Laboratoire National des Champs Magetiques Intenses, CNRS, MIKE SPRINKLE, CLAIRE BERGER, WALTER DE HEER, School of Physics,Georgia Institute of Technology, Atlanta, LIANG TAN, STEVEN LOUIE, Department of Physics, University of California at Berkeley — Absolute magneto-optical transmission measurements have been performed in the far-infra-red range under magnetic fields up to 32 T and at a temperature of 1.8 K on a series of multi-layer epitaxial graphene samples. In all samples, transmission data show for the main optical transition involving the n=0 landau level a clear splitting of the transition in the field range 17-18 T corresponding to an energy of about 150 meV which coincides with that of the K zone boundary phonon of graphene. A global analysis of the data using a multi-dielectric model, to fit them with a single transition, reveals in that range of energies an additional increase of the line-width accompanied by a softening of the transition energy. The energy variation of these quantities is characteristic of the emission of phonons. Possible origins of this effect will be discussed but seems to be the consequence of electron-electron interactions between the two valleys K and K' assisted by K-phonons between these two valleys.

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P37 DMP: Focus Session: Graphene Structure, Dopants, and Defects: Strain Engineering II C146

8:00AM P37.00001 Beller Lectureship Talk: Gauge fields in graphene , FRANCISCO GUINEA, CSIC - Madrid — Graphene is a unique material with many special features not found in other systems. Elastic strains, and also topological defects, act on the charge carriers in the same way as effective gauge fields. The emergence of these fields, their dependence on sample parameters, and their relevance to experiments will be reviewed.

8:36AM P37.00002 Limits on electron quality in suspended graphene due to flexural phonons , EDUARDO V. CASTRO, H. OCHOA, Instituto de Ciencia de Materiales de Madrid (CSIC), Spain, M.I. KATSNELSON, Radboud University Nijmegen, Institute for Molecules and Materials, The Netherlands, R.V. GORBACHEV, D.C. ELIAS, K.S. NOVOSELOV, A.K. GEIM, School of Physics & Astronomy and Manchester Centre for Mesoscience & Nanotechnology, University of Manchester, UK, F. GUINEA, Instituto de Ciencia de Materiales de Madrid (CSIC), Spain — The temperature dependence of the mobility in suspended graphene samples has been investigated. In clean samples, flexural phonons become the leading scattering mechanism at temperature $T > 10$ K, and the resistivity increases quadratically with T. Flexural phonons limit the intrinsic mobility down to a few m^2/Vs at room T, a value that is routinely achievable for graphene on a substrate. Their effect can be eliminated by applying strain. Similar qualitative behavior, even though with important quantitative differences, has been found for suspended bilayer graphene.

8:48AM P37.00003 Topological defect clustering and plastic deformation mechanisms in functionalized graphene[1] , RICARDO NUNES, JOICE ARAUJO, HELIO CHACHAM, UFMG-Brazil — We present ab initio results suggesting that strain plays a central role in the clustering of topological defects in strained and functionalized graphene models. We apply strain onto the topological-defect graphene networks from our previous work [1], and obtain topological-defect clustering patterns which are in excellent agreement with recent observations in samples of reduced graphene oxide [2]. In our models, the graphene layer, containing an initial concentration of isolated topological defects, is covered by hydrogen or hydroxyl groups. Our results also suggest a rich variety of plastic deformation mechanism in functionalized graphene systems.

[1] Joice da Silva-Araujo, H. Chacham, and R. W. Nunes, Phys. Rev. B 81, 193405 (2010).
[2] C. Gomez-Navarro et al., Nano Lett. 10, 1144 (2010).

[1]We acknowledge support from the Brazilian agencies: CNPq, Fapemig, and INCT-Materiais de Carbono.

9:00AM P37.00004 Electronic states of graphene grain boundaries , ANDREJ MESAROS, Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands, STEFANOS PAPANIKOLAOU, LASSP, Physics Department, Clark Hall, Cornell University, Ithaca, NY 14853-2501, C.F.J. FLIPSE, Department of Applied Physics, Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands, DARIUS SADRI, JAN ZAANEN, Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands — Recent scanning tunneling spectroscopy measurements on graphite grain boundaries have identified zero energy peaks in the local density of states. These features are tied to intriguing magnetic properties observed in such samples, but are not found in existing theoretical models. We therefore study amorphous grain boundaries in graphene, and find stable structures along the boundary, responsible for local density of states enhancements both at zero and finite energies. We also consider the low energy continuum theory of arrays of dislocations forming a grain boundary in graphene. It predicts the appearance of localized zero energy states, pending the atomic scale dislocation core structure. We discuss possible stable dislocation core structures that actually carry such states.

9:12AM P37.00005 Spectromicroscopy measurements of surface morphology and band structure of exfoliated graphene , KEVIN KNOX, ANDREA LOCATELLI, Elettra Synchrotron, Trieste, Italy, DEAN CVETKO, University of Ljubljana, TEVFIK MENTES, MIGUEL NINO, Elettra Synchrotron, Trieste, Italy, SHANCAI WANG, Renmin University of China, MEHMET YILMAZ, Fatih University, Istanbul, Turkey, PHILIP KIM, RICHARD OSGOOD, Columbia University, ALBERTO MORGANTE, TASC National Laboratory, Trieste, Italy — Monolayer-thick crystals, such as graphene, are an area of intense interest in condensed matter research. However, crystal deformations in these 2D systems are known to adversely affect conductivity and increase local chemical reactivity. Additionally, surface roughness in graphene complicates band-mapping and limits resolution in techniques such as angle resolved photoemission spectroscopy (ARPES), the theory of which was developed for atomically flat surfaces. Thus, an understanding of the surface morphology of graphene is essential to making high quality devices and important for interpreting ARPES results. In this talk, we will describe a non-invasive approach to examining the corrugation in exfoliated graphene using a combination of low energy electron microscopy (LEEM) and micro-spot low energy electron diffraction (LEED). We will also describe how such knowledge of surface roughness can be used in the analysis of ARPES data to improve resolution and extract useful information about the band-structure.

9:24AM P37.00006 Snap-through instability of graphene on corrugated substrates , CESAR CHIALVO, SCOTT SCHARFENBERG, NIKHITA MANSUKHANI, RICHARD WEAVER, NADYA MASON, University of Illinois at Urbana Champaign — We discuss atomic force microscopy measurements of the interplay between interfacial bonding energy and strain energy in few-layer-graphene (FLG) placed on micro-scale corrugated metallic substrates. For fixed corrugation amplitude and wavelength, the theoretical strain energy of conformed FLG scales with the third power of its thickness. We present evidence of a so-called "snap-through instability," where the behavior of the FLG abruptly changes, as a function of thickness, from fully conformed, to completely detached. The large FLG thickness, and by implication strain energy, at the snap-through point implies that the FLG-substrate bonding is larger than expected for van der Waals forces.

9:36AM P37.00007 A Quantitative Characterization of Thermally Excited Ripples in Graphene , DONALD PRIOUR, JR, University of Missouri, Kansas City — In the framework of an atomistic model, we calculate the amplitude and typical wavelength of undulations in graphene sheets with length scales similar to those encountered in experiment. As part of a quantitative treatment, bond bending and stiffness constants are fixed by appealing to phonon frequency dispersion curves measured experimentally and from *ab initio* electronic structure calculations. Equilibrium thermodynamic quantities, such as mean square atomic deviations and the average length scale (i.e. the typical "wavelength") of graphene ripples, are calculated in the context of statistical mechanical Monte Carlo simulations. Thermally induced rippling is examined for suspended graphene, as well as graphene in the presence of a substrate, where the attractive coupling of atomic species to the substrate layer is modeled with a Lennard-Jones potential. The contribution of quenched substrate disorder to undulations in the graphene sheet relative to the component of graphene ripples due purely to thermal fluctuations is studied by examining graphene sheets bound to substrates with various levels of intrinsic positional disorder.

9:48AM P37.00008 Wrinkling of graphene membranes supported by silica nanoparticles on substrates[1] , MAHITO YAMAMOTO, WILLIAM CULLEN, MICHAEL FUHRER, THEODORE EINSTEIN, Materials Research Science and Engineering Center and Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, DEPARTMENT OF PHYSICS, UNIVERSITY OF MARYLAND TEAM — The challenging endeavor of modulating the morphology of graphene via a patterned substrate to produce a controlled deformation has great potential importance for strain engineering the electronic properties of graphene. An essential step in this direction is to understand the response of graphene to substrate features of known geometry. Here we employ silica nanoparticles with a diameter of 10-100 nm to uniformly decorate SiO_2 and mica substrates before depositing graphene, to promote nanoscale modulation of graphene geometry. The morphology of graphene on this modified substrate is then characterized by atomic force spectroscopy. We find that graphene on the substrate is locally raised by the supporting nanoparticles, and wrinkling propagates radially from the protrusions to form a ridge network which links the protrusions. We discuss the dependence of the wrinkled morphology on nanoparticle diameter and graphene thickness in terms of graphene elasticity and adhesion energy.

[1]Supported by NSF-MRSEC, Grant DMR 05-20471

10:00AM P37.00009 Magnetoresistance of Metal-Shunted Graphene Devices , PAUL CAMPBELL, ADAM FRIEDMAN, F. KEITH PERKINS, JEREMY ROBINSON, US Naval Research Laboratory — Graphene, a single atomic layer of hexagonally arranged carbon atoms, presents the optimal platform to study magnetoresistance (MR) effects because of its temperature-independent mobility and linear band structure with zero band gap. Extraordinary magnetoresistance (EMR) can be realized in metal-shunted graphene devices. Here, due to the different magnetic-field-dependent resistances of the metallic shunt, graphene, and shunt-graphene interface, current flows easily through the shunt in zero and low magnetic field, while in high magnetic field, more current flows around the shunt and is redistributed in the graphene. Devices made from chemical vapor deposition (CVD) graphene grown on copper and transferred to a SiO_2/Si substrate with Ti/Au shunts display gate-tunable longitudinal MR of $\sim$600% at 12 T and also show promise for use as Hall sensors. Graphene magnetoresistance devices have many possible applications including magnetic field sensors and magnetic read-heads. In contrast with the many proposed electronic uses for graphene, which necessitate the creation of a band-gap, graphene magnetoresistance devices that exploit LMR or EMR provide a use for as-grown or deposited graphene.

10:12AM P37.00010 A Graphene-Based Biosensor , AMAL KASRY, Visiting Scientist at IBM T. J. Watson Research Center, ALI AFZALI, GEORGE TULEVSKI, Research Staff Member, BERNHARD MENGES, Project Leader, SATOSHI OIDA, Postdoc, MATTHEW COPEL, LIBOR VYKLICKY, Research Staff Member, EGYPT NANOTECHNOLOGY CENTER COLLABORATION, IBM RESEARCH COLLABORATION, MAX PLANCK INSTITUTE FOR POLYMER RESEARCH COLLABORATION — Graphene, a single layer of carbon atoms, has attracted significant interest in several applications including biosensors. In this work graphene was grown by the CVD method. Optical parameters of graphene such as refractive index and extinction coefficient were measure by a mix of techniques including ellipsometer, XPS, Raman Spectroscopy, SPR and MEIS. Determining the optical properties of graphene allowed for study of its ability to sense biomolecular interactions. We also examined graphene modification by electrostatic interaction utilizing a molecule synthesized by IBM Research. Successful modification was proven by XPS, Raman Spectroscopy, and SPR. Studies of the chemical modification, along measurement of electrical and optical properties of graphene are components of our work to develop highly sensitive graphene-based sensors.

10:24AM P37.00011 ABSTRACT WITHDRAWN –

10:36AM P37.00012 Graphene-Silicon Schottky Diodes , CHUN CHUNG CHEN, MEHMET AYKOL, CHIA-CHI CHANG, A.F.J. LEVI, STEPHEN B. CRONIN, University of Southern California — By depositing mechanically exfoliated graphene on top of silicon substrates, the graphene-silicon Schottky barriers are observed. The resulting current-voltage characteristics exhibit rectifying diode behavior with a barrier energy of 0.41 eV on n-type silicon and 0.45 eV on p-type silicon at room temperature. The ideality factor is also evaluated for bilayer, three layer, and multiple layer graphene-silicon Schottky diodes at various temperatures. These results indicate that the number of graphene layers and the ambient temperature are major influences for the ideality factor of graphene-silicon Schottky diodes. In this work, photocurrents are observed under 532 nm laser illumination. The transparency of the thin graphene layer allows the underlying silicon substrate to absorb the laser light and generate a photocurrent. The full current-voltage characteristics under illumination are also reported. Spatially resolved photocurrent measurements also reveal the importance of inhomogeneity and series resistance in these devices.

10:48AM P37.00013 Conductance-Based Temperature Programmed Desorption with Single Defect Resolution , DENG PAN, PATRICK C. SIMS, BRAD L. CORSO, PHILIP G. COLLINS, Department of Physics and Astronomy, Univ. of California at Irvine, Irvine, CA 92697-4576 — The controlled functionalization of nanotubes and graphene requires methods of chemically attacking these inert surfaces and of removing unwanted oxidation damage. The appeal of reversible chemistries is rarely achieved: the degraded electrical properties of reduced graphene oxide compared to pristine graphene indicates residual damage that remains poorly understood. Using a high temperature, UHV apparatus to perform electrical measurements in situ, we investigate the thermal desorption of adducts that can restore conductivity in oxidized nanographites. The majority of our measurements are accomplished using SWCNTs, due to their enhanced sensitivity to even single point defects. Discrete conductance jumps accompanying the removal of different types of adducts provide a characterization method that directly distinguishes the relative electronic effects of phenolic, epoxide, and carboxylic defects. The electronic measurements complement more traditional, temperature programmed desorption from bulk material, which is insensitive to electronic disorder.

Wednesday, March 23, 2011 8:00AM - 10:48AM –

Session P38 DCP DBP: Focus Session: Quantum Coherence in Biology III A130/131

8:00AM P38.00001 Barrier compression and tunneling in enzyme catalysed reactions , NIGEL SCRUTTON, University of Manchester — Nuclear quantum mechanical tunneling is important in enzyme-catalysed H-transfer reactions. This viewpoint has arisen after a number of experimental studies have described enzymatic reactions with kinetic isotope effects that are significantly larger than the semi-classical limit. Other experimental evidence for tunneling, and the potential role of promoting vibrations that transiently compress the reaction barrier, is more indirect, being derived from the interpretation of e.g. mutational analyses of enzyme systems and temperature perturbation studies of reaction rates/kinetic isotope effects. Computational simulations have, in some cases, determined exalted kinetic isotope effects and tunneling contributions, and identified putative promoting vibrations. In this presentation, we present the available evidence – both experimental and computational – for environmentally-coupled H-tunneling in several enzyme systems, from our recent work on redox enzyme systems. We then consider the relative importance of tunneling contributions to these reactions. We find that the tunneling contribution to these reactions confers a rate enhancement of approx. 1000-fold. Without tunneling, a 1000-fold reduction in activity would seriously impair cellular metabolism. We infer that tunneling is crucial to host organism viability thereby emphasising the general importance of tunneling in biology.

8:36AM P38.00002 The control of electron transfer pathways in biomolecular systems: the role of fluctuations , SPIROS SKOURTIS, Department of Physics, University of Cyprus — Electron transfer reactions are ubiquitous in biology. They are observed in both protein and DNA systems. Biological electron transfer mechanisms range from tunnelling to thermally activated hopping. Due to the floppiness of biomolecules, molecular motion is an important determinant of the electron transfer rate. The electronic couplings that enable electron transfer in biomolecular systems can be understood in terms of competing and interfering electron transfer pathways that are controlled by structure, dynamics, and initial state preparation. We review recent theoretical progress on the effects of conformational distributions, excited-state polarization, and electron-nuclear dynamics on tunneling electron transfer reactions in different biomolecular systems. We discuss how electron-transfer-rate control can be achieved in the presence of a highly fluctuating environment.

[1] S. S. Skourtis, D. H. Waldeck, and D. N. Beratan. Fluctuations in biological and bioinspired electron-transfer reactions. Ann. Rev. Phys. Chem. Vol. 61 461-485 (2010).
[2] I. A. Balabin, D.N. Beratan, and S. S. Skourtis. The persistence of structure over fluctuations in biological electron transfer reactions. Phys. Rev. Lett. 101, 158102 (2008).

9:12AM P38.00003 A molecular breakwater enhances electron transfer between proteins , NATHAN S. BABCOCK, University of Calgary, AURÉLIEN DE LA LANDE, Universite Paris-Sud, JAN ŘEZÁČ, Academy of Sciences of the Czech Republic, BARRY C. SANDERS, DENNIS R. SALAHUB, University of Calgary — Does natural selection optimize molecular biomachinery at the quantum level? We present statistical characterizations of molecular dynamics at an interprotein electron transfer (ET) interface. In simulations of the wild-type protein complex, we find that the most frequently occurring molecular configurations afford superior electronic coupling due to the consistent presence of a single water molecule hydrogen-bonded between the donor and acceptor sites. We attribute the persistence of this water bridge to a "molecular breakwater" composed of several hydrophobic residues surrounding the acceptor site. The breakwater supports the function of solvent-organizing residues by limiting the exchange of water molecules between the sterically constrained ET region and the surrounding bulk. When the breakwater is affected by a mutation, bulk solvent molecules disrupt the water bridge, resulting in reduced electronic coupling. These results suggest that protein surface residues may stabilize interprotein solvent dynamics to enable coherent ET along a single molecular pathway.

9:24AM P38.00004 Mixed quantum classical simulations of vibrational energy transport in alpha-helices[1] , ANNE GOJ, ERIC BITTNER, University of Houston — We use mixed classical/quantum simulations to study the time dependence of an excitation of a C=O vibration on a 3-10 helix of α-Aminoisobutyric acid (AIB), a system which represents a test case for the formation of self-trapped vibrational excitation states on protein helices. Due to the inherent disorder in the system caused by the finite temperature and fluctuations in hydrogen bonding, the excitation tunnels randomly among C=O sites along the helix. Quantum forces are insufficient to establish a coherent relationship between the location of the excitation and the contraction of hydrogen bonds around this site. Our simulations indicate that the excitation frequently becomes localized on the end of the helix due to the defect in helical structure caused by unwinding. Our results generally do not support the existance of Davydov type solitons in biological helix systems under physiological conditions.

[1]This work was funded by the National Science Foundation (CHE-1011894) and the Robert Welch Foundation (E-1334) .

9:36AM P38.00005 Quantum processes as a mechanism in olfaction for smell recognition?[1] , JENNIFER BROOKES, Massachussetts Institute of Technology — The physics of smell is not well understood. The biological processes that occur following a signalling event are well understood (Buck 1991). However, the reasons how and why a signalling event occurs when a particular smell molecule and receptor combination is made, remains un-established. Luca Turin proposes a signalling mechanism which determines smell molecules by quantum mechanics (Turin 1996). Investigation of this mechanism shows it to be physically robust (Brookes,et al, 2007), and consequences of the theory provides quantitative measurements of smell and interesting potential experiments that may determine whether the recognition of smell is a quantum event. Brookes, J.C, Hartoutsiou, F, Horsfield, A.P and Stoneham, A.M. (2007). Physical Review Letters 98, no. 3 038101 Buck, L. (1991) Cell, 65, no.1 (4): 175-187. Turin, L. (1996) Chemical Sences 21, no 6. 773-791

[1]With many thanks to the Wellcome Trust

10:12AM P38.00006 Recent developments in the physics of your sense of smell[1] , ANDREW HORSFIELD, Imperial College London, LUCA TURIN, MIT, YEONG-AH SOH, Imperial College London, MARION SOURRIBES, MARSHALL STONEHAM, LIANHENG TONG, PAUL WARBURTON, UCL — A radical proposal in 1996 [L. Turin, Chem. Senses 21, 773 (1996)] was that human olfactory receptors use phonon assisted electron tunnelling to probe the vibrational spectrum of odorants in order to determine their chemical identity. A development of this model [J. C. Brookes et al., Phys. Rev. Lett., 98, 038101 (2007)] showed that this Turin mechanism is indeed physically possible, even robust, but left a number of questions open. One such question is: between which sites does the tunnelling electron pass? Our recent calculations support a particular pair of likely sites. Because of the complexity of biological environments, probing the receptor is difficult. Thus we have begun to investigate the properties of a semiconductor nanowire device that mimics the key processes [A. P. Horsfield et al., J. Appl. Phys., 108, 014511 (2010)]. We will present the latest findings of this study.

[1]This work is supported by DARPA (Grant N66001-10-1-4062), EPSRC (Grant No. EP/H005544/1) and AFOSR (Grant No. FA8655-08-1-3082).

10:24AM P38.00007 A Quantum of Solace: molecular electronics of benzodiazepines[1] , LUCA TURIN, MIT, ANDREW HORSFIELD, Imperial College London, MARSHALL STONEHAM, University College London — Benzodiazepines and related drugs modulate the activity of GABA-A receptors, the main inhibitory receptor of the central nervous system. The prevailing view is that these drugs bind at the interface between two receptor subunits and allosterically modulate the response to GABA. In this talk I shall present evidence that benzodiazepines work instead by facilitating electron transport from the cytoplasm to a crucial redox-sensitive group in the gamma subunit. If this idea is correct, benzodiazepines should not only be regarded as keys fitting into a lock, but also as one-electron chemical field-effect transistors fitting into an electronic circuit.

[1]Supported by DARPA Grant N66001-10-1-4062.

10:36AM P38.00008 Theoretical investigation of coherent exciton flow dynamics in light harvesting complex 2 (LH2)[1] , SEOGJOO JANG, Queens College, City University of New York — The light harvesting complex 2 (LH2) is a peripheral antenna complex found in photosynthetic unit of purple bacteria. Numerous spectroscopic and computational studies demonstrated that quantum coherence plays an important role in the energetics and the dynamics of excitons created in LH2, but detailed and quantitative understanding is still missing regarding how the quantum coherence influences spectroscopic observables and how it boosts efficient energy transfer despite disorder and soft nature of the system. The present talk reports recent progress in the analysis of the single molecule spectroscopy (SMS) and application of resonance energy transfer theories, which account for multichromophoric and quantum coherence effects. These suggest that spectroscopic modeling allows development of reliable coarse-grained model for LH2 that can capture the major features of the excitons and that LH2 is a highly optimized natural system where the interplay between quantum coherence and disorder/fluctuation is maximally utilized.

[1]This research was supported by the Department of Energy, Office of Basic Energy Sciences and the National Science Foundation.

Wednesday, March 23, 2011 8:00AM - 10:24AM –

Session P39 DBP: Physics of Proteins IV: Folding, Dynamics and Function A124/127

8:00AM P39.00001 Competition between chemical denaturation and macromolecular crowding effects on the folding dynamics of proteins[1] , ANTONIOS SAMIOTAKIS, MARGARET CHEUNG, University of Houston — It is well known that proteins fold and function in the crowded environment of the cell's interior. In the recent years it has been established that the so-called "macromolecular crowding" effect can enhance the folding stability of proteins by destabilizing their unfolded states. On the other hand, chemical and thermal denaturation are often used in experiments as tools to destabilize protein structures when probing a protein's folding landscape. However, little is known about the combined effects of these competing phenomena on proteins. In this work, we use coarse-grained molecular simulations to study the thermodynamic and kinetic properties of the small peptide Trp-cage, in the combined presence of macromolecular crowders and chemical denaturant. With the use of an energy function derived by all-atomistic simulations in the presence of urea, we investigate the thermodynamics and kinetics of Trp-cage's folding mechanism at several concentrations of urea. The effects of the competition between stabilization by macromolecular crowding and destabilization by chemical denaturation will also be discussed.

[1]This work was supported by the National Science Foundation, Molecular & Cellular Biosciences (MCB0919974).

8:12AM P39.00002 Can understanding the packing of side chains improve the design of protein-protein interactions?[1] , ALICE ZHOU, COREY O'HERN, LYNNE REGAN, Yale University — With the long-term goal to improve the design of protein-protein interactions, we have begun extensive computational studies to understand how side-chains of key residues of binding partners geometrically fit together at protein-peptide interfaces, e.g. the tetratrico-peptide repeat protein and its cognate peptide). We describe simple atomic-scale models of hydrophobic dipeptides, which include hard-core repulsion, bond length and angle constraints, and Van der Waals attraction. By completely enumerating all minimal energy structures in these systems, we are able to reproduce important features of the probability distributions of side chain dihedral angles of hydrophic residues in the protein data bank. These results are the crucial first step in developing computational models that can predict the side chain conformations of residues at protein-peptide interfaces.

[1]CSO acknowledges support from NSF grant no. CMMT-1006527.

8:24AM P39.00003 Insight into the mechanics of the selectivity filter of *Escherichia coli* aquaporin Z[1] , GUODONG HU, L.Y. CHEN, University of Texas at San Antonio — Aquaporin Z (AQPZ) is a tetrameric protein that forms water channels in Escherichia coli's cell membrane. The histinine residue in the selectivity filter (SF) region plays an important role in the transport of water across the membrane. In this work, we perform equilibrium molecular dynamics (MD) simulation to illustrate influences of two different protonation states and the gate mechanics of the SF. We calculate the pore radii in the SF region versus the simulation time. We perform steered MD to compute the free energy profile, i.e., the potential of the mean force (PMF) a water molecule through the SF region. We calculate the binding energy of one water molecule with the SF region residues, using Gaussian. The hydrogen bonds formed between the side chains of Hsd 174 and side chains of Arg189 play important roles in the selectivity filter mechanics of AQPZ. The radii of the pores, hydrogen bond analysis, and free energies show that Hsd is favored than Hse.

[1]The authors acknowledge support from a NIH grant (Grant No. SC3 GM084834), the UTSA Computational Biology Initiative, and the Texas Advanced Computing Center.

8:36AM P39.00004 The Effect of Phosphate Buffered Saline (1x PBS) on Induced Thermal Unfolding and Low Frequency Dielectric Spectra of Lysozyme[1] , KLAIDA KASHURI, HEKTOR KASHURI, GERMANO IANNACCHIONE — It is well known that the folding / unfolding of proteins is related directly to their structure and functionality. Calorimetry (both AC and MDSC) studies as well as low-frequency (1Hz to 100 kHz) dielectric measurements have been performed on hen egg white lysozyme dissolved in PBS (pH 7.4) from 20 to 100 °C. From the heat capacity profile, the temperatures and related an enthalpy change of the protein denaturing is probed. The heat capacity peak broadens and new features are reveled as the temperature scan rate is lowered to +0.017 K/min for the AC calorimetric method. Significant differences are observed using the (M)DSC technique at scan rates of from 1 to 5 K/min. The temperature dependence of the permittivity, ϵ', and the loss factor, ϵ'', at 100 kHz of the diluted protein show features associated with those seen in the heat capacity (AC and MDSC). All results are interpreted in terms of protein denaturing then subsequent gelation that depend on protein sample concentration, which is supported by the frequency dependence of the permittivity at room temperature after thermally cycling

[1]Worcester Polytechnic Institute (WPI)

8:48AM P39.00005 The effect of macromolecular crowding, ionic strength and calcium binding on calmodulin dynamics[1] , QIAN WANG, KAO-CHEN LIANG, University of Houston, NEAL WAXHAM, University of Texas Health Science Center-Houston, MARGARET CHEUNG, University of Houston — The flexibility in the structure of calmodulin (CaM) allows its binding to over 300 target proteins in the cell. To investigate the structure-function relationship of CaM in response to the changing intracellular environment, we use a combined method of computer simulation and experiments based on circular dichroism (CD). The conformation, helicity and EF hand orientation of CaM are analyzed computationally to address the effect of macromolecular crowding, ionic strength and calcium binding in the experiments. We applied a unique solution of charges computed from QM/MM to accurately represent the charge distribution in the transition from apo-CaM to holo-CaM. Computationally, we found that a high level of macromolecular crowding, in addition to calcium binding and ionic strength, can impact the conformation, helicity and the EF hand orientation of CaM. Our result may provide unique insight into understanding the promiscuous behavior of calmodulin in target selection inside cells.

[1]This work is supported by National Science Foundation, Molecular & Cellular Biosciences (MCB0919974).

9:00AM P39.00006 α-Helical to β-Helical Conformation Change in the C-Terminal of the Mammalian Prion Protein , JESSE SINGH, UC Davis, PAUL WHITFORD, Los Alamos National Laboratory, NATHA HAYRE, DANIEL COX, UC Davis Physics, JOSÉ ONUCHIC, Center for Theoretical Biological Physics, UCSD — We employ all-atom structure-based models with mixed basis contact maps to explore whether there are any significant geometric or energetic constraints limiting conjectured conformational transitions between the alpha-helical (αH) and the left handed beta helical (LHBH) conformations for the C-terminal (residues 166-226) of the mammalian prion protein. The LHBH structure has been proposed to describe infectious oligomers and one class of in vitro grown fibrils, as well as possibly self- templating the conversion of normal cellular prion protein to the infectious form. Our results confirm that the kinetics of the conformation change are not strongely limited by large scale geometry modification and there exists an overall preference for the LHBH conformation.

9:12AM P39.00007 Dynamics of Protein Carbonmonoxyhemoglobin on Multiple Length Scales , JYOTSANA LAL, ROBERT FISCHETTI, LEE MAKOWSKI, Argonne National Laboratory, Argonne IL-60439, USA., PETER FOUQUET, MARCO MACCARINI, Institut Laue-Langevin, 38042 Grenoble- Cedex 9, France, NANCY HO, CHIEN HO, Carnegie Mellon Univ., Pittsburgh, PA-15213, USA. — A combination of wide-angle x-ray solution scattering (WAXS) and neutron spin echo spectroscopy (NSE) was used to probe the structure and dynamics of carbonmonoxy hemoglobin (HbCO) in the presence and absence of the allosteric effector inositol hexaphosphate (IHP). IHP shifts the structure of HbCO slightly towards an unliganded, (deoxy)-state conformation. Two potential binding sites for IHP are consistent with the WAXS data, one near each end of the central channel. IHP binding slows the self-correlation times of some protons, most likely those immediately adjacent to the bound IHP, and simultaneously induces an increase in the relaxation rate of correlated motions with length scales comparable to the $\alpha\beta$-dimer. IHP binding increases the spatial extent of these fluctuations by about 20%. This suggests that when hemoglobin binds CO, its conformation is confined to a relatively narrow structural ensemble residing within a functionally well defined energy well. On the other hand, when it binds both CO and IHP, in response to the contradictory stresses applied by these two ligands, it adopts an incommensurate structure with a conformation exploring a broad structural ensemble.

9:24AM P39.00008 Infrared Spectroscopy Measurements of Protein Dynamics and Mechanism , CURTIS W. MEUSE, JOSEPH B. HUBBARD, National Institute of Standards and Technology — Infrared spectroscopy has long been used to deduce the concentration and secondary structures of proteins in a variety of static and time resolved applications. Our focus is on developing new infrared methods to compare the structure, dynamics and function of nearly identical protein samples, in different environments, to apply to the problem of identifying bio-similar protein therapeutics. We have developed an order parameter describing protein conformation variations around the average molecular values. By comparing our order parameter and amide hydrogen/deuterium exchange methods, we explore the relationship between protein stability and the dynamics of the protein conformational distribution. Examples include lysozyme and albumin in solution, cytochrome c interacting with lipid membranes of varying net-negative surface charge density, fibrinogen on different polymer surfaces and bacteriorhodopsin during its photocycle.

9:36AM P39.00009 Comparing potential copper chelation mechanisms in Parkinson's disease protein , FRISCO ROSE, MIROSLAV HODAK, JERRY BERNHOLC, CHiPS/NCSU — We have implemented the nudged elastic band (NEB) as a guided dynamics framework for our real-space multigrid method of DFT-based quantum simulations. This highly parallel approach resolves a minimum energy pathway (MEP) on the energy hypersurface by relaxing intermediates in a chain-of-states. As an initial application we present an investigation of chelating agents acting on copper ion bound to α-synuclein, whose misfolding is implicated in Parkinson's disease (PD). Copper ions are known to act as highly effective misfolding agents in a-synuclein and are thus an important target in understanding PD. Furthermore, chelation therapy has shown promise in the treatment of Alzheimer's and other neuro-degenerative diseases with similar metal-correlated pathologies. At present, our candidate chelating agents include nicotine, curcumin and clioquinol. We examine their MEP activation barriers in the context of a PD onset mechanism to assess the viability of various chelators for PD remediation.

9:48AM P39.00010 Investigating hexameric helicases: Single-molecule studies of DnaB and T4 gp41 , OMAR SALEH, NOAH RIBECK, JOHN BEREZNEY, University of California Santa Barbara — Hexameric, ring-shaped motor proteins serve as replicative helicases in many systems. They function by encircling and translocating along ssDNA, denaturing dsDNA in advance of its motion by sterically occluding the complementary strand to the outside of the ring. We investigate the helicase activity of two such motors using single-molecule measurements with magnetic tweezers. First, we measure the activity of the *E. coli* helicase DnaB complexed with the tau subunit of the Pol III holoenzyme. Tau is known from bulk measurements to stimulate DnaB activity (Kim et al., *Cell*, 1996); we investigate the means of this stimulation. Second, we measure helicase activity of the T4 phage helicase gp41 in multiple tethered DNA geometries. Previous work on DnaB showed a dependence of helicase activity on DNA geometry (Ribeck et al., *Biophys. J.*, 2010); here, we test gp41 for similar behavior to see whether it is a common characteristic of hexameric helicases.

10:00AM P39.00011 Copper attachment to prion protein at a non-octarepeat site , MIROSLAV HODAK, North Carolina State University, JERRY BERNHOLC — Prion protein (PrP) plays a causative role in a group of neurodegenerative diseases, which include "mad cow disease" or its human form variant Creutzfeld-Jacob disease. Normal function of PrP remains unknown, but it is now well established that PrP can efficiently bind copper ions and this ability has been linked to its function. The primary binding sites are located in the so-called octarepeat region located between residues 60-91. While these are by now well characterized, the sites located outside these region remain mostly undetermined. In this work, we investigate the properties of Cu binding site located at His 111 using recently developed hybrid Kohn-Sham/orbital-free density functional simulations. Experimental data indicate that copper is coordinated by either four nitrogens or three nitrogens and one oxygen. We investigate both possibilities, comparing their energetics and attachment geometries. Similarities and differences with other binding sites and implications for PrP function will also be discussed.

10:12AM P39.00012 Pressure and Temperature Effects on Polypeptides and Biomolecules Probed by Micro-Raman Spectroscopy , SANGHOON PARK, ALFONS SCHULTE, Department of Physics and College of Optics, University of Central Florida — We investigate pressure and temperature effects on the secondary structure of Poly-L-glutamic acid (PGA) in D_2O buffer (pH 5.4) solution. Our setup employs a Raman microscope equipped with a micro-capillary high-pressure cell and a variable temperature stage. Raman spectra are acquired over the pressure range from 0.1 to 300 MPa while the temperature can be varied from 270 K to 330 K. The amide I band of PGA is sensitive to pressure and temperature, and by spectral deconvolution we determine the relative contributions due to α-helix and random coil conformations. The amount of α-helix increases with increasing pressure. Extensions of these experiments to model proteins and lipids are presented.

Wednesday, March 23, 2011 8:00AM - 11:00AM –
Session P40 DPOLY: Polymer Melts & Solutions A122/123

8:00AM P40.00001 Radical-cured block copolymer modified thermosets[1] , ERICA REDLINE, LORRAINE FRANCIS, FRANK BATES, Department of Chemical Engineering and Materials Science, University of Minnesota — Poly(ethylene-*alt*-propylene)-*b*-poly(ethylene oxide) (PEP-PEO) diblock copolymers were synthesized and added at 4 wt. % to bisphenol A glycidyl methacrylate (BisGMA). The mixture was thermally cured using free radical chemistry. In separate experiments, 4 wt. % PEP-PEO was added to a combination of poly(ethylene glycol) dimethacrylate (PEGDMA) and BisGMA and cured. Based on small angle X-ray studies of the modified monomers before curing, diblock copolymers self-assembled into well-dispersed spherical micelles with PEP cores and PEO coronas. TEM results showed that these micellar structures were retained during curing. Fracture resistance measurements indicate that the addition of block copolymers does not significantly toughen these thermoset materials. This finding is contrary to the large increase in fracture resistance observed in block copolymer-modified epoxies. We propose that differences in network structure, originating during polymerization, are responsible.

[1]This work was supported primarily by the MRSEC Program of the National Science Foundation under Award Number DMR-0212302 and DMR-0819885.

8:12AM P40.00002 Cavitation in Filled Styrene-butadiene Rubber: A Real Time SAXS Observation , HUAN ZHANG, ESPCI ParisTech, Paris, France, ARTHUR K. SCHOLZ, MRL-UC Santa Barbara, CA, FABIEN VION-LOISEL, Michelin, Clermont-Ferrand, France, EDWARD J. KRAMER, MRL-UC Santa Barbara, CA, COSTANTINO CRETON, ESPCI ParisTech, Paris, France — Cavitation of filled and unfilled elastomers under confinement at the macroscopic scale has been experimentally reported and theoretically modeled. However, cavitation occurring at the nanometer length scale has not yet been demonstrated conclusively in rubbers. Real time SAXS with synchrotron radiation was employed to probe the structure changes in carbon black filled styrene-butadiene rubber (SBR) under uniaxial loading. The scattering invariant was calculated and increased sharply at a critical extension depending on both filler content and crosslinking density around q = 0.1 nm-1, which we attributed to the formation of voids. At very large strains, a sharp and wide streak developed perpendicular to the tensile axis in reciprocal space, suggesting the deformation of the voids in elliptical voids along the tensile direction. In step cycle test, we observed that voids only appeared when the current strain exceeded the maximum historical strain (Mullins effect) and attributed the increase of the scattering invariant outside the Mullins region to the creation of new voids rather than to the reopening of old ones.

8:24AM P40.00003 Why is the tube model inapplicable for entangled polymer dynamics at large deformation , SHI-QING WANG, YANGYANG WANG, University of Akron — Accumulating experimental revelation of the phenomenology governing dynamics of entangled linear polymers at large deformations has caused us to question the legitimacy of the tube model as an acceptable theoretical description of nonlinear polymer rheology. Upon an explicit investigation of its premise, we have come to realize that the tube model did not overcome the difficulty confronted by other theories and did not contain the basic physics required to explain why and how the entanglement network must break down during large deformations. It considered an unrealistic situation where a load-bearing chain relaxed fast in an affinely deformed tube so that only the chain segment orientation produced the shear stress for applied rates lower than the Rouse rate. A non-monotonic relation between the resulting shear stress and imposed strain for startup shear and step deformations arose from excessive chain orientation not collapse of the entanglement network. In the tube model, the nature of the overshoot is not yielding (transition from elastic deformation to flow), but an elastic instability. Accumulating experimental observations contradict this picture. This presentation will elucidate how the emerging physical picture differs from that of the unrealistic tube model.

8:36AM P40.00004 Non-Gaussian Stretching Behavior of Entangled Polymers , YANGYANG WANG, SHI-QING WANG, The University of Akron — The behavior of entangled SBR melts and solutions in rapid uniaxial extension has been studied by rheometric and rheo-optical measurements. A yield-to-rupture transition occurs around the same Rouse Weissenberg number of nine for all samples when the failure mechanism changes from chain disentanglement (yielding) to chain scission. Our results show that elastic rupture takes place only when chains between entanglements are near full extension, the strain at rupture grows with increasing entanglement spacing, and the critical stress for rupture is proportional to the polymer concentration. These characteristics validate the well-known idea to represent entangled polymers in terms of a transient network.

8:48AM P40.00005 Parameters of slip-springs model of polymer entanglement from the maximum likelihood principle , TIMOTHY PALMER, ALEXEI LIKHTMAN, University of Reading, JORGE RAMIREZ, Technical University of Madrid, MARK MATSEN, University of Reading — The slip-spring model for polymer entanglements proposed by A.E.Likhtman [Macromolecules; 2005; 38(14); 6128] replaces entangling chains with slip-links, which are anchored via springs. The use of such models allows reduction of complex multi-chain problem to a simpler single chain problem. In this work we test the slip-spring model on the simplest possible situation: replacing two entangled chains by one chain with one slip-link. We demonstrate how Maximum Likelihood Estimation (MLE) can be used to generate parameters for the slip-spring model by observing a multi-chain system. The test system being considered consists of two Rouse polymer chains that are anchored by the ends in an entangled state. The effect of the entanglement is enforced by rejecting all steps that lead to topology violation. We show how the results of this MLE indicate that slip-link models with slip-links fixed in space are not satisfactory, and demonstrate analytically the dependence of the plateau modulus upon the strength of the slip-spring. Our results contradict recent calculations of Schieber and Horio [JCP; 2010; 132(7); 074905] who claimed that the plateau modulus must be independent of the slip-spring strength.

9:00AM P40.00006 Segmental orientation dynamics in bidisperse entangled linear polymer melts , ZUOWEI WANG, JING CAO, ALEXEI LIKHTMAN, Department of Mathematics and Statistics, University of Reading, Whiteknights, RG6 6AX, UK, RONALD LARSON, Department of Chemical Engineering, University of Michigan, Ann Arbor, MI 48109-2136 — Extensive molecular dynamics simulations were performed to investigate the segmental orientation dynamics in mono- and bidisperse entangled linear polymer melts. The binary blends consist of short probe chains diluted in long chain matrices of chain length up to 30 entanglements. With increase of the chain length in monodisperse melts, the bond vector autocorrelation function was found to approach a distinctive time-dependent power law, which is compared with recent NMR experiments. When introduced into long chain matrices, the segmental orientation relaxation and monomer diffusion of short probe chains slowed down strongly due to the suppression of constraint release (CR) effects. The same trend was observed for the end-to-end vector correlation function, reflecting the CR effects on contour length fluctuations. On the other hand, the time-dependent orientation coupling parameter in the entangled systems demonstrates the similar universal behaviour as that discovered in unentangled melts. Considering the stress-optical law was recovered in all simulated systems, our simulations should clarify the connection between rheology and other experimental techniques, which are essential for progress in modeling entangled polymers.

9:12AM P40.00007 Simulations of polymer melts modeled as chains of interacting soft-colloids , ANTHONY CLARK, MARINA GUENZA, University of Oregon — The range of time and length scales accessible to dynamical simulations of melts of long polymer chains is strongly limited by the computational demands of calculating large numbers of forces between monomers. Simulations modeling each polymer as a point particle interacting by an analytical soft pair potential have previously been successfully developed to extend this range. For many effects in polymer systems, however, submolecular degrees of freedom remain relevent to molecular-level behavior even at long times and large length scales. To allow for the inclusion of relevant submolecular degrees of freedom, we use analytical effective potentials based on our model of the structure of polymer melts on the level of large chain sub-blocks to simulate homopolymer melts. We demonstrate that structure on the block and center of mass level consistent with the structural model and monomer-level simulation data can be reproduced for large systems and long times at much lower computational cost than monomer-level simulations. Using this model, we also test the effects of additional short-range repulsive interactions between chain subunits on structure and dynamics.

9:24AM P40.00008 Renormalized dynamics of overdamped driven elastic media , JONATHAN LANDY, UCLA Dept. of Physics and Astronomy, ALEX J. LEVINE, UCLA Dept. of Chemistry & Biochemistry and California Nanosystems Institute — We present the results of a dynamical renormalization group calculation used to explore the fluctuations of an elastic body steadily driven through a viscous background fluid. Direct applications of this work involve the study of the fluctuation spectrum of semiflexible filament networks driven through a background fluid by e.g. polymerization, but also include the motion of one-dimensional driven elastic objects (e.g. polymers, flux vortices etc.) In that case, a previous linear stability analysis suggests that, when such elastic lines are driven in a direction perpendicular to their axis, they become unstable at any non-zero driving force [1]. We discuss the affect of nonlinearities on these conclusions, showing that such terms can stabilize the system at finite drive velocities. We similarly explore the dynamics of lines driven parallel their axis showing that these systems exhibit "weak dynamic scaling" [2]. Turning to the case of driven elastic solids, we report on the effect of molecular motor-induced forces on the long length scale and long time scale dynamics of the driven system. [1] R. Lahiri and S. Ramaswamy, Are steadily moving crystals unstable?, Phys. Rev. Lett. 79, 1150 (1997) [2] D. Das et al., Weak and strong dynamic scaling in a one-dimensional driven coupled-field model: Effects of kinematic waves, PRE 64, 021402 (2001).

9:36AM P40.00009 Thermodyanmic Scaling of Polymer Dynamics versus Shifting by T-Tg , JIAXI GUO, SINDEE SIMON, Texas Tech University — A universal scaling law for the relaxation time (τ) of amorphous liquids as a function of temperature and volume has been proposed by Roland and coworkers: τ(T,V) = F(TV$^{\gamma}$), where γ is a material-dependent constant. We test this law for four materials, linear polystyrene, star polystyrene, and two polycyanurate networks using PVT data obtained in our laboratory coupled with the temperature dependent shift factors used to reduce the viscoelastic bulk modulus at different pressures and the dynamic shear properties at ambient pressure. In all cases, τ can be reduced both by the scaling law and by shifting to account for the changes in T_g with pressure, i.e., by plotting versus T - T_g(P). In the polycyanurate case, time-crosslink density superposition holds and τ for the two materials can be reduced simply by shifting the temperature with respect to T_g to account for the changes in $T_g$with crosslink density; however, the thermodynamic scaling for the two materials does not superpose unless the thermodynamic function is normalized by $T_g V_g^{\gamma}$. The validity of the scaling function and its relationship to T - T_g will be further examined. In addition, the impact of errors in T, T_g, and V on the ability to satisfactorily reduce data and obtain universal scaling will be discussed.

9:48AM P40.00010 The linear rheological responses of dense branched brush polymers with different side chain lengths and structures , MIAO HU, GREGORY MCKENNA, Department of Chemical Engineering, Texas Tech University, YAN XIA, CHRIS DAEFFLER, ANDREW BOYDSTON, ROBERT GRUBBS, JULIA KORNFIELD, Division of Chemistry and Chemical Engineering, California Institute of Technology — We examined the linear rheological responses of three kinds of dense and regular branched brush polymers. Brush polymers with different degree of polymerization were synthesized from the ω-Norbornenyl macromolecule (as main chain) with linear, three combined short arms, and dendronized brush structures. The master curves for these brush polymers were obtained by time temperature superposition (TTS) of the dynamic moduli from the glassy plateau region to the terminal flow region. The glassy modulus and rubbery modulus for these brush polymers were greatly influenced by the side chain properties. Two different relaxation processes can be observed for those samples with the higher molecular weight, slightly entangled, side chains. The dilution effect of the side chain which is related to the side chain volume fraction doesn't follows theoretical expectations.

10:00AM P40.00011 Analytical rheology of metallocene-catalyzed polyethylenes[1] , SACHIN SHANBHAG, ARSIA TAKEH, Florida State University — A computational algorithm that seeks to invert the linear viscoelastic spectrum of single-site metallocene-catalyzed polyethylenes is presented. The algorithm uses a general linear rheological model of branched polymers as its underlying engine, and is based on a Bayesian formulation that transforms the inverse problem into a sampling problem. Given experimental rheological data on unknown single-site metallocene- catalyzed polyethylenes, it is able to quantitatively describe the range of values of weight-averaged molecular molecular weight, M_W, and average branching density, b_m, consistent with the data. The algorithm uses a Markov-chain Monte Carlo method to simulate the sampling problem. If, and when information about the molecular weight is available through supplementary experiments, such as chromatography or light scattering, it can easily be incorporated into the algorithm, as demonstrated.

[1]Financial support from NSF DMR 0953002

10:12AM P40.00012 Pressure-Volume-Temperature Behavior of Hyperbranched Polyols: Experiment and Modelling , MUKUL KAUSHIK, SERGEI NAZARENKO, BRIAN OLSON, School of Polymers and High Performance Materials The University of Southern Mississippi, Hattiesburg, MS 39406 — The pressure volume temperature behavior of two generations of hyperbranched polyesters Boltorn^{TM} H40 and H20 was studied by PVT measurements using high pressure dilatometer. Volumetric expansivity, and free volume parameters were determined for both generations in the melt state. The PVT data were fitted to Simha-Somcynsky (SS) equation of state (EOS) and Sanchez–Lacombe (SL) equation of state (EOS) to calculate occupied volume and fractional free volume. The values of occupied volume and fractional free volumes obtained through both the equations of states were similar. Simulated atmospheric pressure V-T data were generated by using Discover module of Accelrys®. Quality of equilibrium was confirmed by energy stabilization and closeness of experimental and simulation densities. WAXD and temperature-volume curves obtained by molecular dynamics simulations were comparable to the experimental data. Well relaxed amorphous cell was further utilized to study hydrogen bond network and determination of O-O pair correlation function of terminal hydroxyl groups.

10:24AM P40.00013 Influence of the Hofmeister Series on Lower Critical Solution Temperature (LCST) Polymers , RYAN TOOMEY, LEENA PATRA, University of South Florida — Lower critical solution temperature (LCST) polymers can serve as model systems for probing the effect of ions on the stability of biological macromolecules. In this talk, we show how permutations in the chemical structure of poly(N-isopropylacrylamide), including n-propylacrylamide, cyclopropylacrylamide, and N-vinylisobutyramide influence the action of ions in the Hofmeister series. By using a combination of ellipsometry and FTIR, we show that ions salt out neutral polymers by enhancing the surface tension of the hydrophobic portions of the polymer. Weakly hydrated ions (known as chaotropes) can also lead to salting-in effects through interactions with amide dipoles. This salting-in effect is strongly modulated by the surrounding hydrophobic groups. The larger the hydrophobic group the weaker the salting-in effect, indicating that the specificity of the Hofmeister series results from a combination of ion-dipole interactions and hydrophobicity.

10:36AM P40.00014 Ionic Liquids for the Imaging of Wet Polymer Morphology[1] , DAVID HOAGLAND, JOHN HARNER, MALVIKA BIHARI, Univ. of Massachusetts Amherst — Unlike convention aqueous and organic solvents, ionic liquids are essentially nonvolatile and thus compatible with the high vacuum environments of electron microscopy. Here is described the room temperature imaging of wet polymer systems such as patterned gels, gel networks, polymeric vesicles, and proteins. Both TEM and SEM images will be offered, along with a discussion of difficulties in applying the two techniques. Via SEM, imprinted surface structures as small as 100-300 nm can be captured for chemically crosslinked gels (polyHEMA), and via TEM, the structure of a physical gel (PEG) is viewed at the 50-to-10-nm scale, revealing network connectivity established by PEG crystallinity. Self-assembled vesicle and micelle structures will be presented for dispersed block copolymers, and the same approach will be applied toward discerning the quality of dispersion for proteins (ferritin) and other nanoparticles.

[1]Funding: UMass MRSEC

10:48AM P40.00015 Biaxial Strain Testing of Extremely Soft Gels , KENJI URAYAMA, YOHSUKE BITOH, TOSHIKAZU TAKIGAWA, Dept. Mater. Chem., Kyoto Univ. — We present a biaxial tensile tester to characterize the nonlinear stress–strain behavior of extremely soft polymer gels with very low shear moduli, of the order of 100 Pa, under general (equal and unequal) biaxial strain. Stretching of gel sheet specimens in a solvent bath can avoid finite self-weight bending deformations that have precluded biaxial tensile experiments with such extremely soft gels. General biaxial strain covers a wide range of physically accessible deformations in contrast to conventional uniaxial strain that is only a special one among them. The biaxial data for fully swollen chemical gels reveal that the exceptional agreement of uniaxial data with predictions of the simplest rubber elasticity model (ideal gas model), which has been known for over 60 years, is superficial because the model evidently fails to describe the biaxial data. This new biaxial tester will be a powerful tool for the full characterization of the large deformation behavior of extremely soft materials, including biological soft tissues.

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P41 DCP: Focus Session: Fundamental Issues in Interfacial Charge Transport for Energy Applications I A115/117

8:00AM P41.00001 Excitons at Interfaces , XIAOYANG ZHU, University of Texas at Austin — Solar photovoltaics based on molecular and nano materials commonly involve excitons. This results from strong Coulomb attraction between an electron and a hole due to the low dielectric constants of molecules or quantum confinement of nano materials. In this lecture, I will address the question of how excitons dissociate at donor/acceptor interfaces. The first example deals with charge separation in organic photovoltaics. Due to the low dielectric constant of organic materials, an electron-hole pair across an organic donor/acceptor interface is bound by the Coulomb potential. This gives rise to a set of H-atom like states called charge-transfer excitons, as observed experimentally. The lowest energy charge transfer exciton state has a binding energy much higher than kT at room temperature. This leads to the conclusion that hot charge transfer exciton states must be involved in charge separation in organic photovoltaics. The second example deals with hot exciton dissociation due to electron transfer from photo-excited semiconductor nanocrystals (PbSe) to an electron acceptor (TiO2), an issue of particular interest to hot carrier solar cells with theoretical solar conversion efficiency surpassing the Shockley-Queisser limit. We show that, with appropriate chemical treatment of the nanocrystal surface, ultrafast transfer of a hot electron can be competitive with hot exciton relaxation due to phonon scattering. The last example will show recent development on hot carrier scattering and multiple exciton generation (MEG) in semiconductor nanorystals.

8:36AM P41.00002 The Effect of Photoexcitation and Population Relaxation on Carrier Multiplication Efficiency in Semiconductor Nanocrystals and Bulk , ANDREI PIRYATINSKI, KIRILL VELIZHANIN, Los Alamos National Laboratory — The carrier multiplication (CM) is the process of production of two or more electron-hole pairs (excitons) per single absorbed photon. Detailed understanding of the mechanisms of this process is of importance for developing novel cheap and efficient photovoltaic devices. To model the CM dynamics, we have developed an exciton scattering model which accurately treats the contributions of different multi-exciton generation pathways on the same footing. Furthermore, the model allows one to study CM in nanocrystalline and bulk semiconductor materials. Using this model, we performed a numerical study of photogeneration and population relaxation processes contributing to CM in PbSe nanocrystals and bulk. It is found that the photogeneration provides small contribution to the total quantum efficiency compared to the population relaxation process. The resonant incoherent biexciton production is found to be main mechanism of CM in both cases of direct biexciton photogeneration and during the population relaxation. Comparison to the published experimental data shows that the calculations reproduce experimentally observed trends providing insight into the mechanisms of CM.

8:48AM P41.00003 Non-radiative Energy Transfer in Colloidal Nanocrystals/Silicon Hybrid Structures , HUE MINH NGUYEN, The University of Texas at Dallas, Department of Physics, OLIVER SEITZ, DAMIEN AUREAU, AMANDEEP SRA, YVES CHABAL, The University of Texas at Dallas, Department of Materials Science, ANTON MALKO, The University of Texas at Dallas, Department of Physics — The integration of organic and inorganic materials at the nanoscale offers the possibility of developing new photonic devices that could potentially combine the advantages of both classes of materials. Such optoelectronic structures could work both in photovoltaic as well as in light emitting modes depending on the direction of non-radiative *exciton* energy transfer (NRET). In present work, we studied hybrid structures consisting of a monolayer of the colloidal nanocrystal quantum dots (NQDs) grafted on hydrogenated Si surface via amine modified carboxy-alkyl chains linkers. Such approach allowed us to passivate Si surface to suppress non-radiative surface state defects ($N_s << 10^{11}$ cm^2) and provided with the controllable spacer lengths between NQDs and Si. We performed systematic measurements of NRET via time-resolved and steady-state photoluminescence (PL) in the range of 10K to 300K and as a function of spacer lengths and quantified NRET rates. Local field effects due to the acceptor surface (Si) are discussed.

9:00AM P41.00004 Quantum Dot Solar Cells. Understanding Charge Transfer at Nanostructure Interface[1] , PRASHANT KAMAT, University of Notre Dame — Quantum dot solar cells are designed using a chemical approach. Different size CdSe quantum dots are assembled on mesoscopic TiO_2 films either by direct adsorption or with the aid of molecular linkers. Upon bandgap excitation, CdSe quantum dots inject electrons into TiO_2 nanoparticles and nanotubes, thus enabling the generation of photocurrent in a photoelectrochemical solar cell. The interfacial processes that dictate the photoelectrochemical performance of these solar cells have now been evaluated by comparing photoelectrochemical behavior with charge transfer dynamics between different size CdSe quantum dots and various oxide substrates. The primary photochemical event in these solar cells is the charge injection from excited CdSe quantum dots into nanostructured metal oxide films. This process can be modulated by varying the particle size of CdSe quantum dots or the conduction band of the acceptor oxide. The difference in the conduction band energy of two semiconductors serves as a driving force for the interparticle electron transfer. According to Marcus theory, for a non-adiabatic reaction in the activation limit, the rate of electron transfer depends on the electronic coupling between the donor and acceptor states, the density of states (DOS) per unit volume and the driving force. Because of the quasi continuum of states in the metal oxide conduction band, the total electron transfer rate depends on the sum of all possible electronic transitions. The dependence of electron transfer rate constant on the energy gap and its implication in photoconversion efficiency of quantum dot solar cells will be presented.

[1]Supported by the Office of Basic Energy Sciences of the US Department of Energy

9:36AM P41.00005 Ab initio theory of impact ionization applied to silicon nanocrystals[1] , MARTON VOROS, Budapest University of Technology and Economics, ADAM GALI, Hungarian Academy of Sciences, Research Institute for Solid State Physics and Optics, DARIO ROCCA, GERGELY ZIMANYI, GIULIA GALLI, UC Davis — Achieving multi exciton generation (MEG) in semiconducting nanocrystals may lead to overcome the well-known Shockley-Queisser limit when building semiconductor-based solar cells. A thourough, theoretical understanding of the experiments that reported MEG in e.g. Si and PbSe nanocrystals, is still missing and could significantly contribute to clarify the several controversial results in the field. Several theoretical and numerical studies have addressed the origin of the MEG formation, mostly supporting an impact ionization mechanism. However, impact ionization rates have only been evaluated for model nanocrystals by using empirical pseudopotentials fitted to bulk properties, and model dielectric functions to describe the screened Coulomb interaction. We present an ab-initio scheme based on Density Functional Theory in a plane-wave pseudopotential implementation that includes static screening within the random-phase approximation. We will discuss how impact ionization rates are affected by the shape and surface structure of few nm Si nanocrystals.

[1]Support from Grant NSF DMR-1035468 is acknowledged.

9:48AM P41.00006 Optical properties of crystalline and amorphous silicon slabs with adsorbed metal clusters and with dopants: A combined ab-initio electronic structure and density matrix treatment[1] , DIMITRI KILIN, University of South Dakota, DAVID MICHA, JESSICA RAMIREZ, University of Florida — The optical absorbance and surface photovoltage of slabs of Si with varying number of layers have been calculated starting from their atomic structure. Results have been obtained for nanostructured surfaces with adsorbed metal clusters and for group III and V dopants, from ab initio DFT with periodic boundary conditions for extended systems, and from time-dependent DFT for supercells. Density matrix equations of motion (EOM) have been parametrized in a basis set of Kohn-Sham orbitals, for both crystalline and amorphous Si slabs [1]. Results for properties and from electronic charge distributions provide insight on slab confinement effects for electronically excited states and for particle-hole creation. In addition, the integrodifferential EOMs have been solved for an initial femtosecond pulse excitation [2] to analyze the nature of electron transfer at the surfaces, relevant to photovoltaics.

[1] T. W. LaJoie, J. J. Ramirez, D. S. Kilin, and D. A. Micha Intern. J. Quantum Chem. 110, 3005 (2010).
[2] A. S. Leathers, D. A. Micha, and D. S. Kilin, J. Chem. Phys. 132, 114702-1(2010)]

[1]Work supported by the NSF and by the Dreyfus Foundation to DM.

10:00AM P41.00007 Ultrafast Single and Multiple Exciton Dissociation in CdSe and PbS Quantum Dots[1] , TIANQUAN LIAN, Emory University — Charge transfer to and from quantum dots (QDs) is of intense interest because of its important roles in QD-based devices, such as solar cells and light emitting diodes. Recent reports of multiple exciton generation (MEG) by one absorbed photon in some QDs offer an exciting new approach to improve the efficiency of QD-based solar cells and to design novel multi-electron/hole photocatalysts. However, two main challenges remain. First, the efficiency of MEG process remains controversial and may need to be significantly improved for practical applications. Second, the utilization of the MEG process requires ultrafast exciton dissociation prior to the exciton-exciton annihilation process, which occurs on the 10s to 100s ps time scale. In this presentation we report a series of studies of exciton dissociation dynamics in quantum dots by electron transfer to adsorbed electron acceptors. We show that excitons in CdSe can be dissociated on the a few picosecond timescale to various adsorbates. As a proof of principle, we demonstrated that multiple excitons (generated by multiple photons) per QD can be dissociated by electron transfer to adsorbed acceptors (J. Am. Chem. Soc. 2010, 132, 4858-4864). We will discuss the dependence of these rates on the size and the nature of the quantum dots and possible approaches to optimize the multiple exciton dissociation efficiency.

[1]This work is supported by National Science Foundation (CHE-0848556).

10:36AM P41.00008 Short time evolution of electronic charge transfer and separation, and quantum coherences, at photoexcited crystalline and amorphous Si surfaces: Adsorbate and dopant effects[1] , DAVID MICHA, ANDREW LEATHERS, University of Florida, DMITRI KILIN, University of South Dakota — The short time evolution of populations of electronic states and their quantum coherence at nanostructured surfaces of semiconductors provide insight on mechanisms of electronic charge transfer and separation. Starting from atomic structure, density matrix (DM)equations of motion (EOM) have been generated from a general formulation of dissipative quantum dynamics and have been parametrized in a basis set of Kohn-Sham orbitals, for both crystalline and amorphous Si slabs [1] with metal cluster adsorbates and with group III and V dopants. Integrodifferential EOMs have been solved for an initial ground state excited by femtosecond light pulses [2] to provide the time evolution of direct and indirect electron transfer at the surfaces. Results show that one of the transfer mechanisms can lead to long term separation of electronic charge, and what material properties contribute to large charge transfer and separation.

[1] T. W. LaJoie et al., Intern. J. Quantum Chem. 110, 3005 (2010).
[2] A. S. Leathers et al. J. Chem. Phys. 132, 114702-1(2010)]

[1]Work partly supported by the NSF Chemistry Division and by the Dreyfus Foundation to DM.

10:48AM P41.00009 Investigation of electron-hole recombination in multi-layered quantum dots using explicitly correlated wavefunction based methods , ARINDAM CHAKRABORTY, Syracuse University — Electron-hole pairs are generated by photoexcitation of electrons to excited electronic states. Accurate calculations of electron-hole binding energies and recombination probabilities can give important insights into the photovoltaic properties of semiconductor nanocrystals and quantum dots. In the present work, the challenge of accurate treatment of electron-hole correlation is addressed by developing explicitly correlated electron-hole wavefunction that depends on electron-hole interparticle distance. The explicitly correlated ansatz for the electron-hole wavefunction is used to calculate eigenvalues and eigenfunction of the electron-hole Hamiltonian in multi-layered quantum dots using self-consistent field (SCF) and configuration interaction (CI) techniques. These methods are applied to investigate influence of the core/shell structure and chemical composition on electron-hole binding energies and recombination probabilities. The calculations indicate that for a given chemical composition there exists a optimum core/shell structure than minimizes electron-hole recombination. Comparison with experimental studies on similar system show good agreement between the experimental and computed results.

Wednesday, March 23, 2011 8:00AM - 10:48AM –

Session P42 DMP DPOLY: Focus Session: Organic Electronics and Photonics – Organic Photovoltaic Devices A302/303

8:00AM P42.00001 Increasing Transport Efficiencies of Polymer Based Solar Cells by Electrophoresis , TERRENCE WONG, CSUEB — Organic polymer photovoltaic (PV) cells are an active area of Applied Physics research because of four unique characteristics: (1) relatively inexpensive costs, (2) transparent properties, (3) flexibility, and (4) ease of mass production. We are studying the effects of incorporating single-walled carbon nanotubes (SWCNs) into a mixture of poly-(3-hexylthiophene) (P3HT), to test the affects on transport characteristics. The experiment will be segregated into parallel trials, with fixed volume ratios of P3HT:SWCNs to test the effects of (1) random orientation of SWCNs or the control, and (2) an aligned orientation of SWCNs. An electrophoresis-based technique, similar to gel electrophoresis, used to separate DNA fragments of variable masses, is used for partial alignment of the SWCN. Fixed geometry metalized substrates in a four striped copper patternare used for the transport studies and the P3HT:SWCN film's resistivity is monitored in-situ. The oriented films show enhanced conductivity, indicating this plays a major role in the increased efficiencies found in P3HT:SWCN based polymer solar cells.

8:12AM P42.00002 Transparent Carbon Nanotube layers as cathodes in OLEDs , ALEXIOS PAPADIMITRATOS, ALBERT NASIBULIN, ESKO KAUPPINEN, ANVAR ZAKHIDOV, SOLARNO INC COLLABORATION, AALTO UNIVERSITY COLLABORATION, UT DALLAS COLLABORATION — Organic Light Emitting diodes (OLEDs) have attracted high interest in recent years due to their potential use in future lighting and display applications. Reported work on OLEDs traditionally utilizes low work function materials as cathodes that are expensive to fabricate because of the high vacuum processing. Transparent carbon nanotube (CNT) sheets have excellent mechanical and electrical properties. We have already shown earlier that multi-wall (MWCNT) as well as single CNT (SWCNT) sheets can be used as effective anodes in bright OLEDs [1,2]. The true advantage of using the CNT sheets lies in flexible devices and new architectures with CNT sheet as layers in tandem devices [3] with parallel connection. In this work, we are investigating the possibility of using SWCNT as cathodes in OLEDs. SWCNT sheets have been reported to show lower work function compared to MWCNT. Our work attempts to demonstrate transparent OLED devices with CNT anodes and cathodes. In the process, OLEDs with CNT cathodes have been fabricated in normal and inverted configurations using inorganic oxides (MoO3,ZnO) as invertion layers.[1] C.D. Williams et al., Appl.Phys.Lett. 93, 1, 2008.[2] A. Kaskela et al. Nano Lett., 10,11, 4349 ,2010.[3] A. Papadimitratos et al. 8th ICEL,2010.

8:24AM P42.00003 Nanoscale electro-optical measurements of photovoltaic materials using scanning probe microscopy , NIKOLAI ZHITENEV, BEHRANG HAMADANI, PAUL HANEY, CNST, NIST, SUYONG JUNG, HUA XU, Nanocenter, UMD/ CNST, NIST — The efficiency of photovoltaic devices based on inorganic thin-films or organic polymer blends is often determined by the nanoscale structure and properties of internal and contact interfaces. Measurements of local photo-conductivity, along with other scanning probe based measurements, can link the structural properties to the performance providing the desired feedback for the device optimization. However, the nature of the tip-to-sample contact can be quite different from contact interfaces in devices strongly affecting the injection and collection of charge carriers and complicating the data analysis. Here, we present the characterization of photoconductive channels in a model bulk heterojunction organic solar cell based on a p-type polymer and n-type small molecule. We directly compare the properties of the tip-to-sample interface to the nanocontact interface. We explore the nanoscale photocurrent response on two complementary device architectures using conductive tips suitable for the appropriate charge (i.e., electrons vs. holes) collection. In addition to the measurements at the top surface, we examine the response from the bulk of the film using novel sectioning technique. Our results provide significant insight into the origin of nanoscale variations in photoresponse and nanoscale morphology of such materials.

8:36AM P42.00004 Organic and hybrid organic-inorganic photovoltaic cells , MICHAEL MCGEHEE, Stanford University — The performance and limitations of the world's best organic and dye sensitized solar cells will be presented along with plans to increase the energy conversion efficiency to 15%. Topics of more detailed discussion could include the formation of polymer-fullerene co-crystals and their implications for recombination, the use of energy transfer to improve light harvesting in dye sensitized solar cells, solution deposited transparent electrodes or the use of plasmonics to improve light absorption.

9:12AM P42.00005 Studying recombination in the bulk heterojunction solar cells using lateral solar cell geometries , CHRISTOPHER LOMBARDO, ERIC DANIELSON, ANANTH DODABALAPUR, The University of Texas at Austin — Lateral structures are shown to be a very powerful tool to understand transport and recombination phenomena in bulk heterojunction materials and solar cells. Active layers of phase separated P3HT:PCBM were chosen due to their wide use in research devices and potential for commercialization. Studies of current-voltage curves for varying carrier transit lengths have resulted in information about the movement of charge carriers as well as carrier recombination. By examining typical solar cell parameters (open circuit voltage, short circuit current, fill factor, and power conversion efficiency) combined with photocurrent measurements as a function of electrode spacing, carrier density, applied electric field, and temperature under illumination conditions (0.1 – 100 suns), we have determined how these parameters depend on the carrier concentration, electric field, and temperature. This work provides a clear picture of when bimolecular recombination dominates and also if the recombination is Langevin or non-Langevin.

9:24AM P42.00006 Scaling behavior and transport in bulk heterojunction materials , ERIC DANIELSON, CHRISTOPHER LOMBARDO, ANANTH DODABALAPUR, The University of Texas at Austin — A lateral device geometry has been used to study charge transport in P3HT:C_{71}-PCBM bulk heterojunction devices. Analysis of current-voltage curves have previously been used to study charge transport in these materials. We perform ambipolar field effect transistor measurements on these structures to extract carrier mobilities. We are also able to describe the charge transport and recombination properties of these materials. Assymetric electrodes (Al, Au) separated by 100 nm-20μm enable us to gain considerable insight into transport physics. Photocurrent measruements as a function of channel length, electric field, and illumination intensity (0.1-100 suns) are used to measure the ambipolar mobility-lifetime product and study how this correlates with measured field-effect mobilities at various electric fields. Lateral structures are shown to be a powerful tool to understand transport and the role of carrier mobility on photovoltaic performance.

9:36AM P42.00007 Charge Carrier Lifetime in Poly(3-hexylthiophe)/ZnO Nanowire Array Based Photovoltaic Devices , LEE BUTLER, WILLIAM BAUGHMAN, SHAWN DAVID WILBERT, NICK HARRIS, GANG SHEN, NABIL DAWAHRE, JOSEPH BREWER, PATRICK KUNG, SEONGSIN MARGARET KIM, The University of Alabama — Nanostructured electron donor and acceptor materials have shown potential for greatly improving the efficiency of organic photovoltaic (OPV) devices. Inorganic hybrid OPVs utilizing nanowires, nanorods and nanoparticles have been shown to greatly increase the current through P3HT based devices but have yet to achieve the efficiencies of their corresponding bulk-heterojunction OPVs. Determining the carrier properties and interface structure of these hybrid devices could greatly aid in determining limitation of the device structure on the overall efficiency. Here we report the use of terahertz, micro-Raman and micro-photoluminescence spectroscopy in determining carrier lifetime and optical properties of P3HT/ZnO based OPV devices. We will also discuss the effects of surface functionalization on the available phonon modes, carrier lifetimes and absorption properties.

9:48AM P42.00008 ABSTRACT WITHDRAWN –

10:00AM P42.00009 Spectral aspects of cavity tuned absorption in organic photovoltaics , BRENT VALLE, Case Western Reserve University, STEPHEN LOSER, JONATHAN HENNEK, Northwestern University, KENNETH D. SINGER, Case Western Reserve University, JAMES ANDREWS, Youngstown State University, TOBIN MARKS, Northwestern University — In order to increase the power conversion efficiency of organic photovoltaic devices it is necessary to extend absorption to longer wavelengths and to concentrate and capture light in a thin bulk heterojunction (BHJ) layer. In this work, optical transfer matrix formalism is used to model absorption in organic photovoltaic devices as a function of BHJ thickness and incident wavelength in the optical cavity formed by the BHJ layer sandwiched between the aluminum cathode and indium tin oxide (ITO) anode. We have found that absorption can be finely tuned by adjusting the thicknesses of the BHJ and ITO layers within a relatively narrow range. We have also observed distinct spectral effects due to frequency pulling resulting in enhanced long- wavelength absorption. Because the absorption shifts arise purely from optical interference effects, tuning of the absorption spectrum can be achieved by careful cavity design without affecting the open circuit voltage. We have experimentally verified aspects of our modeling and suggest methods to improve device design. Additionally, we consider the effects of BHJ material gradients versus depth on absorption in these devices.

10:12AM P42.00010 Probing the Thickness Limits of Organic Solar Cells using Monte Carlo Simulation[1] , MIKE HEIBER, ALI DHINOJWALA, The University of Akron — Organic solar cell performance has increased dramatically in recent years, but in order to achieve higher efficiency devices, it is imperative to understand the remaining fundamental challenges. One major shortcoming is that thin film devices cannot absorb all of the targeted incoming light due to the limited optical density of the materials used. To overcome this, thicker devices that can maintain the high quantum efficiency and high fill factor, present in thin state-of-the-art devices, must be developed. We have taken advantage of recent advancements in dynamic Monte Carlo (DMC) simulation methods to study the current-voltage (J-V) behavior of organic solar cells with different thicknesses. This method allows all detailed physical mechanisms of the device to be simulated and as a result, the effects of device morphology and a range of material properties can be captured. Studying device behavior as a function of thickness highlights the importance of the competition between light absorption and charge recombination. The effects of carrier mobility and active layer morphology are also considered. Understanding this tradeoff between absorption and recombination will help direct future experimental efforts to design optimal materials and devices.

[1]Lord Corporation and The University of Akron

10:24AM P42.00011 Dehydration assisted nanoimprint of PEDOT:PSS nanogratings to improve organic photovoltaics , YI YANG, KOYAU LEE, KAMIL MIELCZAREK, WALTER HU, ANVAR ZAKHIDOV, DEPARTMENT OF ELECTRICAL ENGINEERING, THE UNIVERSITY OF TEXAS AT DALLAS TEAM, DEPARTMENT OF PHYSICS,THE UNIVERSITY OF TEXAS AT DALLAS TEAM — We demonstrate the fabrication of oly(3,4-ethylenedioxythiophene) poly(styrenesulfonate) (PEDOT:PSS)nanograting by a dehydration assisted nanoimprint lithographic technique. Dehydration of PEDOT:PSS increases its mechanical strength for high fidelity and fine precision nanoimprinting process, resuling in formation of high quality nanogratings of 60 nmin height, 70 nm in width, and70 nm in spacing. PEDOT:PSS nanograting ar used as hole injection and electron barrier layer in blended poly(3-hexylthiophene-2,5-diyl) (P3HT)[6,6]-penyl-C61-butyric-acid-methyl-ester PCBM) rganic bulk heterojuncton photovoltaic devices (OPV), showing enhancement of photocurrent and increased efficiency in comparison to non-patterned plane PEDOT:PSS film. Improved performance is discussed in terms of increased interface for charge collection and better distribution of internal electric field.

10:36AM P42.00012 High-performance inverted polymer solar cells with ITO coated with a thin layer of oxide for electron collection , JIANYONG OUYANG, HONGMEI ZHANG, National University of Singapore — Solar cells using organic or polymeric materials as the active material have been attracting strong attention due to the low fabrication cost and high mechanical flexibility. The photovoltaic efficiency has been improved to more than 8% under AM1.5 G illumination. However, polymer solar cells are usually not very stable, which severely impedes the practical application. The stability is strongly affected by the electrodes. Both PEDOT:PSS used as the buffer layer on ITO for the hole electron and active metals like Ca for the electron collection are blamed to lower the stability of polymer solar cells. Polymer solar cells with an inverted structure can have much better stability than normal devices because they do not use PEDOT:PSS and active metals. One big challenge in building the inverted polymer solar cells is to lower the work function of ITO for effective electron collection. Here, we report a new method to effectively lower the work function of ITO by depositing a thin layer of oxide and demonstrate high-performance polymer solar cells. The photovoltaic efficiency of the inverted polymer photovoltaic cells is even higher than the normal devices. The mechanism for the oxide effect on the work function of ITO will be presented as well.

Wednesday, March 23, 2011 8:00AM - 11:00AM –
Session P43 DPOLY: Focus Session: Thin Film Block Copolymers III A306/307

8:00AM P43.00001 Effect of Well-defined Roughness on the Microdomain Orientation of Block Copolymer Thin Films , KOOKHEON CHAR, YOUNGWOO CHOO, HYO SEON SUH, TAEHEE KIM, Seoul National University — It is well known that the perpendicular orientation of block copolymer (BCP) films is preferred over the parallel orientation when the BCP films are placed on rough surfaces due to the unfavorable elastic deformation of BCP chains in the parallel oriented microdomains. More recently, the approach to utilize the rough substrate for BCP domains in long range order has been reported. However, the quantitative analysis to explore the effect of each individual roughness factors, such as lateral or vertical displacement, on the microdomain orientation of BCP films has not been thoroughly studied yet. In order to examine the roughness effect systematically, we prepared substrates with well-defined roughness utilizing either nanoparticle monolayers or line patterns generated by e-beam lithographic technique. Based on the detailed observation of the orientational change of BCP films on the well-defined surface roughness, we analyzed the dependence of BCP domain orientation on each roughness parameter. Furthermore, we found that the BCP film thickness, coated on the substrate, is another important parameter determining the orientation of microphase-separated domains of BCP thin films in addition to the surface roughness.

8:12AM P43.00002 Multiple Replicas of Block Copolymer Thin Films from a Brushless Organosilicate Substrate , HYO SEON SUH, HYUNSIK YOON, KOOKHEON CHAR, Seoul National University — The chain end-grafted polymer brushes or cross-linked polymer mats have typically been utilized as the surface modification layers to induce the perpendicular orientation of block copolymer (BCP) thin films. Instead of such polymer-based approaches, we have recently introduced a new concept to control the BCP orientation using the brushless organosilicate (OS) substrates, whose surface energy can be finely tuned with thermal treatment. In this brushless case, the BCP chains do not penetrate into the underlying hard OS substrates during thermal annealing of BCP films, therefore, the BCP chains at the interface have no entangled structure with fairly weak adhesion of BCP films against the substrate. Owing to such weak adhesion of BCP films against the OS substrate, the perpendicularly oriented BCP film on a neutral OS substrate could be easily peeled off and transferred to a UV-curable resin applied onto the BCP film. The OS substrate after the peel-off process of a BCP film could regenerate the perpendicularly oriented BCP films since the surface energy of the OS substrate remains intact during the peel-off process. Furthermore, the direct-assembled BCP films on chemically patterned OS substrates could also be peeled off and transferred on to a UV-curable resin, allowing us to produce multiple replicas of direct-assembled BCP thin films from a single chemically patterned OS substrate.

8:24AM P43.00003 Rational design of block copolymer morphologies via control of the film thickness and substrate patterning: A self consistent field study , XIANGGUI YE, BRIAN J. EDWARDS, BAMIN KHOMAMI, Materials Research and Innovative Laboratory (MRAIL), Department of Chemical and Biomolecular Engineering, University of Tennessee, Knoxville — Chemically patterned substrates can direct the assembly of adsorbed layers or thin films of block copolymers. In this study we have examined the self-assembly of a lamella-forming diblock copolymer on periodically stripe-patterned substrates, and a cylinder-forming diblock copolymer on periodically doted-patterned substrates for various film thicknesses. In general, we have shown that for thin films the morphology of the block copolymer follows the chemical pattern at the substrate; however, with an increase degree of mismatch between the spacing of the pattern and the natural spacing of bulk block copolymer, a host of novel morphologies can been created, which have not to date been experimentally realized. Our studies clearly demonstrate that the film thickness and the pattern of substrate can be judiciously manipulated to rationally design morphologies for various applications such as filtration, conduction, and high-surface area membranes. Overall, these results demonstrate a promising strategy for fabrication of complex interfacial nanostructures from chemically patterned templates.

8:36AM P43.00004 Utilizing low surface energy moieties to control surface composition of a polystyrene-b-poly(2-vinylpyridine) block copolymer , MICHAEL DIMITRIOU, Materials UC Santa Barbara, DANIEL FISCHER, NIST, CRAIG HAWKER, EDWARD KRAMER, Materials UC Santa Barbara — During processing the interaction of a block copolymer film with a free surface affects its final orientation and surface composition. A strategy to control this interaction and hence tailor the final structure of a polymer film is to introduce low surface energy moieties to the system. A lamellar forming polystyrene-b-poly(2-vinylpyridine) (PS-b-P2VP) block copolymer was synthesized with varying amounts of 1-[(3-butenyloxy)methyl]-4-vinylbenzene copolymerized with the 2VP block. Utilizing thiol-ene chemistry the pendant alkene of 1-[(3-butenyloxy)methyl]-4-vinylbenzene was functionalized with 1H,1H,2H,2H-perfluorooctanethiol to efficiently and selectively incorporate fluorinated hydrocarbons into the 2VP block. Near edge X-ray absorption fine structure spectroscopy (NEXAFS) and X-ray photoelectron spectroscopy were used to characterize the polymer surface as a function of 1H,1H,2H,2H-perfluorooctanethiol incorporation. At molar incorporations of the fluorinated monomer in P2VP greater than 4% dynamic secondary ion mass spectrometry and NEXAFS indicate a P2VP rich surface.

8:48AM P43.00005 Flexible Confinement of Block Copolymer Films Between Tunable Surface Energy Elastomeric Films and Xerogel Substrates , MANISH KULKARNI, GURPREET SINGH, Department of Polymer Engineering, University of Akron, Ohio 44325, SUSHIL SATIJA, NIST Center for Neutron Research, Gaithersburg, MD 20899, ALAMGIR KARIM[1], Department of Polymer Engineering, University of Akron, Ohio 44325 — Orientation control of block copolymer (BCP) films is important for advanced technological applications such as nanoscale lithography. Here we present a different strategy whereby both interfaces of the poly(styrene)-block-poly(methylmethacrylate) BCP films are tunably controlled. The BCP films were coated on a roughness and surface energy tunable xerogel substrates and the top surface of the polymer film was conformally covered by crosslinked PDMS elastomer. The surface energies of xerogel substrate and crosslinked PDMS is tunable from 28 and 18 mJ/m^2 to 45 and 55 mJ/m^{2}resp. via UV-Ozone treatment. The confined BCP film was then thermally annealed to induce ordering. Such a unique approach allowed the BCP films to respond in its orientation of cylinders and lamellae from parallel to perpendicular. The morphology of these micro-phase separated BCP films was studied by tapping mode atomic force microscopy and neutron reflectivity.

[1]Corresponding Author

9:00AM P43.00006 Directed Assembly of Block Copolymer on Tunable Surface Energy Flexible Substrate , ARZU HAYIRLIOGLU, ALAMGIR KARIM, Department of Polymer Engineering, The University of Akron, Akron, OH, USA — We examine the ordering properties of micro-phase separated block copolymer (BCP) films on flexible substrates. In particular, we investigated the wettability characteristics and morphology of the BCP films before and after annealing on tunable surface energy PDMS substrates. The surface energy of PDMS substrates was modified to vary from 20 to 68 mJ/m^2 by exposing them to UV-ozone (UVO). Two types of block copolymer systems were examined on these UVO exposed PDMS substrates. Our experiments were carried out with surface energy above 42 mJ/m^2 because the BCP dewets on the PDMS substrate below that surface energy. Atomic Force Microscope (AFM) and Optical Microscope (OM) were used to study of the surface morphology of the BCP films. It was observed that the BCP morphology exhibits perpendicular orientation on PDMS substrate with surface energy in the range of 42 to 66 mJ/m^2 and parallel orientation above 67 mJ/m^2. BCP film morphology on other types of soft substrates and different BCP systems as a function of annealing temperatures and film thickness will be presented.

9:12AM P43.00007 The effect of Surface Neutrality on ODT of PS-b-PMMA films , EUNHYE KIM, SEUNGHOON CHOI, RUI GUO, DU YEOL RYU, Yonsei University, CRAIG J. HAWKER, University of California, Santa Barbara, THOMAS P. RUSSELL, University of Massachusetts, Amherst, YONSEI UNIVERSITY TEAM, UNIVERSITY OF CALIFORNIA COLLABORATION, UNIVERSITY OF MASSACHUSETTS COLLABORATION — The film transitions, the order-to-disorder transition (ODT), has been investigated in a symmetric polystyrene- b-poly(methyl methacrylate) (PS-b-PMMA) on a random copolymer (P(S-r-MMA)) grafted substrate where the interfacial interactions are balanced. With decreasing film thickness less than 25L0, the ODT significantly decreases, because the interfacial interactions by a random copolymer grafted to the substrate provide a surface-induced compatibilization toward two block components. However, a plateau of the ODT for films thicker than 25L0 was observed above the bulk value. The elevation of this ODT indicates a suppression of compositional fluctuations normal to the film surface, more than likely because the dominant orientation of the lamellar microdomains was found to be parallel to the film surface.

9:24AM P43.00008 Surface Affinity Effects On Confined Thin Film Block Copolymers Using Self Consistent Field Theory Modeling , ADAM HANNON, ALFREDO ALEXANDER-KATZ, CAROLINE ROSS, Massachusetts Institute of Technology — Self consistent field theory (SCFT) applied to inhomogeneous thin film block copolymer systems allows for the exploration of a wide array of potential equilibrium ordered morphologies at the nanoscale through varying parameters such as χ, the segmental Flory-Huggins parameter, N, the polymer degree of polymerization, and f, the volume fraction of the minority polymer component. In addition, boundary conditions of the chemical potential fields in the field theory can be specified to model surface features such as polymer brush layers and topological templating features from lithography that enrich the possible morphologies observed [Macromolecules 2010, 43, 8290–8295]. In this presentation, we show how the orientation and surface morphology of diblock copolymers with large χN varies with surface affinity, surface shape, and $f$for confined thin film systems. Surfaces neutral to both polymer species are examined, as well as surfaces preferential to both the minority and majority polymer components with fine variances in the magnitude of the surface affinity. Commensurability of the ordered structures is examined as well by varying simulation cell size. The results of the study will be applied to the generation of complex features for nanolithography applications.

9:36AM P43.00009 Stress induced topographic patterning in thin diblock copolymer films , ANDREW CROLL, North Dakota State University, ALFRED CROSBY, University of Massachusetts, Amherst — When a thin rigid polymer film is attached to a soft elastic substrate and placed in a state of compressive stress, the system wrinkles as a critical stress is surpassed. This simple deformation pattern contains information about the mechanical state of both the polymer film and substrate. Although classical mechanics can be used to relate the global deformation of the film/substrate to the local wrinkle geometry as a function of materials properties, relatively little is known about how the thin capping film material accommodates the localized bending (and therefore localized stress). Here we conduct wrinkling experiments using a model diblock copolymer/elastomer composite. Wrinkling a homogeneous, disordered block copolymer film places the film in a well-defined initial stress state. When heated above its glass transition, the wrinkled film flows, microphase separates, and relaxes from the stress imposed by local wrinkle deformations. The periodic stress relaxation leads to the emergence of a new pattern in the microphase separated surface structure, thus providing new insight into how block copolymers react to stress.

9:48AM P43.00010 Shear-induced sphere-to-cylinder transition in thin films of diblock copolymers and the role of wetting layers , ALEXANDROS CHREMOS, RICHARD REGISTER, Princeton University, PAUL CHAIKIN, New York University, ATHANASSIOS PANAGIOTOPOULOS, Princeton Unversity — The shear-induced sphere-to-cylinder transition in diblock copolymer thin films has been studied using large-scale coarse- grained Langevin dynamics simulations. At zero-shear conditions and below the order-disorder transition temperature the thin film forms a monolayer or bilayer of spheres given the thickness of the film. Mimicking the experimental setup the minority block has an affinity to be adsorbed on the confining surfaces forming brushes which interpenetrate the rest of the film. Once a shear field is applied and above a critical shear rate, the spheres elongate and merge with their neighbors to form cylinders. We find that the mechanism with which the spheres merge is closely related with the stretching of individual diblock chains. In particular, we find that in monolayer thin films it is more difficult to achieve the sphere-to-cylinder transition, which is also an experimental observation, because the brushes restrict the stretching of diblock chains. The simulations were performed with the use of Graphical Processing Units allowing large-scale simulations with long polymer chains to studied.

10:00AM P43.00011 Shear alignment of standing block copolymer lamellae in thin films , SASWATI PUJARI, MICHAEL KEATON, Princeton University, PAUL CHAIKIN, New York University, RICHARD REGISTER, Princeton University — While thin films of cylinder-forming block copolymers (BCPs) can be effective templates for striped patterns (leading to parallel nanowires), a drawback is the modest aspect ratio of the final structures, because of limited etch contrast between the two polymer blocks. Using thin films of lamellar BCPs, with the lamellae standing perpendicular to the substrate, could yield structures with larger aspect ratio. To generate parallel stripes of controlled direction, the in-plane orientation needs to be guided while preserving the out-of-plane perpendicular orientation. In this study, we have produced thin films of standing lamellae of a polystyrene/polymethylmethacrylate BCP of thicknesses up to 1.5 times the domain spacing, by neutralizing the Si substrate with a random terpolymer brush layer. To date, films less than one domain spacing thick have been aligned by shear, while shearing thicker films causes the perpendicular lamellae to switch to parallel orientation. We are currently investigating the alignment as a function of stress, film thickness, terpolymer composition and domain spacing.

10:12AM P43.00012 Defect generation in thin films of block copolymer cylinders: the effect of cylinder spacing and film thickness , VINDHYA MISHRA, EDWARD KRAMER, Univ of California Santa Barbara — Understanding the fundamental physics of disordering and defect generation in block copolymer (BCP) films is important for directed assembly based block copolymer lithography. We investigate the defect generation in, and smectic-nematic-isotropic transition temperature T_m of, monolayers and bilayers of poly (styrene-b-2vinyl pyridine) diblock copolymer cylinders aligned parallel to the substrate in 2 micron wide channels. Quantitative AFM studies were supplemented with grazing incidence small angle X-ray diffraction line-shape analysis to quantify the decay of translational and orientational correlation functions with increasing temperature. We find that T_m decreases, and the dislocation density n below T_m increases, if either the number of layers or the cylinder spacing a decreases. These results are expected since $n \sim \exp(-E_d/kT)$ and E_d, the dislocation formation energy, scales as a^2h, where h is film thickness. Since only a 10% decrease in a produces a dramatic increase in n, these results suggest that using 2D smectic structures such as BCP cylinders aligned parallel to, or BCP lamellae normal to, a substrate to produce more closely spaced features will result in patterns with more and more defects.

10:24AM P43.00013 Micelle Formation of Diblock Copolymer in a Thin Film Homopolymer: a Comparison with Polymer Brush-Coated Nanoparticles , HENGXI YANG, CHELSEA CHEN, PETER GREEN, University of Michigan — We investigated micelle formation of a diblock copolymer polystyrene-*b*-poly(2-vinylpyridine) (PS-*b*-P2VP) of degree of polymerization N, in thin films of homopolymer polystyrenes (PS) of different degrees of polymerization P, supported on substrates, and compared the results with the phase behavior of PS brush-coated Au nanoparticles in homopolymer PS matrix. PS-*b*-P2VP copolymer chains aggregated to form micelles, composed of an inner P2VP core and an outer PS corona. The size of the micelle cores, D_{core}, increased with increasing P, and reached a plateau at very large P. The transition occurred at a larger P/N than expected from brush-melt interaction theories. The organization of micelles at large P regimes suggested attractions between micelles. P2VP block also adsorbed onto the substrate to form a brush layer and the surface adsorption process was affected by micellization of copolymers. We compared the micelle formation of PS-*b*-P2VP in PS with the phase behavior of PS coated Au nanoparticle/PS mixtures: the host chains penetrate into the corona of the micelles more easily than into the PS brush grafted on the particle due to low "grafting density;" what's more, micelles can self-adjust their aggregation number as the interaction between host chains and the corona changes.

10:36AM P43.00014 Bicontinuous nanoporous block copolymer films prepared from a spherical-phase architecture , EASAN SIVANIAH, PAUL ZAVALA, KEVIN CHANNON, SANNA NATARAJ, Cambridge University, SHAHEEN AL-MUHTASEB, Qatar University — In a recent discovery, we have found a way to make a bicontinuous nanoporous polymer network and subsequently transform this into interconnected mesoporous inorganic oxide sheets. Notably, these structures arise from a spherical block copolymer template. Nanoporous materials of such architecture, both polymeric and inorganic, are rare and also extremely useful. Importantly, the process is not restricted to a single block copolymer system or a narrow range of molecular weights or compositions. All of the process steps are scaleable, fast enough to be appropriate to continuous production methods, do not require vacuum technology, and can be achieved by solution processing. We discuss the process and its use to make PLEDs, photovoltaics and filtration membranes.

10:48AM P43.00015 Arrangement of the Microdomains of Block Copolymers Confined at Hemi-sphere Walls , DU SIK BAE, JIN KON KIM, Pohang University of Science and Technology — The arrangement of the microdomains of polystyrene-*block*-poly(methyl methacrylate) copolymer (PS-*b*-PMMA) confined at hemi-sphere walls was investigated by scanning and transmission electron microscopy. The hemi-spherical constraint was introduced by using anodic aluminum oxide template.. The wall surface was modified by thin layers grafted by PS, PMMA, and PS-*ran*-PMMA copolymer. We observed interesting morphologies which have not been observed. The observed microdomain arrangement was compared with theoretical predictions.

Wednesday, March 23, 2011 8:00AM - 11:00AM –

Session P44 DPOLY: Focus Session: Assembly, Structure, & Instabilities in Polymer Films, Network Films, & Interfaces I A309

8:00AM P44.00001 An interplay between self-organization and interfacial modification of diblock copolymers in bi-layered thin film laminates , JAN GENZER, North Carolina State University — We study the interfacial partitioning of poly(styrene-b-methyl methacrylate) (SM) diblock copolymers at interfaces between thin planar films of polystyrene (PS) and poly(methyl methacrylate) (PMMA) homopolymers. SM copolymers with constant PS and varying PMMA block lengths are incorporated into the top PS layer and the resulting dewetting kinetics of the top PS film decrease by reducing the length of the PMMA block and increasing the molecular weight of the host PS homopolymer. Similar behavior is observed when the SM copolymers are added to the bottom PMMA homopolymer. Systems incorporating SM copolymers possessing short PS blocks and long PMMA blocks exhibit dewetting rates that are higher than those of the copolymer-free PS/PMMA bilayer. This behavior is attributed to the segregation of SM aggregates at the PS/PMMA interface, which migrate to and roughen the interface and destabilize the film. The dewetting kinetics of systems with mixtures of asymmetric copolymers (stabilizing and destabilizing) added in the PS homopolymer lie between those of the individual copolymers pure copolymers. Using block copolymer mixtures rather than single copolymers to tune stabilizing/compatibilizing efficacy provides an unexplored route to achieving property control in thin polymer films.

8:36AM P44.00002 Formation of Nanoparticle Stripe Patterns via Flexible-Blade Flow Coating , DONG YUN LEE, HYUN SUK KIM, CASSANDRA PARKOS, CHEOL HEE LEE, TODD EMRICK, ALFRED CROSBY — We present the controlled formation of nanostripe patterns of nanoparticles on underlying substrates by flexible-blade flow coating. This technique exploits the combination of convective flow of confined nanoparticle solutions and programmed translation of a substrate to fabricate nanoparticle-polymer line assemblies with width below 300 nm, thickness of a single nanoparticle, and lengths exceeding 10 cm. We demonstrate how the incorporation of a flexible blade into this technique allows capillary forces to self-regulate the uniformity of convective flow processes across large lateral lengths. Furthermore, we exploit solvent mixture dynamics to enhance intra-assembly particle packing and dimensional range. This facile technique opens up a new paradigm for integration of nanoscale patterns over large areas for various applications.

8:48AM P44.00003 Hierarchically Organized Structures Engineered from Controlled Evaporative Self-Assembly , ZHIQUN LIN, MYUNGHWAN BYUN, WEI HAN, Iowa State University, NED BOWDEN, University of Iowa — By constraining an asymmetric comb block copolymer (CBCP) toluene solution to evaporate in a wedge-on-Si geometry composed of a wedge lens situated on a Si substrate, gradient concentric stripe-like surface patterns of CBCP at the microscopic scale were yielded as a direct consequence of *controlled* evaporative self-assembly of CBCP. The formation of either straight stripes or jagged stripes was dictated by the height of the wedge. Upon subsequent solvent vapor annealing, hierarchically organized structures of CBCP were produced, resulting from the interplay of solvent vapor-assisted, unfavorable interfacial interaction-driven destabilization of CBCP from the Si substrate at the microscopic scale and the solvent vapor-promoted reconstruction of CBCP nanodomains within the stripes at the nanometer scale. This facile approach of combining *controlled* evaporative self-assembly with subsequent solvent vapor annealing offers a new platform to rationally design and engineer self-assembling building blocks into functional materials and devices in a simple, cost-effective manner.

9:00AM P44.00004 Wrinkling instabilities in compressed networks of polymer supported single-wall carbon nanotubes[1] , JOHN HARRIS, SWATHI IYER, NDSU, JI YEON HUH, JEFFREY A. FAGAN, JUN YOUNG CHUN, STEVEN D. HUDSON, JAN OBRZUT, CHRISTOPHER M. STAFFORD, NIST, ERIK K. HOBBIE, NDSU — Strain-induced structural and electronic changes in polymer supported membranes of purified single-wall carbon nanotubes (SWCNTs) are evaluated through the wrinkling instabilities that develop under both uniaxial and isotropic compression. Nanotubes that have been purified by length or electronic type using density-gradient ultracentrifugation are assembled as surfactant-free thin membranes on prestrained polydimethylsiloxane (PDMS) substrates, and the strain response is measured using a broad range of techniques. The small-strain behavior is inferred from kinetic changes in the wrinkling topography of the SWCNT membranes during the slow drying of pre-swelled polymer supports. The measurements suggest a remarkable degree of strain softening that strongly couples to the anisotropic sheet resistance of the films, which we in turn relate to the microscale anisotropy that develops through excluded volume interactions.

[1]Supported by the NSF through CMMI-0969155 and the DOE through DE-FG36-08GO88160

9:12AM P44.00005 Confinement-Induced Molecular Stresses and Wetting Instability in Ultrathin Polymer Films , Y. CHEIN, P.W. LEE, A.C.-M. YANG, Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, Taiwan — Chain packing and molecular behavior of polymers confined below unperturbed coil sizes are still poorly understood. To explore the physical state and condensation process, molecular recoiling stresses in polystyrene films (4-100 nm) were measured through wetting instability at above T_g(100 C). The films demonstrated strikingly different instability mechanisms in regimes divided by entanglement molecular weight (M_e). Moreover, the recoiling stress decreased with chain length above M_e, consistent with the condensation process dominated by solvent evaporation, but plunged below M_e, apparently due to diminishing deformations. A small fraction of MEH-PPV added in films manifested photoluminescence (PL) following the same trend as recoiling stress confirming stress-enhanced PL characteristic of conjugated polymers. As aging temperature lowered but still above T_g, film stability increased but recoiling stress underwent significant changes, in contrast to that below T_g where no changes was observed.

9:24AM P44.00006 Nucleation and growth of creases on swelled polymer gel surfaces , JINHWAN YOON, JUNGWOOK KIM, RYAN HAYWARD, Polymer Sci & Eng, UMass Amherst, UMASS AMHERST TEAM — We have studied the processes by which surface creases form, evolve, and disappear using thin temperature-responsive poly(N-isopropylacrylamide) copolymer hydrogels. For shallow quenches beyond the critical level of compression, creases nucleate and growth, and thus the observed onset and morphology are typically dominated by heterogeneous defects. Measurements of crease growth velocities at different quench depths are used to precisely determine the compression at which the surface first becomes unstable, and this critical strain is found to be slightly elevated as film thickness is reduced. This behavior is captured by a simple model for the energy change upon forming a fold, with a nucleation barrier to fold formation provided by the gel/water surface-energy. While hysteresis between onset and disappearance is often observed in experiments, this reflects predominantly the degree of "undercooling" necessary to yield nucleation and growth of creases.

9:36AM P44.00007 Effect of polymer architecture on the interfacial properties of thin films , EMMANOUIL GLYNOS, BRADLEY FRIEBERG, PETER GREEN, University of Michigan, Ann Arbor — Many physical properties of polymers, such as phase transitions, mechanical properties, dynamics, crystallization and the glass transition, Tg, are influenced by film thickness constraints, and associated with the interactions between the constituent macromolecules and external interfaces. We show that star-shaped molecules, possessing sufficiently high functionality, exhibit significant differences in their average Tg-vs-thickness (H) behavior, both in the magnitude and the thickness dependent trends, from their linear analogs. In this talk, we will discuss the effect of polymer architecture on the interfacial properties of supported thin films, and more specifically how chain segments near the free and the solid interfaces influence the average Tg of the film. These effects are discussed in terms of the role of macromolecular architecture and entropic effects on the structure and dynamics of the polymer chains close to the interfaces, and their influence on the average properties of thin supported films.

9:48AM P44.00008 Interfacial Effects on Pentablock Ionomer Thin Films , THUSITHA ETAMPAWALA, DILRU RATNAWEERA, NARESH OSTI, UMESH SHRESTHA, DVORA PERAHIA, Department of Chemistry, Clemson University, Clemson, SC, JAROSLAW MAJEWSKI, Lujan Neutron Scattering Center, Los Alamos National Laboratory, Los Alamos, NM — The interfacial behavior of multi block copolymer thin films results from a delicate balance between inherent phase segregation due to incompatibility of the blocks and the interactions of the individual blocks with the interfaces. Here in we report a study of thin films of ABCBA penta block copolymers, anionically synthesized, comprising of centered randomly sulfonated polystyrene block to which rubbery poly-ethylenebutalene is connected, terminated by blocks of poly-t-butylstyrene, kindly provided by Kraton. AFM and neutron reflectometry studies have shown that the surface structure of pristine films depends on film thickness and ranges from trapped micelles to thin layered films. Annealing above Tg for the styrene block results in rearrangements into relatively featureless air interface. Neutron reflectivity studies have shown that annealed films forms layers whose plane are parallel to the solid substrate with the bulky block at the air interface and the ionic block at the solid interface.

10:00AM P44.00009 Directed Morphology of Nanofilled Polymer Films on Flexible Substrates , DIYA BANDYOPADHYAY, ARZU HAYIRLIOGLU, MANISH KULKARNI, ALAMGIR KARIM, Department of Polymer Engineering, The University of Akron, Akron, OH, USA — We demonstrate viable meso-patterning techniques that have relevance to electronics and organic photovoltaic applications via tunable control of polymer thin film instabilities. To this end, we examine the influence of fullerene (C_{60}) nanoparticles on multicomponent polymer thin films on patterned and flexible polydimethylsiloxane substrates and compare these results to morphologies on hard silica xerogel substrates of variable roughness and surface energy. Controlled incorporation of nanoparticles (NPs) can be used to tune polymer thin film instabilities and morphology. At NP concentrations below a threshold value, we observe directed dewetting of blend thin films consisting of uniformly aligned dewet domains that mimic the periodicity of the confining media, consistent with our previous experiments where it was observed that C_{60} NPs preferentially segregate to a PS/PB blend interface up to a certain saturation concentration.

10:12AM P44.00010 Fiber Formation From the Melting of Free-standing Polystyrene, Ultra-thin Films: A Technique for the Investigation of Thin Film Dynamics, Rheological Properties and Confinement Effects , JEREMY M. RATHFON, University of Massachusetts Amherst, ROBERT W. COHN, University of Louisville, ALFRED J. CROSBY, JONATHAN P. ROTHSTEIN, GREGORY N. TEW, University of Massachusetts Amherst — The processes of fiber formation from the melting of ultra-thin films are explored in high detail and produce a new technique for the investigation of rheological properties, confinement effects, and the dynamics of thin films and polymer chains. Ultra-thin films of polystyrene are suspended atop micro-arrays of pillars. Films are then annealed above the T_g and studied via optical microscopy. Hole nucleation is quantified with a free energy barrier based on a simple capillary model. Holes then grow exponentially in a shear thinning, high shear strain regime. These holes impinge upon each other to form suspended fibers which thin according to a model for elasto-capillary thinning of fluid filaments. Monitoring fiber thinning allows for the acquisition of rheological properties as well as the apparent extensional viscosity. The breakup of the fiber network indicates the effects of confinement on chain entanglements in ultra-thin films. A transition below a critical film thickness, comparable to the dimensions of a polymer chain, shows reduced interchain entanglements and a remarkably faster breakup of fibers.

10:24AM P44.00011 Self-Repair of Polymer Films Through Monomer Filled Ni-Zn Microcapsules , MARCIA PATCHAN, LANCE BAIRD, YO-RHIN RHIM, ERIN LABARRE, ADAM MAISANO, RYAN DEACON, JASON BENKOSKI, JHU Applied Physics Lab — A novel polymer additive composed of isocyanate resin-filled metal microcapsules has been successfully synthesized through a combination of emulsification, interfacial polymerization, and electroless Ni-Zn deposition. The resulting metallic microcapsules impart self-healing and galvanic protection capabilities to off-the-shelf primers. Once scratched, the microcapsules release their contents into the scratch, where they harden and restore the moisture barrier. If healing is incomplete, the Ni-Zn shell acts as a sacrificial anode to galvanically protect the underlying steel. ASTM adhesion, wear resistance, and moisture resistance tests evaluated the ability of microcapsule-filled primers to heal scratches, provide galvanic protection, and prevent corrosion. We found that self- healing was most effective for broad, shallow scratches (3 mm) and narrow scratches (75 μm).

10:36AM P44.00012 Structural Rearrangement of Semifluorinated Diblock copolymer Thin Films Exposed to Selective Solvents , UMESH SHRESTHA, DVORA PERAHIA, Clemson University, STEPHEN CLARSON, University of Cincinnati — A neutron reflectometry study reveals the response of a semifluorinated diblock co-polymer poly trifluoro propyl methyl siloxane -*b*- polystyrene co-polymer thin films of ca. 50-70nm, to selective solvents. This diblock forms surface induced layered structure at volume fractions of the F segment ranging from 0.03 to 0.50. When exposed to toluene, a selective solvent for PS, the film swelled instantaneously, while retaining its layered structure. The solvent however penetrates into both the PS and the semifluorinated layers. In contact with decane vapor, the solvent penetrates predominantly the top fluorinated layers. The rate of penetration increases with increasing volume fraction of the fluorinated segment. In contrast with toluene, the solvent remains at the top layer only for extended periods again retaining the layered structure. The incompatibility and specific affinity of different blocks drive structural rearrangements at the interface as a response to external stimuli, retaining the layers structure.

10:48AM P44.00013 Wetting induced instabilities in miscible polymer blends , NIGEL CLARKE, Durham University, KATHERINE THOMAS, ULLRICH STEINER, ROSA POETES, University of Cambridge, MIHAI MORARIU, DSM — The behaviour of miscible blends of polystyrene (PS)/poly(vinyl methyl ether)(PVME) of varying compositions has been investigated [1] at temperatures where PS and PVME are miscible. The PVME is seen to enrich the polymer-air surface, forming a layer with a width that is comparable to the correlation length. Further heating close to the demixing temperature results in the formation of a capillary instabilities at the polymer surface exhibiting a spinodal-like pattern with a characteristic wavelength that depends on the blend composition. Formation of these instabilities is seen for all blend compositions. We propose that these wetting induced instabilities result from coupled height and composition fluctuations in the PVME enriched surface layer, driving the build-up of long wavelength fluctuations.

[1] Thomas, K.R.; Clarke, N.; Poetes, R.; Morariu, M.; Steiner, U.; Soft Matter, 6, 3517, 2010

Wednesday, March 23, 2011 8:00AM - 11:00AM –
Session P45 DAMOP: Unitary Fermi Gases and the BCS-BEC Crossover A310

8:00AM P45.00001 Universal physics in the dilute Fermi gases[1] , SOON YONG CHANG, MOHIT RANDERIA, NANDINI TRIVEDI, The Ohio State University — Using Quantum Monte Carlo techniques, we investigate universal properties of the repulsive upper branch as well as the superfluid ground state across the Feshbach resonance. We test the Tan relations by computing (a) the equation of state, (b) the short distance behavior of the two-particle density matrix, and (c) the large-k tail of the momentum distribution $n(k)$. We have used twisted boundary conditions to improve the approach to the thermodynamic limit, which allows us to probe $n(k)$ at a dense set of k values. We find consistent estimates of the $1/k_F a$ dependence of the contact C at $T = 0$ from all three methods. We show that, just like the superfluid ground state across the BCS-BEC crossover, the repulsive upper branch also obeys these relations, albeit with different values of C. This reflects the universal behavior of dilute Fermi gases with a short range potential, in contrast to, for instance, the hard sphere gas in the $k_F a \sim 1$ regime.

[1]We acknowledge support from ARO W911NF-08-1-0338 and NSF-DMR 0706203 and the use of computational facilities at the Ohio Supercomputer Center.

8:12AM P45.00002 Thermal distribution and the contact of Fermi gases at large scattering lengths , JOAQUIN DRUT, TIMO LAHDE, Aalto University, TIMOUR TEN, UIC — A few years ago, Tan and others derived a set of exact relations valid for strongly interacting non-relativistic Fermi gases in the regime of short interaction range and large scattering length. Recent developments have shown that a central quantity in these identities, the so-called "contact" C, actually plays a crucial role in the characterization of these systems, as it determines multiple thermodynamic properties as well as linear-response sum rules. However, computing the "contact" presents a challenge as it requires non-perturbative methods such as Quantum Monte Carlo. In this contribution, we present our first results for C as a function of temperature in the limit of infinite scattering length.

8:24AM P45.00003 Investigating the Effect of Density Inhomogenity on Photoemission Spectroscopy , TARA DRAKE, JOHN GAEBLER, RABIN PAUDEL, JILA, University of Colorado, JAYSON STEWART, JILA, University of Colorado, Los Alamos NL, DEBORAH JIN, JILA, University of Colorado — Ultracold atomic gases realize clean and controllable model systems for investigating many-body quantum physics. However, trapped gases are intrinsically spatially inhomogeneous in their density, and in many cases, one would like to compare measurements of these systems with theoretical understanding for a homogeneous gas. In particular, density inhomogeneity can complicate the interpretation of data taken in momentum space, as the original spatial information is lost during time of flight expansion. The effect of density inhomogeneity due to a harmonic trapping potential is studied in a degenerate gas of 40K atoms. Using a method to select only the atoms in the center of the trap, we study how a more homogenous sample changes what can be seen in time of flight experiments, including photoemission spectroscopy.

8:36AM P45.00004 Spectral functions in ultracold Fermi gases[1] , WILLIAM SCHNEIDER, MOHIT RANDERIA, The Ohio State University — We study the fermion spectral function in the superfluid state across the BEC-BCS crossover and in the normal Fermi liquid phase in highly imbalanced Fermi gases. We focus on features that can be measured in momentum-resolved radio frequency spectroscopy experiments. We go beyond mean field theory and include the effects of Gaussian order parameter fluctuations in a manner that gives excellent agreement with asymptotically exact results for the $T = 0$ equation of state in the BEC and BCS limits, as well as quantum Monte Carlo (QMC) results near unitarity. We show that sharp Bogoliubov quasiparticles, with a substantial coherent spectral weight, exist near unitarity. We argue that this is true generally even beyond the Gaussian approximation. In addition, quasiparticle scattering and interaction with collective modes produces incoherent spectral weight. We show that the dispersion is strongly renormalized at unitarity with its minimum shifted up from its mean field value $\sqrt{2m\mu}$ and compare our results with existing QMC data. We discuss how the spectral function changes qualitatively compared with its mean field form as $1/(k_F a)$ increases and the chemical potential changes sign.

[1]Supported by NSF-DMR 0706203 and ARO W911NF-08-1-0338.

8:48AM P45.00005 Short-range correlations and entropy in ultracold atomic Fermi gases , ZHENHUA YU, Physics Department, the Ohio State University, GEORG BRUUN, GORDON BAYM — We relate short-range correlations in ultracold atomic Fermi gases to the entropy of the system over the entire temperature, T, vs. coupling strength, .1/kF a, plane. In the low temperature limit the entropy is dominated by phonon excitations and the correlations increase as T4. In the BEC limit, we calculate a boson model within the Bogoliubov approximation to show explicitly how phonons enhance the fermion correlations. In the high temperature limit, we show from the virial expansion that the correlations decrease as 1/T. By interpolating between the two limits, we predict that the correlations reach a maximum at a finite temperature. We infer the general structure of the isentropes of the Fermi gas in the T,.1/kF a plane, and the temperature dependence of the correlations in the unitary, BEC, and BCS limits. Our results compare well with measurements of the correlations via photoassociation experiments at higher temperatures.

9:00AM P45.00006 Momentum Resolved Radio Frequency Spectroscopy in Trapped Polarized Gases , KATHRYN LEVIN, James Franck Institute and Department of Physics, University of Chicago, CHIH-CHUN CHIEN[1], HAO GUO, James Franck Institute and Department of Physics, University of Chicago — With recent advances in momentum resolved radio frequency (RF) spectroscopy, both experiment and theory, one can consider doing analogous experiments on polarized Fermi gases. In this talk we present predictions for the behavior of the fermionic spectral functions in the majority and minority bands. By truncating the integrated trap contributions at varying radii, the spectral functions will reflect the increase in the local polarization from nearly zero at the center to large values at the edges. We present predictions for these spectral functions and discuss their implications for future experiments.

[1] Stewart, J T et al. Nature 454, 744 (2008)
[2] Chen, Q. and Levin, K. Phys. Rev. Lett. 102, 190402 (2009)
[3] Chen, Q. et al. Rep. Prog. Phys. 72, 122501 (2009)

[1]Los Alamos National Laboratory

9:12AM P45.00007 Observation of shock waves in a unitary Fermi gas , JAMES JOSEPH, Duke University, MANAS KULKARNI, ALEXANDER ABANOV, Stony Brook University, JOHN THOMAS, Duke University — We study the nonlinear hydrodynamics of a strongly interacting (unitary) Fermi gas comprising a 50-50 mixture of the lowest two hyperfine states of ^{6}Li near a broad Feshbach resonance at 834 G. The gas is is cooled via forced evaporation in a cigar-shaped CO_2 laser trap with a repulsive optical sheet potential at the center creating two separate clouds. When the repulsive potential is turned off and the two clouds collide we observe exotic nonlinear hydrodynamics distinguished by the formation of a very sharp and stable density peak at the center of the trap and subsequent evolution into a box-like shape with sharp edges. We attribute these characteristics to shock-wave formation in the unitary gas. By solving the hydrodynamic equations numerically we can reproduce the time dependence of the observed density profiles.

9:24AM P45.00008 Theory of shock waves in a unitary Fermi gas , ALEXANDER ABANOV, Stony Brook University, MANAS KULKARNI, Stony Brook University and Brookhaven National Laboratory, JAMES JOSEPH, JOHN THOMAS, Duke University — We present here evidence of shock wave formation during the collision of two clouds of a unitary Fermi gas. A unitary Fermi gas is an ideal test ground for extreme quantum hydrodynamics. By its very nature the system exhibits universality, i.e., the properties of the gas, constrained by an underlying scale invariance, depend entirely on the density and temperature. The nonlinear hydrodynamics exhibited in this experiment is understood by using a dimensionally reduced quasi- 1D form of the quantum hydrodynamic equations of motion. We found a near perfect agreement with the experiment. The evidence of shock wave formation is a hallmark of nonlinear physics in a universal quantum hydrodynamic system. The hydrodynamic approach works well deep in the nonlinear regime even at low density and for a system far from equilibrium.

9:36AM P45.00009 Finite Size Effects in the BCS-BEC Crossover from Functional Renormalization , MICHAEL SCHERER, Institute for Theoretical Solid State Physics, RWTH Aachen — We apply the functional renormalization group approach to the BCS-BEC crossover for an ultracold gas of fermionic atoms. Formulated in terms of a scale-dependent effective action, the functional RG interpolates continuously between the atomic or molecular microphysics and the macroscopic physics on large length scales. A systematic derivative expansion provides for both a description of the many-body physics and its expected universal features as well as an accurate account of the few-body physics and the associated BEC and BCS limits. Furthermore we put the system into a finite volume and employ periodic boundary conditions to study the effect of a finite size on the few-body scattering physics as well as the critical temperature for the phase transition to superfluidity.

9:48AM P45.00010 Effects of particle-hole channel on the behavior of BCS-BEC crossover[1] , QIJIN CHEN, Zhejiang University — BCS-BEC crossover is effected by increasing pairing strength between fermions from weak to strong. Such pairing is associated primarily with the particle-particle channel. Effects of the particle-hole channel is often dropped. On the other hand, Gor'kov et al argued that the particle-hole channel can cause a substantial reduction in both Tc and the pairing gap. However, this result has largely been neglected until recent years when BCS-BEC crossover has been realized experimentally in ultracold Fermi gases. In this talk, we study the effects of the particle-hole channel on BCS-BEC crossover in a G_0G scheme. While in the BCS limit, such effects may be approximated by a shift in the pairing strength, the situation becomes more complex as the interaction becomes stronger where the gap is no longer very small. References: Q.J. Chen, I. Kosztin, B. Janko, and K. Levin, Phys. Rev. Lett. 81, 4708 (1998); Q.J. Chen, J. Stajic, S.N. Tan, and K. Levin, Physics Reports 412, 1-88 (2005).

[1]Supported by NSF of China and Ministry of Education of China.

10:00AM P45.00011 Microscopic Approach to Viscosities in Superfluid Fermi Gases: From BCS to BEC , PETER SCHERPELZ, HAO GUO, DAN WULIN, James Franck Institute and Department of Physics, University of Chicago, CHIH-CHUN CHIEN, Los Alamos National Laboratory, KATHRYN LEVIN, James Franck Institute and Department of Physics, University of Chicago — We compute the shear viscosity, η, in a BCS-BEC crossover scheme which is demonstrably consistent, via sum rules, with conservation laws. The onset of a normal state pairing gap and the contribution from bosonic (non-condensed pair) degrees of freedom lead to a considerable reduction in the magnitude of these viscosities at general temperatures T. When quantitatively compared with shear viscosity experiments (we independently infer an estimated lifetime from radio frequency data) the agreement is reasonable, as is a comparison of η/s, where s is the trap entropy density. Our fermionic picture is to be contrasted with that of others in the literature which presume that Goldstone bosons are crucial. As in conventional BCS superconductors, we show these Goldstone bosons do not couple to transverse probes such as the shear viscosity. As a result our calculated viscosity at low T becomes arbitrarily small, rather than exhibiting the upturn predicted by others.

10:12AM P45.00012 Triply degenerate quantum mixture of ^{41}K, ^{40}K and ^{6}Li , PEYMAN AHMADI, CHENG-HSUN WU, IBON SANTIAGO, JEE WOO PARK, MARTIN ZWIERLEIN, Massachusetts Institute of Technology — We report the observation of a triply quantum degenerate mixture of ^{41}K, ^{40}K and ^{6}Li atoms. It is demonstrated that bosonic ^{41}K atom is an efficient coolant for sympathetic cooling of fermionic ^{40}K and ^{6}Li atoms. The ^{40}K and ^{6}Li mixture provides access to a strongly correlated Fermi-Fermi mixture allowing us to study superfluidity and Cooper pairing with imbalanced masses. We also present our investigation of ^{41}K and ^{40}K, a Bose-Fermi mixture where a 12 G p-wave resonance and a 40 G s-wave resonance are observed. Negligible differential gravitational sag between ^{41}K and ^{40}K makes these resonances excellent candidates for studying unexplored properties of Bose-Fermi mixtures such as Boson mediated Cooper pairing.

10:24AM P45.00013 The superfluid-insulator transition in disordered Fermi gases near unitarity , SARANG GOPALAKRISHNAN, University of Illinois at Urbana-Champaign — Superfluids, whether composed of weakly interacting fermions (i.e., in the BCS limit) or bosons (i.e., in the BEC limit), undergo quantum phase transitions into an insulating phase in the presence of strong disorder. In the BCS limit, such a transition occurs when the disorder is strong enough to overcome the fermions' kinetic energy; in the BEC limit, it occurs when the disorder is strong enough to overcome the bosons' interaction energy. We address the fate of the disorder-driven superfluid-insulator transition in the intermediate "unitary" regime, discuss the conditions under which the superfluid-insulator phase boundary is non-monotonic in this regime, and investigate the properties of the insulating phase. Our analysis is quantitatively valid at high densities or for narrow Feshbach resonances, but its qualitative implications are expected to hold beyond these regimes; it can also be adapted to show that the superfluid-insulator transition occurs at infinitesimally weak disorder for a unitary Fermi gas in four dimensions.

10:36AM P45.00014 ABSTRACT WITHDRAWN –

10:48AM P45.00015 Population imbalance and pairing in the BCS-BEC crossover of three-component ultracold fermions , TOMOKI OZAWA, GORDON BAYM, University of Illinois at Urbana-Champaign — We investigate the phase diagram and the BCS-BEC crossover of a homogeneous three-component ultracold Fermi gas with a U(3) invariant attractive interaction. We show that the system at sufficiently low temperatures exhibits population imbalance, as well as fermionic pairing. We describe the crossover in this system, connecting the weakly interacting BCS regime of the partially population-imbalanced fermion pairing state and the BEC limit with three weakly interacting species of molecules, including pairing fluctuations within a t-matrix calculation of the particle self-energies.

Wednesday, March 23, 2011 11:15AM - 1:39PM –

Session Q1 DCMP: Gapless Spin Liquids Ballroom A1

11:15AM Q1.00001 Thermal-transport Studies of Quantum Spin Liquids , MINORU YAMASHITA, Department of Physics, Kyoto University — Quantum spins, coupling antiferromagnetically on a 2D triangular lattice, cannot simultaneously satisfy all interactions. This frustrated situation is expected to give rise to mysterious fluid-like states of spins without long- range order, so called quantum spin liquid (QSL). The ground state of QSL and its exotic phenomena, such as fractionalized excitation with an artificial gauge field, have been extensively discussed for decades, yet to be identified by lack of any real materials. This is why the recent discoveries of materials possessing an ideal 2D triangular lattice have spurred a great deal of interest. To understand the nature of QSL, knowledge of the low-lying excitation, particularly the presence/absence of an excitation gap, is of primary importance. We employ thermal transport measurements on newly discovered QSL candidates, κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ and EtMe$_3$Sb[Pd(dmit)$_2$]$_2$, and report that the two organic insulators possess different QSLs characterized by different elementary excitations. In κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ [1], heat transport is thermally activated in low temperatures, suggesting presence of a spin gap in this QSL. In stark contrast, in EtMe$_3$Sb[Pd(dmit)$_2$]$_2$ [2], a sizable temperature-linear term of thermal conductivity is clearly resolved in the zero-temperature limit, showing gapless excitation with long mean free path ($\sim$1,000 lattice distances), analogous to excitations near the Fermi surface in normal metals. These results are consistent with theoretical suggestions including 2D gapless spinons with a Fermi surface. This work was done in collaboration with N. Nakata, Y. Senshu, M. Nagata, Y. Kasahara, S. Fujimoto, T. Shibauchi, Y. Matsuda, T. Sasaki, N. Yoneyama, N. Kobayashi, H. M. Yamamoto and R. Kato.

[1] M. Yamashita *et al.*, Nature Physics **5**, 44- 47 (2009).
[2] M. Yamashita *et al.*, Science **328**, 1246 (2010).

11:51AM Q1.00002 Spin liquids, spin-orbit coupling, and band topology , LEON BALENTS, Kavli Institute of Theoretical Physics — Much of the search for quantum spin liquids has focused on spin-rotationally invariant model Hamiltonians, appropriate for weakly spin-orbit coupled materials. With strong spin-orbit interactions, distinct theoretical approaches are required, and novel spin liquid states may occur. Some such candidate states will be discussed, along with the mechanisms leading to them.

12:27PM Q1.00003 Time-reversal symmetry breaking and spontaneous Hall effect without magnetic dipole order in $Pr_2Ir_2O_7$, SATORU NAKATSUJI, Institute for Solid State Physics, University of Tokyo — An electric current flowing through a conductor in a magnetic field produces a transverse voltage drop known as the Hall effect. In the absence of the field, this effect also appears in ferromagnets in a plane normal to its spontaneous magnetization vector owing to the spin-orbit coupling. Generally, it may also detect a nontrivial order parameter breaking the time-reversal symmetry on a macroscopic scale, for example, scalar spin chirality. In this talk, we present our recent results in the study of the frustrated magnetism and Hall transport of the metallic pyrochlore magnet $Pr_2Ir_2O_7$.[1,2] Strikingly, a spontaneous Hall effect is observed in the absence of both an external magnetic field and conventional magnetic long-range order.[3] This strongly suggests the existence of a chiral spin liquid, a spin-liquid phase breaking the time-reversal symmetry. Both our measurements indicate that spin-ice correlations in the liquid phase lead to a non-coplanar spin texture forming a uniform but hidden order parameter: the spin chirality. Interesting phenomena seen under high field will also be discussed. This is the work performed in collaboration with Y. Machida, Y. Ohta, T. Sakakibara, T. Tayama, Y. Uwatoko (ISSP, Univ. of Tokyo), S. Onoda (Riken, Tokyo), L. Balicas (NHMFL), D. E. MacLaughlin (UC, Riverside) and C. Broholm (JHU).

[1]S. Nakatsuji, Y. Machida, Y. Maeno, T. Tayama, T. Sakakibara, J. v. Duijn, L. Balicas, J. N. Millican, R. T. Macaluso, and Julia Y. Chan, *Phys. Rev. Lett.* **96**, 087204 (2006).

[2]Y. Machida, S. Nakatsuji, Y. Maeno, T. Tayama, T. Sakakibara, and S. Onoda, *Phys. Rev. Lett.* **98**, 057203 (2007).

[3]Y. Machida, S. Nakatsuji, S. Onoda, T. Tayama, and T. Sakakibara, *Nature* **463**, 210 (2010).

1:03PM Q1.00004 Fractional spin textures in the frustrated magnet SCGO , ARNAB SEN, Boston University — Spin liquids are remarkable states of matter that do not order magnetically even at very low temperatures and show collective phenomena like emergent gauge fields and topological order. Impurities can potentially reveal the underlying correlations in such states that appear deceptively featureless in their ground state properties. We consider the archetypal frustrated antiferromagnet $SrCr_{9p}Ga_{12-9p}O_{19}$ (SCGO) in which Ga ions act as non-magnetic impurities in the magnetic lattice composed of Cr^{3+} S=3/2 spins for disordered $p < 1$ samples. We demonstrate that a spin in direct proximity to a pair of vacancies is cloaked by a spatially extended spin texture that encodes the correlations of the parent spin liquid. In this spin liquid regime, our analytic theory predicts that the combined object has a magnetic response identical to a classical spin of length S/2=3/4, which dominates over the small intrinsic susceptibility of the pure system. We calculate the full texture on the lattice in the spin liquid regime and check that it agrees well with Monte-Carlo simulations. This fractional-spin texture leaves an unmistakable imprint on the measured ^{71}Ga nuclear magnetic resonance (NMR) lineshapes, which we compute using Monte-Carlo simulations and compare with experimental data. We also study the long-ranged interactions between these spin textures at low temperatures to gain a better understanding of the case of finite dilution in the parent spin liquid.

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q3 DCMP DMP: The Kavli Foundation Special Symposium: Superconductivity Centennial: Future Research Opportunities Ballroom A3

11:15AM Q3.00001 Superconductivity: A Continuous Surprise or "How I Learned to Love the Surprises" , ROBERT DYNES, University of California, San Diego — When I was invited to give this talk, I thought I would talk about new materials, or new opportunities, or the electron-phonon interaction, or non electron phonon interactions. Then when I looked at the speakers in this symposium and the subjects that they were scheduled to talk about, I realized that they were better equipped to talk individually about each of these subjects than I was, and it was my role to introduce the subject and give a perspective on the future of research and applications in superconductivity. My experience over the past decades has been that it is very dangerous to make predictions in this field. There are many examples of our distinguished colleagues who have engaged in this practice only to be proven wrong by surprise after surprise Fortunately, this has not harmed their reputations or their courage to continue to make predictions. In this talk I will reflect on my personal experience over several decades of research in superconductivity and how my own thinking has changed. Hopefully, I will

1. Transmit a flavor of this field and stimulate other younger investigators to be adventuresome
2. Prepare the audience for the talks that follow
3. Motivate the following speakers to reveal their own predictions and surprises.

11:51AM Q3.00002 Research opportunities in new superconducting materials[1] , L.H. GREENE, University of Illinois at Urbana Champaign — Since the discovery of superconductivity 100 years ago, new superconducting materials have rarely successfully been designed, with almost every new superconductor being discovered serendipitously. Through the years we have developed a variety of guidelines based on observations, but some of these guidelines remain disparate - such as, reduced dimensionality seems to give rise to higher Tc but isotropic materials would be better for applications. It is encouraging to note that this is an area where physicists, chemists, and material scientists seamlessly work together without boundaries, and ideas between groups are exchanged freely. Just as the theory of superconductivity and its development has had a major impact on how we do theoretical physics, our approach, with consilience, in searching for "better" superconductors may change the way we do experimental physics. I will present some of our guidelines and how our approach will help to provide exciting new research opportunities in superconducting materials.

[1]This work was supported by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-AC0298CH1088.

12:27PM Q3.00003 Iron-based superconductors and relevant materials:progress and opportunity[1] , HIDEO HOSONO, Tokyo Institute of Technology — Iron, a representative magnetic element, was believed to the last constituent for emergence of superconductivity because long range magnetic ordering competes with the formation of Cooper pair requisite for superconductivity. However, once LaFeAs(O,F) with Tc=26K was discovered, many iron-pnictide (chalcogenide) superconducting materials have been found and the maximum Tc reached 56K, which is next to the high Tc cuprates exceeding MgB_2. I think there are two significances in discovery of iron-based superconductors. First, we realized that magnetic element is not a hateful enemy but a powerful friend to realize high Tc superconductors. Second it provides a large opportunity to find new high Tc materials because there exist several hundreds of layered compounds containing square lattice of transition metal cations taking tetrahedral coordination with non-oxide anions. We expect materials with higher Tc and/or novel class of superconductors would be hidden among these. To our interest, the crystal structure of 122 is the same as that of a representative heavy fermion superconductor $CeCu_2T_2$(T=Si,Ge). One may expect some clue to bridge these two superconducting systems would be found. What we have not to forget is a historical fact that most of ground-breaking materials including high Tc superconductors have been discovered by serendipity in the course of concentrated exploration effort. I am anticipating new material functions would be discovered as a result of concentrated material exploration with a help of theoretical modeling and advanced characterization. Iron is the most important element led to leap of civilization. I hope iron would serve as the same role in the history of superconductivity. *Strike while the iron is hot*. I think this saying is still true for superconductivity research.

[1]This work was supported by the FIRST program, JSPS.

1:03PM Q3.00004 Exploring electron-phonon interactions in superconductors[1] , MARVIN COHEN, University of California, Berkeley — Superconductors can be roughly assigned to two classes. The first class contains materials in which the electronic pairing induced by electron-phonon interactions is the fundamental mechanism giving rise to the superconductivity. The BCS theory, together with its extensions, explains the properties of these superconductors extremely well . The second class is all other superconductors including the cuprate, Fe based, and heavy Fermion superconductors. Again, electronic pairing appears to be evident, but there is no consensus on the correct underlying theory of the superconducting mechanism at this time. I will discuss calculations for materials in the former class and describe the progress made in explaining and predicting their superconducting properties. I will emphasize calculations of the transition temperature and discuss some suggestions for raising the maximum transition temperature for materials in this class.

[1]This work was supported by National Science Foundation Grant No. DMR10-1006184 and the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

1:39PM Q3.00005 Electronic Pairing Interactions[1] , D.J. SCALAPINO, University of California, Santa Barbara — The heavy fermion, actinide, cuprate, iron-pnictide/chalcogenide and Bechgaard organic salts form a class of superconducting materials which are believed to share an electronic pairing mechanism. While the early electronic pairing interactions which were suggested involved charge fluctuations, it appears that for these materials it is the spin (and orbital) fluctuations that play a central role. Here I will discuss some of what is known about the electronic pairing interaction in this class of materials and conclude with some questions for future research.

[1]Support from the Center for Nanophase Materials Science at ORNL, sponsored by the Division of Scientific User Facilities, U.S. DOE.

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q4 DPOLY DBP: Macromolecular Crowding Effects in the Cytoplasm Ballroom A4

11:15AM Q4.00001 Formation of protein-complexes in crowded environments: from in vitro to in vivo[1] , GIDEON SCHREIBER, Dept Biological Chemistry, the Weizmann Institute of Science — Rates of protein interactions are one to five orders of magnitude slower than the theoretically calculated collision rate of spheres of the same size. The rates can be increased by favorable electrostatic forces between the two proteins. Recent studies have established that the association reaction proceeds through transient complexes, which may be specific or diffusive in nature. To bring binding studies closer to the in vivo environment, we investigated the role of crowding on binding. For crowding we added various polymers to the solution, including Dextran and PEGs of different molecular weights. While crowding enhances oligomerization and polymerization of macromolecules, it has only a small effect on the binding rates and affinities of transient protein-protein interactions. We suggest that the limited effect of crowders, which is much bellow the expected from the increased viscosity of the solutions, is a result of the occluded volume effect in high crowder concentrations. Direct measurements of the stability of the encounter complex shows that crowders slow both k1 and k-1, resulting in an increased half-life of the encounter complex. High crowder concentrations also slow k2, suggesting an increased size of the encounter region. These results fit double-mutant cycle measurements on the activated complex, which suggest an increased size of the fruitful encounter region. These results are in line with the suggested occluded volume effect of crowders. We contrasted these with the effect of crowding on the weak binding pair CyPET-YPET. On this pair, aggregation, and not enhanced dimerization, was detected in PEG solutions. The results suggest that typical crowding agents have only a small effect on specific protein-protein dimerization reactions while promoting aggregation. To further validate these results, we performed real time binding assays in living cells, showing that even in the crowded cellular environment binding can be fast and specific.

[1]This research is supported by the Israel Science Foundation.

11:51AM Q4.00002 Crowding effects on protein association , ARUN YETHIRAJ, University of Wisconsin–Madison — The cell cytoplasm is a dense environment where the presence of inert cosolutes can significantly alter the rates of protein folding and protein association reactions. These crowding effects can either increase or decrease the rates of association reactions (or protein folding) depending on the nature of the crowding agents and the type of reaction. Our work aims to obtain a quantitative understanding of crowding effects. We present the first kinetic study of the effect of hard sphere crowding agents on protein association reactions where reactants and crowding agents are both hard spheres. If every collision results in a reaction, crowding always decreases the reaction rate but if the probability of a reaction is low then crowding increases the reaction rate. We find that the thermodynamics of crowding are relatively insensitive to interactions between the crowding agents suggesting that the hard sphere model of crowding agents has a surprisingly large regime of validity, and should be sufficient for a qualitative understanding of the thermodynamics of crowding effects.

12:27PM Q4.00003 Protein structure, stability and folding in the cell – *in silico* biophysical approaches[1] , MARGARET CHEUNG, University of Houston — How the crowded environment inside a cell affects the structural conformation of a protein with aspherical shape is a vital question because the geometry of proteins and protein-protein complexes are far from globules in vivo. Here we address this question by combining computational and experimental studies of several aspherical proteins (calmodulin, VlsE, and phosphoglycerate kinase) under crowded, cell-like conditions. The results show that macromolecular crowding affects protein folding dynamics, structures and functions. Our work demonstrates the malleability of "native" proteins and implies that crowding-induced shape changes may be important for protein function and malfunction in vivo.

[1]Source of Support: National Science Foundation, Molecular & Cellular Biosciences (MCB0919974).

1:03PM Q4.00004 Phosphoglycerate kinase in crowded and cellular environments , SIMON EBBINGHAUS, Ruhr-University Bochum — We developed the temperature-jump fluorescence microscope to spatio-temporally resolve fast biomolecular kinetics and stability inside a single mammalian cell. We measured the reversible fast folding kinetics as well as folding thermodynamics of a fluorescent phosphoglycerate kinase construct in a bone marrow cell with subcellular resolution. The same instrument was also used to perform the comparative in vitro measurement in dilute buffer and crowded environments. Investigating an ensemble of cells, each cell has its own unique kinetic signature that can differ substantially from the in vitro result. Variations in the cytoplasmic environment are significant modulators of the protein energy landscape. We quantitate these variations with a statistical analysis of multiple cells and compare folding dynamics on the nm length scale with μm length scale diffusion processes. Cytoplasmic energy landscape modulation may be a candidate for non-genetic regulation of proteins but also challenges protein homeostasis.

1:39PM Q4.00005 Crowding and hydrodynamic interactions likely dominate in vivo macromolecular motion , JEFFREY SKOLNICK, Georgia Institute of Technology — To begin to elucidate the principles of intermolecular dynamics in the crowded environment of cells, employing brownian dynamics (BD) simulations, we examined possible mechanism(s) responsible for the great reduction in diffusion constants of macromolecules in vivo from that at infinite dilution. In an Escherichia coli cytoplasm model comprised of 15 different macromolecule types at physiological concentrations, BD simulations of molecular-shaped and equivalent sphere representations were performed with a soft repulsive potential. At cellular concentrations, the calculated diffusion constant of GFP is much larger than experiment, with no significant shape dependence. Next, using the equivalent sphere system, hydrodynamic interactions (HI) were considered. Without adjustable parameters, the in vivo experimental GFP diffusion constant was reproduced. Finally, the effects of nonspecific attractive interactions were examined. The reduction in diffusivity is very sensitive to macromolecular radius with the motion of the largest macromolecules dramatically slowed down; this is not seen if HI dominate. In addition, long-lived clusters involving the largest macromolecules form if attractions dominate, whereas HI give rise to significant, size independent intermolecular dynamic correlations. These qualitative differences provide a testable means of differentiating the importance of HI vs. nonspecific attractive interactions on macromolecular motion in cells.

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q5 FIAP: The Physics of Confronting Weapons of Mass Destruction: Chemical, Biological and Nuclear Ballroom C1

11:15AM Q5.00001 Physics in the Confrontation of Nuclear Weapons , JAMES TOEVS, James W. Toevs Consulting — Had the detonations on 9/11 involved nuclear explosives rather than jet fuel the number of deaths and the costs would have been multiplied by 100 or 1,000. This talk will briefly describe the nuclear threat and then focus on the technologies, both extant and evolving, for the detection and interdiction of clandestine trafficking of nuclear weapons and nuclear and radiological material. The methods vary from passive detection of heat, gamma radiation, neutrons, or other signatures from nuclear material, through radiological approaches to examine contents of vehicles and cargo containers, to active interrogation concepts that are under development. All of these methods have major physics components ranging from simple gamma ray detection as learned in a senior undergraduate lab to the latest ideas in muon production and acceleration.

11:51AM Q5.00002 Discrimination and classification of bio-aerosol particles using optical spectroscopy and scattering , JAY D. EVERSOLE, Naval Research Laboratory — For more than a decade now, there has been significant emphasis for development of sensors of agent aerosols, especially for biological warfare (BW) agents. During this period, the Naval Research Laboratory (NRL) and other labs have explored the application of optical and spectroscopic methods relevant to biological composition discrimination to aerosol particle characterization. I will first briefly attempt to establish the connection between sensor performance metrics which are statistically determined, and aerosol particle measurements through the use of computational models, and also describe the challenge of ambient background characterization that would be needed to establish more reliable and deterministic sensor performance predictions. Greater attention will then be devoted to a discussion of basic particle properties and their measurement. The NRL effort has adopted an approach based on direct measurements on individual particles, principally of elastic scatter and laser-induced fluorescence (LIF), rather than populations of particles. The development of a LIF instrument using two sequential excitation wavelengths to detect fluorescence in discrete spectral bands will be described. Using this instrument, spectral characteristics of particles from a variety of biological materials including BW agent surrogates, as well as other "calibration" particles and some known ambient air constituents will be discussed in terms of the dependence of optical signatures on aerosol particle composition, size and incident laser fluence. Comparison of scattering and emission measurements from particles composed of widely different taxa, as well as from similar species under different growth conditions highlight the difficulties of establishing ground truth for complex biological material compositions. One aspect that is anticipated to provide greater insight to this type of particle classification capability is the development of a fundamental computational model of fluorescent emission for a particle of known composition but arbitrary size and shape. Finally if time permits, I will review the recent development and use of a 40 MHz mode-locked 524 nm laser source to evaluate the utility of sub-picosecond excitation of fluorescence with 2-photon absorption in biological aerosols.

12:27PM Q5.00003 Minimizing the bioterrorist threat: Fear, fancy, folly, and physics , PHILIP WYATT, Wyatt Technology Corporation — There can be little doubt that a bioterrorist attack represents one of the most significant dangers facing the Nation today. It is cheap, relatively easy to use, and can produce huge casualties and significant financial losses. Because of its apparent simplicity, there has been a great amount of attention directed towards developing means for early detection of an attack in progress. Most developmental funding for protective strategies comes from the Federal government: DoD is focused on protecting the military (personnel and facilities) whereas DoHS is most concerned with civilian response (police, triage, epidemiology, cure). Associated with such activities are some pretty amazing ideas both concerning the threat and means to detect its presence. These include the belief that certain bioterrorist attacks could equal the consequences of a nuclear weapon, that crop dusters with the proper agents could wipe out a city, that if it "glows" (i. e. is fluorescent) it must be an agent, or even that gravitational forces are actually far greater than believed. From the early warning side of things, the huge costs associated with a false positive call have resulted in the generally recognized need to identify before any alarm is triggered. Some consequences of this strategy have been the development of so-called smart chips and even handheld mass spectrometers! A brief review of some of these devices and the physics required for their success is discussed. An approach based upon some simple features of inverse scattering theory is proposed whereby identification may be unnecessary.

1:03PM Q5.00004 Physics and National Security: The Spectrum of Opportunities , JAY DAVIS, The Hertz Foundation — Physicists reflexively tend to approach their role in addressing national security problems by reaching for technologies and inventing devices or systems. While this is appropriate, the space for contribution is much larger. The application of technology is frequently constrained by doctrinal, operational, financial, and logistic constraints, not to mention those of security. The speaker, who has played a role in technology development, field operations, advisory processes, and policy considerations will discuss the role physicists can have in definition of the threat space, creation and assessment of technologies needed, and helping with response and recovery. In particular, he will address the opportunities and risks for both academic and industrial physicists in trying to assist in these matters, i.e., when in career to address such problems, what are the obstacles or consequences, and when do you know you have contributed?

1:39PM Q5.00005 Detecting Chemical Weapons: Threats, Requirements, Solutions, and Future Challenges , BRIAN BOSO, Smiths Detection — Although chemicals have been reportedly used as weapons for thousands of years, it was not until 1915 at Ypres, France that an industrial chemical, chlorine, was used in World War I as an offensive weapon in significant quantity, causing mass casualties. From that point until today the development, detection, production and protection from chemical weapons has be an organized endeavor of many of the world's armed forces and in more recent times, non-governmental terrorist organizations. The number of Chemical Warfare Agents (CWAs) has steadily increased as research into more toxic substances continued for most of the 20^{th} century. Today there are over 70 substances including harassing agents like tear gas, incapacitating agents, and lethal agents like blister, blood, chocking, and nerve agents. The requirements for detecting chemical weapons vary depending on the context in which they are encountered and the concept of operation of the organization deploying the detection equipment. The US DoD, for example, has as a requirement, that US forces be able to continue their mission, even in the event of a chemical attack. This places stringent requirements on detection equipment. It must be lightweight (<2 lbs), detect a large array of chemical warfare agents and toxic industrial chemicals, detect and warn at concentration levels and time duration to prevent acute health effects, meet military ruggedness specifications and work over a wide range of temperature and humidity, and have a very high probability of detection with a similarly low probability of false positives. The current technology of choice to meet these stringent requirements is Ion Mobility Spectrometry. Many technologies are capable of detecting chemicals at the trace levels required and have been extensively developed for this application, including, but not limited to: mass spectroscopy, IR spectroscopy, RAMAN spectroscopy, MEMs micro-cantilever sensors, surface acoustic wave sensors, differential mobility spectrometry, and amplifying fluorescence polymers. In the future the requirements for detection equipment will continue to become even more stringent. The continuing increase in the sheer number of threats that will need to be detected, the development of binary agents requiring that even the precursor chemicals be detected, the development of new types of agents unlike any of the current chemistries, and the expansion of the list of toxic industrial chemical will require new techniques with higher specificity and more sensitivity.

Wednesday, March 23, 2011 11:15AM - 2:15PM –
Session Q6 DCOMP: Hydrogen Storage Materials Ballroom C2

11:15AM Q6.00001 First-Principles Prediction of Crystal Structures, Reaction Pathways, and Intermediate Products in Hydrogen Storage Reactions[1] , CHRIS WOLVERTON, Northwestern University — Practical hydrogen storage for mobile applications requires materials that exhibit high hydrogen densities, low decomposition temperatures, and fast kinetics for absorption and desorption. Unfortunately, no reversible materials are currently known that possess all of these attributes. Here we present an overview of our recent efforts aimed at developing a first-principles computational approach to the discovery of novel hydrogen storage materials. We have developed computational tools which enable accurate prediction of decomposition thermodynamics, crystal structures for unknown hydrides, and thermodynamically preferred decomposition pathways. We present examples that illustrate each of these three capabilities. Specifically, we focus on recent work on crystal structure and dehydriding reactions of (i) borohydride materials, such as $Ca(BH_4)_2$ and $Mg(BH_4)_2$, (ii) amidoboranes and their decomposition products, and (iii) mixtures of complex hydrides.

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11:51AM Q6.00002 Towards predictor based design of thermodynamic and kinetic properties of complex materials for hydrogen storage , JENS HUMMELSHOEJ, Technical University of Denmark — A calculational approach for the design of new complex materials for hydrogen storage with favorable thermodynamic stability and enhanced diffusion kinetics is presented. By combining density functional theory (DFT) calculations on stable crystal structures and local coordination models with database methods, we perform large-scale screening studies to determine a number of potential alloys/mixtures with favorable thermodynamic stabilities and identify simple descriptors for subsequent materials prediction. Predictors for the kinetic properties of the materials are derived from combining materials screening with path techniques and harmonic transition state theory (TST) to indentify materials parameters, e.g. the hydrogen binding energy, which correlate with the macroscopic diffusion rates. These predictors are then used to design new alloy/mixture compositions and ratios to favor structures with optimal diffusion kinetics. We present results from binary and ternary alkali-transition metal borohydrides and Perovskite based hydrogen permeable membranes, as well as results from studies of binary and mixed metal ammines. Results from the modeling of pathways and rates of dynamical processes involved in the ab-/desorption mechanisms will also be presented and compared to quasi elastic neutron scattering data.

12:27PM Q6.00003 Theory of molecular hydrogen sorption for hydrogen storage[1] , SHENGBAI ZHANG, Department of Physics, Applied Physics and Astronomy, Rensselaer Polytechnic Institute — Molecular hydrogen (H_2) sorption has the advantage of fast kinetics and high reversibility. However, the binding strength is often too weak to be operative at near room temperatures. Research into such hydrogen sorption materials has branched into the study of pure van der Waals (vdW) physisorption and that of weak chemisorption (known to exist in the so-called Kubas complexes). In either case, however, theoretical tools to describe such weak interactions are underdeveloped with error bars that often exceed the strength of the interaction itself. We have used quantum-chemistry (QC) based approaches to benchmark the various available DFT methods for four classes of weak chemisorption systems [Sun et al., Phys. Rev. B **82**, 073401 (2010)]. These involve complexes containing Li, Ca, Sc, and Ti with increased strength of H_2 binding from predominantly vdW to mostly Kubas-like. The study reveals that most of the DFT functionals within the generalized gradient approximation underestimate the binding energy, oppose to overestimating it. The functionals that are easy to use yet yielding results reasonably close to those of accurate QC are the PBE and PW91. I will also discuss the effort of implementing vdW interaction into the currently available density functional methods [Sun, J. Chem. Phys. **129**, 154102 (2008)]. The rationale is that while the true vdW is an electron-electron correlation, a DFT plus classical dispersion approach may be too simple and unnecessary within the DFT. A local pseudopotential approach has been developed to account for the core part of the polarizability of the elements. Applications to a number of benchmark systems yield good agreement with QC calculations. The application of this method and the QC methods to vdW hydrogen binding will also be discussed.

[1]Work supported by DOE/BES and DOE/EERE Hydrogen Sorption Center of Excellence under RPI subcontracts No. J30546/J90336.

1:03PM Q6.00004 Point-defect-mediated dehydrogenation of alane[1] , LARS ISMER, University of California, Santa Barbara — For the engineering of better hydrogen storage materials a systematic understanding of their hydrogen sorption kinetics is crucial. Theoretical studies on metal hydrides have indicated that in many cases point defects control mass transport and hence hydrogen uptake and release. Manipulating point-defect concentrations thus allows control over hydrogen sorption kinetics, opening up new engineering strategies. However, in some cases the relevance of kinetic limitations due to point defects is still under debate; kinetic inhibition of hydrogen sorption has also been attributed to surface effects, e.g. oxide layers or low recombination rates. We present a systematic analysis of the dehydrogenation kinetics of alane (AlH3), one of the prime candidate materials for hydrogen storage. Using hybrid-density functional calculations we determine the concentrations and mobilities of point defects and their complexes. Kinetic Monte Carlo simulations are used to describe the full dehydrogenation reaction. We show that under dehydrogenation conditions charged hydrogen vacancy defects form in the crystal, which have a strong tendency towards clustering. The vacancy clusters denote local nuclei of Al phase, and the growth of these nuclei eventually drives the AlH3/Al transformation. However, the low concentration of vacancy defects limits the transport of hydrogen across the bulk, and hence acts as the rate-limiting part of the process. The dehydrogenation is therefore essentially inactive at room temperature, explaining why AlH3 is metastable for years, even though it is thermodynamically unstable. Our derived activation energy and dehydrogenation curves are in excellent agreement with the experimental data, providing evidence for the relevance of bulk point-defect kinetics.

[1]Work performed in collaboration with A. Janotti and C. G. Van de Walle, and supported by DOE.

1:39PM Q6.00005 Kinetics of hydrogen transport in metal hydrides, crystalline alloys, and amorphous metals , DAVID SHOLL, Georgia Tech — The diffusion of hydrogen is critical in the kinetics of hydrogen uptake and release in metal hydrides and in membrane-based approaches to hydrogen purification. First principles calculations have become a valuable counterpart to experimental methods to study hydrogen diffusion. Examples will be presented of using first principles calculations to understand hydrogen diffusion in a diverse range of solid materials, including metal hydrides in their bulk state and near interfaces, crystalline alloys for membrane applications, and amorphous metals for membrane applications.

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q7 DBP DCP: System Biology III: The Physics of Evolution Ballroom C3

11:15AM Q7.00001 Does Tumor Development Follow a Programmed Path?[1] , ROBERT AUSTIN, Princeton University — The initiation and progression of a tumor is a complex process, resembling the growth of a embryo in terms of the stages of development and increasing differentiation and somatic evolution of constituent cells in the community of cells that constitute the tumor. Typically we view cancer cells as rogue individuals violating the rules of the games played within an organism, but I would suggest that what we see is a programmed and algorithmic process. I will then question If tumor progression is dominated by the random acquisition of successive survival traits, or by a systematic and sequential unpacking of "weapons" from a pre-adapted "toolkit" of genetic and epigenetic potentialities? Can we then address this hypothesis by data mining solid tumors layer by layer?

[1]Support of the NSF and the NCI is gratefully acknowledged.

11:51AM Q7.00002 Adaptation Driven by Spatial Heterogeneities[1] , RUTGER HERMSEN, Center for Theoretical Biological Physics, University of California, San Diego, CA, USA — Biological evolution and ecology are intimately linked, because the reproductive success or "fitness" of an organism depends crucially on its ecosystem. Yet, most models of evolution (or population genetics) consider homogeneous, fixed-size populations subjected to a constant selection pressure. To move one step beyond such "mean field" descriptions, we discuss stochastic models of evolution driven by spatial heterogeneity. We imagine a population whose range is limited by a spatially varying environmental parameter, such as a temperature or the concentration of an antibiotic drug. Individuals in the population replicate, die and migrate stochastically. Also, by mutation, they can adapt to the environmental stress and expand their range. This way, adaptation and niche expansion go hand in hand. This mode of evolution is qualitatively different from the usual notion of a population climbing a fitness gradient. We analytically calculate the rate of adaptation by solving a first passage time problem. Interestingly, the joint effects of reproduction, death, mutation and migration result in two distinct parameter regimes depending on the relative time scales of mutation and migration. We argue that the proposed scenario may be relevant for the rapid evolution of antibiotic resistance.

[1]This work was supported by the Center for Theoretical Biological Physics sponsored by the National Science Foundation (NSF) (Grant PHY-0822283).

12:27PM Q7.00003 Experimental Ignition of Evolution on Fitness Landscapes , KRISTELLE ROBIN, Institute for Advanced Studies, HKUST — Microbiologist are starting to revise the single cell centered view of evolution to a multicellular view, considering it at entire population scale, and even whole ecosystem. Indeed, as Darwin recognized on the Galapagos Island, evolution of a community of bacteria is strongly influenced by the global spatial stress and depends of the neighboring communities. This collective dynamical process can be studied using micro-nanofabricated landscape to create stressed conditions. Our microfluidic device consists of interconnected chambers in 2D hexagonal geometries. The design of our ecology enables to combine gradients of antibiotic and nutrient, thus generating population gradient and motion of bacteria across them. We study here evolution of resistance to the antibiotic ciprofloxacin in highly-stressed conditions. Non-random mutations are induced in the collectivity to develop resistance to the antibiotic. Channels between microhabitats allow motion of bacteria between different islands, and once evolution is ignited in a local metapopulation, a very fast spread through the collectivity happens. In such environments, evolution is observed in typical time scales of few hours. Knowing the complexity of natural world, we believe that our approach provide a model to understand the rapid emergence of resistance to antibiotic and its spread in the entire population.

1:03PM Q7.00004 Towards a Quantitative Endogenous Network Theory of Cancer Genesis and Progression: beyond "cancer as diseases of genome"[1] , PING AO, Shanghai Jiaotong University — There has been a tremendous progress in cancer research. However, it appears the current dominant cancer research framework of regarding cancer as diseases of genome leads impasse. Naturally questions have been asked that whether it is possible to develop alternative frameworks such that they can connect both to mutations and other genetic/genomic effects and to environmental factors. Furthermore, such framework can be made quantitative and with predictions experimentally testable. In this talk, I will present a positive answer to this calling. I will explain on our construction of endogenous network theory based on molecular-cellular agencies as dynamical variable. Such cancer theory explicitly demonstrates a profound connection to many fundamental concepts in physics, as such stochastic non-equilibrium processes, "energy" landscape, metastability, etc. It suggests that neneath cancer's daunting complexity may lie a simplicity that gives grounds for hope. The rationales behind such theory, its predictions, and its initial experimental verifications will be presented.

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[1]Supported by USA NIH and China NSF.

1:39PM Q7.00005 Understanding the distribution of fitness effects of mutations by a biophysical-organismal approach , SHIMON BERSHTEIN, Harvard University — The distribution of fitness effects of mutations is central to many questions in evolutionary biology. However, it remains poorly understood, primarily due to the fact that a fundamental connection that exists between the fitness of organisms and molecular properties of proteins encoded by their genomes is largely overlooked by traditional research approaches. Past efforts to breach this gap followed the "evolution first" paradigm, whereby populations were subjected to selection under certain conditions, and mutations which emerged in adapted populations were analyzed using genomic approaches. The results obtained in the framework of this approach, while often useful, are not easily interpretable because mutations get fixed due to a convolution of multiple causes. We have undertaken a conceptually opposite strategy: Mutations with known biophysical and biochemical effects on E. coli's essential proteins (based on computational analysis and in vitro measurements) were introduced into the organism's chromosome and the resulted fitness effects were monitored. Studying the distribution of fitness effects of such fully controlled replacements revealed a very complex fitness landscape, where impact of the microscopic properties of the mutated proteins (folding, stability, and function) is modulated on a macroscopic, whole genome level. Furthermore, the magnitude of the cellular response to the introduced mutations seems to depend on the thermodynamic status of the mutant.

Wednesday, March 23, 2011 11:15AM - 2:15PM –
Session Q8 GMAG: New Developments in Organic Spintronics Ballroom C4

11:15AM Q8.00001 Spin Injection/detection using organic-based magnetic semiconductor , ART EPSTEIN, Ohio State University — This abstract not available.

11:51AM Q8.00002 Magnetic Field Effect in Organic Devices: the Role of Hyperfine, Exchange and Spin Orbit Interactions , EITAN EHRENFREUND, Physics Dept., Technion-Israel Institute of Technology — Recently we have observed a novel phenomenon in both magneto-electroluminescence (MEL) and magneto-conductance (MC) in a variety of organic light emitting diodes that consists of a sign reversal at very small magnetic fields ($B \leq$1 mT), dubbed hereafter ultra-small magnetic field effect (USMFE) [1]. Similar response has been obtained in MC(B) of unipolar organic diodes [2]. As B is reduced below the zero crossing field, the magnitude of the obtained MEL and MC increases to a maximum value at $B = B_m$, before diminishing at B=0. We found that B_m is isotope dependent: it is lower when the protons in the organic material are replaced by deuterons having a smaller nuclear magnetic moment and reduced hyperfine interaction (HFI), and is higher when the ^{12}C atoms (nuclear spin I=0, no HFI) are replaced by ^{13}C atoms (I=$1/2$, with finite HFI). We also found that B_m scales with the half width at half maximum, ΔB, of the high field response. From the MEL(B) and MC(B) responses, the marked isotope effect, and voltage and temperature dependencies we explain the USMFE as well as the width ΔB, as due to loosely coupled pairs of polarons (either with same or opposite charges) of which spins are intermixed via the HFI [1,2]. The model captures the sign reversal and its dependence on the HFI strength. The role of the HFI anisotropy, exchange interaction between the polaron pair spins, and spin orbit interaction effect on the USMFE will be discussed. *Supported by the Israel Science Foundation grant 745/08, and NSF grant DMR 08-03325. **In collaboration with T. D. Nguyen, B. R. Gautam, and Z. V. Vardeny, University of Utah.

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12:27PM Q8.00003 Molcular spntronics: tailoring spin polarization with molecules , PIERRE SENEOR, Unite Mixte de Physique CNRS/thales — Organic/molecular spintronics is a rising research field at the frontier between spintronics and organic chemistry. Organic molecules and semiconductors were first seen as promising for spintronics devices due to the expected long spin lifetime. An exciting challenge is now to find opportunities arising from chemistry to develop new spintronics functionalities that were unavailable with inorganic materials. Here one can hope to control the spin dependent transport by using the chemical versatility brought by molecules and molecular engineering. Starting from the use of Alq3 and Phthalocyanine molecules we will show how the ferromagnetic metal/molecule hybridization can strongly influence the interfacial spin properties: from spin polarization enhancement to its sign control. CNRS/Thales team: C. Barraud, P. Seneor, R. Mattana, S. Tatay, K. Bouzehouane, S. Fusil, C. Deranlot, F. Petroff, A. Fert in collaboration with ISMN, Bologna, Italy & IPCMS, Strasbourg, France

1:03PM Q8.00004 Spin relaxation in organic semiconductors , PETER BOBBERT, Technische Universiteit Eindhoven — Intriguing magnetic field effects in organic semiconductor devices have been reported: anomalous magnetoresistance in organic spin valves and large effects of small magnetic fields on the current and luminescence of organic light-emitting diodes. Influences of isotopic substitution on these effects points at the role of hyperfine coupling. We performed studies of spin relaxation in organic semiconductors based on (i) coherent spin precession of the electron spin in an effective magnetic field consisting of a random hyperfine field and an applied magnetic field and (ii) incoherent hopping of charges. These ingredients are incorporated in a stochastic Liouville equation for the dynamics of the spin density matrix of single charges as well as pairs of charges. For single charges we find a spin diffusion length that depends on the magnetic field, explaining anomalous magnetoresistance in organic spin valves. For pairs of charges we show that the magnetic field influences formation of singlet bipolarons, in the case of like charges, and singlet and triplet excitons, in the case of opposite charges. We can reproduce different line shapes of reported magnetic field effects, including recently found effects at ultra-small fields.

1:39PM Q8.00005 Coherent spin spectroscopy in organic thin film semiconductor devices[1] , CHRISTOPH BOEHME, University of Utah, Department of Physics and Astronomy — With the emergence of organic spintronics and renewed interest in magnetoresistive effects, there is much need to illuminate the properties of spins in molecular electronic materials. Examples include spin-relaxation times, spectral diffusion times, spin dephasing times and spin interactions. In this presentation, an overview is given about the concepts of pulsed, electrically and optically detected magnetic resonance spectroscopy as techniques to manipulate and observe and thus characterize these fundamental properties of electron and nuclear spins in organic semiconductors [1]. By coherent (pulsed) magnetic resonant perturbation of spin states one may cause the spins to coherently propagate in a defined manner [2]. Spin-dependent charge carrier-transport or -recombination allow the observation of this coherent spin motion through electrical or optical measurements in working devices, such as organic light-emitting diodes. The ubiquitous presence of hydrogen nuclei gives rise to strong hyperfine interactions, which appear to provide the basis for many of the magnetoresistive effects observed in these materials. Since hyperfine coupling influences resonantly driven quantum spin beating in electrically or optically detectable electron-hole pairs, an extraordinarily sensitive probe for hyperfine fields in such pairs is given [3]. This allows scrutinizing the various existing models for these electronic processes. Qualitative as much as quantitative insights are gained into some of the physical intricacies of organic semiconductor device fabrication such as the influence of contact materials on spin-orbit coupling.

[1] D. R. McCamey, et al. Nature Mat. 7, 723, (2008).
[2] C. Boehme et al. Phys. Stat. Sol B. 246, 11-12, 2750 (2009).
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[1]Acknowledgment is made to the US Department of Energy, Office of Science (grant #DESC0000909) and the National Science Foundation (grant #0953225).

Wednesday, March 23, 2011 11:15AM - 2:03PM –
Session Q9 DFD: Fluid Dynamics at Interfaces D220

11:15AM Q9.00001 Slosh dynamics and rebound suppression of a partially filled sphere , TAYLOR KILLIAN, Brigham Young University Dept. Mathematics, ROBERT KLAUS, TADD TRUSCOTT, Brigham Young University Dept. Mechanical Engineering — We introduce a study on the slosh dynamics of a partially filled elastic sphere. Currently the physical design of fluid-filled containers utilizes clever construction and machinery to mitigate sloshing motions. There are numerous cases that have been observed but we focus on the impact of a sphere under free fall with an initially undisturbed free surface. The study focuses on measurement and simulation of the force distribution between the fluid and the sphere through the use of high-speed imaging and finite element analysis. Using the cavity shape data, a potential flow numerical model is developed that predicts the unsteady forces. Our hypothesis is that the sphere's movements can be counteracted or cancelled by the exchange of energy between the sphere and the fluid. Forces are modulated by the formation of a parabolic cavity in the fluid, formed after the first impact. The second impact results in a collapse of this cavity forming a powerful jet which effectively dampens the motion of the sphere.

11:27AM Q9.00002 Shrinking Instabilities of Toroidal Liquid Droplets in The Stokes Flow Regime , ZHENWEI YAO, MARK BOWICK, Syracuse University — We analyze the stability and dynamics of toroidal liquid droplets. In addition to the Rayleigh instabilities akin to those of a cylindrical droplet there is a shrinking instability that is unique to the topology of the torus and dominates in the limit that the aspect ratio is near one (fat tori). We first find an analytic expression for the pressure distribution inside the droplet. We then determine the velocity field in the bulk fluid, in the Stokes flow regime, by solving the biharmonic equation for the stream function. The flow pattern in the external fluid is analyzed qualitatively by exploiting symmetries. This elucidates the detailed nature of the shrinking mode and the swelling of the cross-section following from incompressibility. Finally the shrinking rate of fat toroidal droplets is derived by energy conservation.

11:39AM Q9.00003 Normal elasticity of liquid bridge by atomic force microscope[1] , BONGSU KIM, WONHO JHE, Seoul National University, CENTER FOR NANO-LIQUID TEAM — The quartz tuning-fork based atomic force microscope (QTF-AFM) has previousely been established as a suitable measurement technique for investigating liquid bridges. By operating a QTF-AFM in the non-contact tapping mode, we are able to measure the normal elasticity of liquid bridges that are formed via capillary condensation or that result from an adsorbed liquid layer. Elasticity, a property typically associated with solids, is studied here for the case of the nano-scale water bridge. We present results that add to our understanding of the origin of the elasticity in nano liquid bridges.

[1]Work supported by Korean Ministry of Science and Technology.

11:51AM Q9.00004 Droplet impact and the dynamics of rapidly moving contact lines , SHMUEL M. RUBINSTEIN, JOHN M. KOLINSKI, Harvard University , SHREYAS MANDRE, Brown University , LAKSHMINARAYANAN MAHADEVAN, DAVID A. WEITZ, Harvard University — When a liquid drop approaches a flat solid surface, the air beneath it is compressed, flattening the bottom of the drop and forcing initial contact to occur in a ring-shape, trapping a pocket of air in its center as two wetting fronts rapidly expand both outward and inwards to completely wet the surface. We combine total internal reflection (TIR) microscopy with a novel virtual frame technique (VFT) to directly observe the sub-micron length scales above a solid surface as the drop approaches, impacts and then spreads over it.

12:03PM Q9.00005 Interfacial Effects on Droplet Dynamics in Poiseuille Flow , JONATHAN SCHWALBE, KENDRA ERK, National Institute of Standards and Technology, JEFFREY MARTIN, Unilever, PETIA VLAHOVSKA, Brown University, STEVEN HUDSON, National Institute of Standards and Technology — Interfacial rheology governs many properties of emulsions, and here we report theory and experiments that account for and measure surface viscous and elastic forces. For the theoretical portion, Stokes flow is assumed in bulk phases and a jump in hydrodynamic stress at the interface is balanced by Marangoni and surface viscous forces according to the Boussinesq-Scriven constitutive law. Our model employs linear equation of state for the surfactant. Our analysis predicts slip, cross-stream migration and droplet-circulation velocities for a spherical drop in plane Poiseuille flow. These results and the corresponding interfacial parameters are separable: e.g., cross- stream migration occurs only if surfactant is present; slip velocity depends on viscosity contrast and dilatational Boussinesq number, but not shear Boussinesq number. Drop dynamics in plan Poiseuille flow are measured experimentally using microfluidics, particle velocimetry, and shape analysis. Several types of surfactant-stabilized aqueous drops in oil are examined and the interfacial properties depend on interfacial composition.

12:15PM Q9.00006 ABSTRACT WITHDRAWN –

12:27PM Q9.00007 Nonequilibrium molecular dynamics of vapor–liquid interface , TAKERU YANO, Osaka University, Japan — Evaporation and condensation at a vapor–liquid interface are studied by moderately large-scale nonequilibrium molecular dynamics simulations for a vapor–liquid two phase system composed of about 0.3 million Lennard-Jones molecules. Constant evaporation and condensation are realized by driving two vapor regions on the either side of a planar liquid film, and thereby the simulation is free from artificial controls of molecular motions in the liquid film and in the neighborhood of the interfaces. This enables us to evaluate the mass, momentum, and energy fluxes across the system, which are relevant to the velocity distribution of molecules leaving the interface at the vapor–liquid nonequilibrium states.

12:39PM Q9.00008 Evaporation out of a 2D model soil , BERTRAND SELVA, REMI DREYFUS, Complex Assemblies of Soft Matter, CNRS-Rhodia-UPenn UMI 3254, Bristol, Pennsylvania 19007, USA — Our goal is to improve our understanding of water transport in the soil-plant-atmosphere continuum. For this purpose, we focus on water losses due to evaporation at the soil surface. Such losses are known to be important at places where plants do not entirely cover the surface. Our model soil is a 2D porous medium with controlled wettability and humidity. It has been reported that evaporation is characterized by three stages: a first stage with a strong and constant evaporation flux, a second stage where mass transfer is dominated by diffusion mechanisms, and a third stage that occurs when the medium is almost empty. Here we focus on the first two stages and the transition between them which occurs when an intermediate unsaturated zone has reached its maximum width. This width strongly depends on the wettability distribution of the porous medium. In our experiments, we have explored a regime where gravity effects and capillary forces have similar contributions. In this particular regime we found that the first stage is characterized by a continuously decreasing evaporation flux and the second stage by usual diffusion transfer mechanisms. In order to understand this behavior, we have developed a model which allows us to predict the transition between the two stages and which is in agreement with the decreasing values of the first stage evaporation flux.

12:51PM Q9.00009 Effects of Sub-Phase Thickness on Interfacial Microrheology , PAUL CHRISTOPHEL MARTIN, KENNETH W. DESMOND, ERIC R. WEEKS, Emory University — The interface between two fluids is known to have a rheological response. In our work, we study human serum albumin protein molecules (HSA) at an air-water interface. Prior experimental work showed that the ratio of the surface viscosity to the sub-phase "bulk" viscosity influences the rheology of the HSA interface. Recent theoretical work has shown that the thickness of the sub-phase h can also influence the rheology of the interface. The finite thickness of the sub-phase only becomes important once h is on the order of the ratio of the surface viscosity to the sub-phase "bulk" viscosity, which is on the order of 100 microns for an HSA-air-water interface. To characterize the interfacial rheology, we suspend tracer particles at the interface, measure their correlated motions, and investigate how the results depend on h for water layers O(100 microns) thick.

1:03PM Q9.00010 Probing single- and multi-phase flow at the pore level , SUJIT DATTA, Department of Physics, Harvard University, AMBER KRUMMEL, Department of Chemistry, Colorado State University, DAVID WEITZ, Department of Physics, Harvard University — We use a new experimental technique to study 3D flow behavior in a porous medium in situ with high spatiotemporal resolution. At the multi-pore level, we probe the fluid configurations resulting from two-phase flow conditions imposed upon the system and correlate these to bulk flow measurements.

1:15PM Q9.00011 Viscous flow and heat transfer in channels with structured walls , VLADIMIR AJAEV, Southern Methodist University, STEFFEN HARDT, PETER STEPHAN, Center of Smart Interfaces, TU Darmstadt — We develop a mathematical model of pressure-driven flow in channels with walls structured by arrays of parallel grooves filled with air or gas. Motivated by cooling applications, we study heat transfer from a heater embedded in the wall to the liquid. The flow in the liquid is described using a Stokes flow model, and thermocapillary effects due to presence of the liquid-gas interface segments in the grooves are also taken into account. The rate of heat transfer is determined by a competition of two physical effects: the insulating effect of the gas in the grooves, due to small thermal conductivity of the gas phase, and the reduction of the effective slip length at the channel wall due to the presence of the liquid-gas interface segments in the grooves. Criteria for heat transfer enhancement are formulated for different parameters of the structuring.

1:27PM Q9.00012 Utilizing an Automated Home-Built Surface Plasmon Resonance Apparatus to Investigate How Water Interacts with a Hydrophobic Surface , ADELE POYNOR, Allegheny College — By definition hydrophobic substances hate water. Water placed on a hydrophobic surface will form a drop in order to minimize its contact area. What happens when water is forced into contact with a hydrophobic surface? One theory is that an ultra-thin low- density region forms near the surface. We have employed an automated home-built Surface Plasmon Resonance (SPR) apparatus to investigate this boundary.

1:39PM Q9.00013 Quantification of slip at a liquid-solid interface – a novel approach[1] , ALEKS PONJAVIC, MOURAD CHENNAOUI, JANET WONG, Imperial College — Much effort has been spent recently on experimentally proving the existence of interfacial slip of a Newtonian fluid. A constant limitation is the proximity to the surface at which the velocity of a fluid can be measured. A new technique is developed to maximise this proximity. The objective is to acquire velocity measurements of a fluid as close as possible to the liquid-solid interface while still using a direct method of observation. To ensure proximity to the surface the technique of photobleaching is adopted. Dye-doped water is pumped through a microfluidic channel. A short, intense pulse from a laser causes dye within the focal volume to bleach, creating a spot. The geometry of this spot evolves depending on the velocity profile of the fluid. By fitting the evolution of the spot with a Poiseuille velocity profile with slip the slip length is extracted. The hydrophobicity of the channel is varied by flowing silane through the channel prior to measurement, forming a self-assembled monolayer. Effects of shear rate and wettability on interfacial slip length are investigated.

[1]This research is supported by an EPSRC grant.

1:51PM Q9.00014 Effects of Interfacial Translation-rotation Coupling for Confined Ferrofluids[1] , ANGBO FANG, Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay Road, Kowloon, Hong Kong — Ferrofluids have wide applications ranging from semiconductor fabrications to biomedical processes. The hydrodynamic spin diffusion theory for ferrofluids has been successful in explaining many experimental data, but it suffers from some fatal flaws. For example, it fails to predict the incorrect flow direction for a ferrofluid confined in a concentric cylinder channel in the presence of a rotating magnetic field. In this work we develop a method to establish the general hydrodynamic boundary conditions (BCs) for micro-polar fluids such as ferrofluids. Through a dynamic generalization of the mesoscopic diffuse interface model, we are able to obtain the surface dissipation functional, in which the interfacial translation-rotation coupling plays a significant role. The generalized hydrodynamic BCs can be obtained straightforwardly by using Onsager's variational approach. The resulted velocity profile and other quantities compares well with the experimental data, strikingly different from traditional theories. The methodology can be applied to study the hydrodynamic behavior of other structured fluids in confined channels or multi-phase flows.

[1]The work is supported by a research award made by the King Abdullah University of Science and Technology.

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q10 DCMP: Chemisorption and Surface Reactions D221

11:15AM Q10.00001 Catalytic Reactions of DNT and TNT Molecules on Porphyrin Complexes

, KEITH WARNICK, BIN WANG, Vanderbilt University, SOKRATES PANTELIDES, Vanderbilt University, Oak Ridge National Laboratory — Reactions of molecules with substrates can be used to identify them, as in sensor applications. Here we examine reactions of DNT and TNT molecules on porphyrin and metal-porphyrin via first-principles DFT calculations. We find that the oxidation of DNT by O_2 using Fe-porphyrin as a catalyst is exothermic. The affinity of O_2 to Fe-porphyrin weakens the O_2 intramolecular bond, which lowers the oxidation reaction barrier is lowered by $\sim$1 eV. Substrate effects on this process are accounted for. One way to use this selective oxidation reaction for DNT/TNT sensor applications is to exploit the metal-semiconductor transition in thin-film VO_2 to detect the energy deposited by the exothermic reaction between the adsorbed molecules. This work was supported in part by DTRA grant HDTRA1-10-0047.

11:27AM Q10.00002 Reactivity of TiO_2 Rutile and Anatase Surfaces toward Nitroaromatics

, SHAO-CHUN LI, ULRIKE DIEBOLD[1], Department of Physics and Engineering physics, Tulane University, New Orleans, LA 70118, USA — The Au-TiO_2 system is a promising catalyst for the synthesis of nitro-aromatic compounds. The adsorption of azobenzene (C_6H_5N-NH_5C_6) and aniline ($C_6H_5NH_2$) on two single-crystalline TiO_2 surfaces, anatase (101) and rutile (110), has been investigated with scanning tunneling microscopy (STM), low energy electron diffraction (LEED), and X-ray photoemission spectroscopy (XPS), and synchrotron Ultraviolet photoemission (UPS). While azobenzene adsorbs as an intact molecule at low coverages, ordered overlayers of phenyl imide (C_6H_5N) form at saturation coverage, indicating that TiO_2 surfaces cleave the N-N bond even without the presence of Au. The same superstructures, p(1 $\times$ 2) on anatase and c(2 $\times$ 2) on rutile and the same electronic structures, form upon adsorption of aniline, suggesting the formation of the same, or a very similar, reaction intermediate. These results suggest that the main role of the supported Au in catalytic aniline $\leftrightarrow$ azobenzene conversion is the activation of O_2/H_2 for de/hydrogenation reactions.

[1]Institute of Applied Physics, Vienna University of Technology, Wiedner Hauptstrasse 8-10, Vienna, Austria

11:39AM Q10.00003 The role of subsurface oxygen in the selectivity enhancement of ethylene epoxidation on Ag-Cu Catalysts

, NGOC LINH NGUYEN, STEFANO DE GIRONCOLI, International School for Advanced Studies (SISSA), via Bonomea 265 Trieste Italy, SIMONE PICCININ, CNR-IOM, DEMOCRITOS National Simulation Center, Theory@Elettra Group, Trieste, Italy — The role of subsurface oxygen on the Ag-Cu alloy catalysts for the ethylene epoxidation reaction has been studied by means of first principles Density Functional Theory (DFT) calculations. We find that in presence of oxygen and ethylene reactants, the subsurface oxygen adsorption is energetically favorable on fcc sites under the thin oxide-like CuO layer formed at the catalyst surface. On this substrate the reaction proceeds via the formation of a common oxametallacycle precursor. The calculated activation energies show favorable energetics for the pathway leading to the formation of the desired product, ethylene oxide, with respect to the one leading to the formation of the undesired product, acetaldehyde, while the opposite order is obtained on pure Ag catalyst. These findings provide an understanding, at the atomistic level, of the selectivity enhancement of Ag-Cu alloy with respect to pure Ag catalysts. Furthermore, we find that under temperature and partial pressure conditions close to the experimental ones, the ethylenedioxy intermediate is present on the phase diagram of Ag-Cu (111) surface. Our calculations indicate, however, that the formation of this structure could poison the catalyst surface.

11:51AM Q10.00004 Surface defects activate new reaction paths: formation of formate during methanol oxidation on defective Ru(0001)

, I. PALACIO, O. RODRÍGUEZ DE LA FUENTE, Complutense University Madrid-SPAIN — An optimum understanding of the existing molecular mechanisms taking place while reactions occur on surfaces, should preferably be based on a correct identification of the intermediate species and the reaction paths, so to avoid trial-and-error approaches. Otherwise, a good control of the chemical activity is not easily attainable. We have adsorbed methanol on Ru(0001), with surfaces having a variable density of defects. In this way, with Auger Electron Spectroscopy (AES), Low Energy Electron Diffraction (LEED) and Infrared Reflection-Absorption Spectroscopy (IRAS) we have identified reaction paths in the methanol/Ru(0001) system. While the sole methanol adsorption leads to its complete dehydrogenation towards CO, we show that oxygen coadsorption stabilizes intermediate products, namely methoxy (CH_3O), formaldehyde (CH_2O) and formyl (CHO). We show as well that a new reaction path appears just on the defective surface: the formation of formate (HCOO). The presence of the defects (mainly steps) catalyzes the oxidation of formaldehyde to formate. This particular case shows how surface defects profoundly affect the catalytic activity, opening new reaction channels which are not available when the density of defects is low.

12:03PM Q10.00005 Dynamics of Low-Energy Electron Induced Reactions in Condensed

, MICHAEL BOYER, CHANMYAEMYAE SOE, KRISTAL CHAMBERLAIN, YOMAY SHYUR, CHRISTOPHER ARUMAINAYAGAM, Wellesley College — We present insights into the dynamics of low-energy electron-induced reactions in thin films of methanol (CH_3OH). Low-energy electrons in matter can initiate chemical reactions though electron impact ionization of a molecule, electron impact excitation of a molecule, or through dissociation of a transient negative ion formed by electron attachment to a molecule. Our studies focus on the dynamics by which low-energy electron interaction with condensed methanol initiates chemical reactions which lead to the formation of methoxymethanol (CH_3OCH_2OH) and ethylene glycol ($HOCH_2CH_2OH$). The results of our post-irradiation temperature programmed desorption experiments indicate that both products can form from irradiating methanol with electrons at subionization energies. In addition, we find evidence that dissociative electron attachment plays a role in the formation of methoxymethanol but not in ethylene glycol.

12:15PM Q10.00006 X-ray Induced Reorganization/Polymerization of Resorcinol on the TiO_2 Rutile (110) Surface

, VINOD KUMAR PALIWAL[1], SHAO-CHUN LI, ULRIKE DIEBOLD[2], Department of Physics and Engineering Physics, Tulane University, New Orleans, LA 70118, USA. — The room-temperature adsorption of resorcinol (1, 3 benzenediol, $C_6H_4(OH)_2$) on the (110) surface of rutile TiO_2 was investigated with STM and x-ray photoemission (XPS). The saturation coverage of resorcinol is smaller as compared to catechol (1,2 benzenediol) with a C1s/Ti2$p_{3/2}$ ratio of $\sim$ 7.3% and 12%, respectively. This indicates that resorcinol occupies on average more than two Ti sites on the surface. STM suggests that resorcinol molecules are mobile at lower coverage, whereas a weakly-ordered overlayer with a periodicity of 3 unit-cells along [001] is observed at higher coverages. Interestingly, exposure of resorcinol-saturated TiO_2 surface to an XPS Mg-Kα beam (1253.6 eV) induces a reorganization of adsorbed resorcinol molecules. STM shows well-resolved double chains that run across [001]-oriented rows of TiO_2(110) surface. These results suggest that irradiation induces a polymerization reaction of adsorbed resorcinol molecules, where neighboring aromatic rings are arranged in a zig-zag configuration.

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[2]Institute of Applied Physics, Vienna University of Technology, Wiedner Hauptstrasse 8-10, Vienna, Austria.

12:27PM Q10.00007 Propane-1,3-diol Adsorption and Dissociation on Rutile TiO_2(110): A Scanning Tunneling Microscopy Study , ZHENRONG ZHANG, Department of Physics, Baylor University, XIAO LIN, BRUCE KAY, ZDENEK DOHNÁLEK, Chemical and Materials Sciences Division, Fundamental and Computational Sciences Directorate, Pacific Northwest National Laboratory — Titanium Dioxide (TiO_2) has attracted great attention in the past decades due to its importance in heterogeneous catalysis. Here the adsorption and dissociation of Propane-1,3-diol molecules on partially reduced rutile TiO_2(110) surfaces are studied via variable temperature scanning tunneling microscopy (VT-STM). STM images of TiO_2(110) surfaces obtained before and after *in-situ* doses of melecules at room temperature show that the molecules preferentially bind in bridge-bonded oxygen vancanies (BBO_V's) *via* one O-H bond scission. The dynamics of Propane-1,3-diol molecules motion has been investigated at room and elevated temperatures. Propane-1,3-diol molecules swing on TiO_2 surface with one end (-CH_2-O^-) anchored on vacancies. Strong interaction of the other end (-O-H) with Ti_{5c} reduces the swing rate when compared with octanol.

12:39PM Q10.00008 First-Principles Studies of Electric Field Effects in Heterogeneous Catalysis: NH_3on Ru(0001) , AARON SISTO, Department of Mechanical Engineering, Purdue University, West Lafayette, IN 47906, ALEXEY ZAYAK, JEFFREY NEATON, Molecular Foundry, LBNL, Berkeley, CA 94720 — The catalytic dissociation of NH_3 has been the focus of recent studies due to the prospect of efficient hydrogen storage and generation. The effects of a static electric field on the surface electronic structure and energy barriers of reactions are examined using density functional theory calculations with gradient corrections. It is found that the interaction strength between the adsorbate and surface can be tuned based on the magnitude and polarity of the field, as evidenced by a field-induced shift of the d-electron band. Correspondingly, energy barriers along minimum energy pathways for desorption and dissociation reactions are significantly affected by the change in substrate-adsorbate interaction. It is concluded that the application of an electric field enhances the catalytic performance of Ru through increased activity and selectivity of NH_3 dissociation. We acknowledge support from DOE, DOE CSGF Fellowship. Computational resources provided by NERSC.

12:51PM Q10.00009 Adsorption and dissociation of molecular oxygen on α-Pu (020) surface: A density functional study[1] , JIANGUANG WANG, ASOK RAY, University of Texas at Arlington — Molecular and dissociative oxygen adsorption on the (020) surface of α-Pu have been studied using the full-potential linearized augmented-plane-wave plus local orbitals (FP-LAPW+lo) basis method. Four adsorption sites and three approaches of O_2 molecule have been considered. Adsorption energies have been optimized according to the distance of the adsorbates from the Pu surface as well as the oxygen dimer bond length. Dissociative adsorption is found for two horizontal approaches (O_2 is parallel to the surface and parallel/perpendicular to a lattice vector) and to be more energetically favorable at the scalar and "fully" relativistic (NSOC vs. SOC) levels of theory. Hor2 approach on the top site was the preferred adsorption site among all cases studied here. Molecular adsorption occurs at the Vert (O_2 is vertical to the surface) approach. The work functions, net spin magnetic moments, and charge transfer are also calculated.

[1]This work is partially supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525) and by the Department of Energy.

1:03PM Q10.00010 ABSTRACT WITHDRAWN –

1:15PM Q10.00011 Structure and Adsorption on Hydrated Alumina Surfaces , VINCENZO LORDI, PATRICK HUANG, ERIC SCHWEGLER, Lawrence Livermore National Lab — Understanding the mechanisms of adsorption of chemical agents on environmental materials under different atmospheric conditions is important for applications in environmental remediation, industrial catalysis, and protection against chemical warfare. In this work, we study molecular adsorption of the chemical agent simulant dimethyl-methylphoshonate (DMMP) on various alumina surfaces, using density functional theory-based molecular dynamics simulations. Both alpha and gamma alumina surfaces of different orientations (and thus surface terminations/reconstructions) are studied, under both wet and dry conditions. Adsorption from the gas phase onto dry and hydroxylated surfaces is compared to adsorption from an aqueous layer in the limit of a fully bulk-like liquid water layer. Interfacial structure and dynamics are directly compared to previous synchrotron X-ray scattering and sum-frequency vibrational spectroscopy experiments, from which specific contributions of different surface functional groups are identified and resolved. Differences in site reactivity on the various surfaces are also compared. Prepared by LLNL under Contract DE-AC52-07NA27344.

1:27PM Q10.00012 Ag/Al_2O_3/FeAl(110): Electronic structure and NO_2 adsorption , MATTHEW PATTERSON, Department of Physics and Astronomy, Louisiana State University, ORHAN KIZILKAYA, Center for Advanced Microstructures and Devices, Louisiana State University, RICHARD KURTZ, PHILLIP SPRUNGER, Department of Physics and Astronomy and Center for Advanced Microstructures and Devices, Louisiana State University — Ag/Al_2O_3 systems are widely studied as catalysts in the selective catalytic reduction of NO_x with hydrocarbons. The exact nature of the active sites and the role of the Ag clusters in such reactions is still not fully understood. In this study, we characterize thermally evaporated Ag clusters on the ultrathin alumina film produced by oxidizing FeAl(110). ARPES demonstrates the evolution of Ag cluster electronic structure and morphology with increasing Ag coverage. Changes in electronic binding energy distinguish charged from metallic clusters. Vibrational EELS of NO_2 adsorbed on the Ag/Al_2O_3/FeAl(110) system elucidates the nature of the NO_x binding site and the changes in the surface chemistry both as a function of Ag cluster size and NO_x adsorption temperature.

1:39PM Q10.00013 Neutron and Thermodynamic Studies of Hydrogen on Pd Decorated Metal Oxides , PAIGE LANDRY, University of Tennessee, A. RAMIREZ-CUESTA, ISIS, E. CRUZ SILVIA, B. SUMPTER, Oak Ridge National Lab, J.Z. LARESE, University of Tennessee — We report our investigations of thermodynamic, inelastic and quasielastic neutron scattering (INS and QENS) studies of H2 adsorbed on bare and Pd decorated metal oxide (MO) surfaces, specifically ZnO, SBA-15 silica, and alumina. Guided by our volumetric adsorption measurements, we used INS and QENS to probe the dynamics of the adsorbed hydrogen molecules. These measurements provide insight into how the microscopic behavior of hydrogen is changed when it is confined at interfaces or interacts with a Pd catalyst. Using INS, the motion of the adsorbed hydrogen are examined as a function of surface adsorbate composition. For rotational motion we use the ortho-to-para transition as a guide and find that the rotational barrier for H2 adsorbed on some of these MO surfaces shift to lower energy (relative to bulk H2). For comparison, the hydrogen adsorption and microscopic behavior when the MO are decorated with 1% Pd metal will be discussed. Evidence for the presence of adsorbed H2, Zn hydroxide and the potential role of spillover will be discussed. This work was partially supported by the U.S. DOE, BES under contract No. DE-AC05-00OR22725 with ORNL managed and operated by UT-Battelle, LLC, the NSF under grant DMR-0412231 and a grant from the University of Tennessee, JINS.

1:51PM Q10.00014 Atomistic Mechanism of Surface Oxide Formation on Pt(111) , ZHENGZHENG CHEN, CHAO WU, Department of Chemical and Biomolecular Egineering, University of Notre Dame, WILLIAM SCHNEIDER, Department of Chemical and Biomolecular Egineering, Department of Chemistry and Biochemistry, University of Notre Dame — A detailed understanding of the interaction of oxygen with Pt surfaces is essential for understanding its catalytic activity and deactivation in oxidizing environments. Here we analyze the transition between metallic and oxidized Pt surfaces. Using first-principles calculations, we characterize the chain-like oxide reconstruction on the Pt(111) surface associated with O coverage $>$50%. We describe the sensitivity of the reconstruction energy to the occupancy of adjacent fcc and hcp sites and present a phenomenological model that relates the reconstruction to the balance between elastic strain energy and screening of O-O repulsions. Core level shift calculations indicate the reconstruction generates two O states with different binding energies and reactivity. Finally, we analyze the thermodynamic stability and equilibrium states of the reconstruction a cluster expansion model. The results are important in developing models of oxidation catalysis on Pt (111) surface.

2:03PM Q10.00015 Tuning Semiconductor Band Edge Energies via Surface Ligand Passivation[1] , SHENYUAN YANG, DAVID PRENDERGAST, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory — Semiconductor band gaps and band edge energies are key parameters that can dictate the efficiency of photocatalysis in solar energy conversion applications. CdSe is a representative semiconducting system with an ideal band gap for solar photon absorption, but with band edge energies that are not positioned for efficient water splitting. Using first-principles calculations within density functional theory, we present a study of the electronic structure of passivated CdSe surfaces and nanostructures, exploring the ability to tune band edge energies in this system via chemisorbed ligands. We predict substantial shifts in band edge energies that are electrostatic in origin, and due to the induced dipole at the CdSe-ligand interface and the intrinsic dipole of the ligand. We further show that, by changing the size and orientation of the ligand's intrinsic dipole moment via novel functionalization strategies, we can control the magnitude and direction of the shifts of CdSe energy levels. The effect of ligands on energy levels of two-dimensional CdSe surfaces and nanocrystal surfaces are thoroughly discussed.

[1]Partially supported by the DOE Helios SERC and under U.S. DOE contract DE-AC02-05CH11231. Computational support from NERSC.

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q11 FIAP: Fractional Quantum Hall Effect II D222

11:15AM Q11.00001 Unexpected Roles for Spin Degrees of Freedom in Competing Phases of the Second Landau Level[1] , TREVOR D. RHONE, J. YAN, U. WURSTBAUER, Columbia University, Y. GALLAIS, Université de Paris 7, A. PINCZUK, Columbia University, L. PFEIFFER, K. WEST, Princeton University, PINCZUK GROUP TEAM — Competing liquid and solid ground states as well as intriguing quantum Hall fluids such as that at ν=5/2 create great current interest in the N=1 Landau level. The spin degrees of freedom in quantum phases of the 2nd Landau level is probed by resonant light scattering. The long wavelength spin wave mode, which monitors the degree of spin polarization, is at the Zeeman energy in the spin polarized state at ν=3. At lower filling factors the intensity of the Zeeman mode collapses indicating loss of spin polarization. At filling factors slightly lower the intensity of the spin wave attenuates and a broad continuum of low-lying excitations emerges - sharp and broad modes coexist. While the coexistence of spectral features has not been explained, the observation could manifest the presence of mixed quantum phases and some loss of spin polarization. A continuum of low-lying excitations emerges that dominates near ν=8/3 and ν=5/2. Resonant Rayleigh scattering reveals that the quantum fluids away from ν=3 break up into robust domains. It is conceivable that these domains could comprise both spin polarized and depolarized quantum fluids. While the state at ν=5/2 is considered to be polarized, these results reveal unprecedented roles for spin.

[1]Work supported by NSF and DOE.

11:27AM Q11.00002 Electron teleportation via Majorana Bound States in a Mesoscopic Superconductor , LIANG FU, Harvard University — Majorana fermions are non-Abelian anyons in 5/2 fractional quantum Hall states and superconductors, which can store quantum information in an inherently nonlocal way. We describe a phase-coherent electron transport phenomena through two spatially separated Majorana bound states in a mesoscopic superconductor. This striking nonlocal effect arises from the interplay between topological order, superconducting order parameter and mesoscopic effects. We discuss its implications for experimental detection of Majorana fermions and topological quantum computation. Ref: Liang Fu, Phys. Rev. Lett. 104, 056402

11:39AM Q11.00003 Entanglement Entropy as a Function of the Aspect Ratio in the First and Second Landau Level , BARRY FRIEDMAN, CURTIS BALUSEK, DARWIN LUNA, Physics Department, Sam Houston State University — Entanglement entropy as a function of aspect ratio has been studied by direct diagonalization in the first and second Landau levels. The torus geometry is used and spin polarized electrons interact via long range Coulomb interaction . As previously noted by Haque et al. (N J Phys 12, 2010 075004), in the first Landau level there is very smooth behavior as a function of aspect ratio making it possible to obtain the topological entanglement entropy. In the second Landau level, the entanglement entropy is much less regular, with possible signatures of quantum phase transitions.

11:51AM Q11.00004 The phase diagram and particle-hole asymmetry of the reentrant integer quantum Hall states of the second Landau level , A. KUMAR, M.J. MANFRA, Department of Physics, Purdue University, L.N. PFEIFFER, K. W. WEST, Princeton University, G.A. CSATHY, Department of Physics, Purdue University — The second Landau level of a two-dimensional electron gas reveals a rich set of competing ground states. Besides an increasing number of fractional quantum Hall states, there are also eight reentrant integer quantum Hall states observed. These reentrant integer states are currently not understood, although they are believed to be collective insulators akin to the field induced Wigner solid with one or more electrons per site. These states are strongly affected by tilt in magnetic field and carrier density but surprisingly there is very limited data on their temperature dependence. We present a detailed study of the melting of the reentrant integer quantum Hall states of the second Landau level from which we extract the phase diagram in the temperature versus filling factor plane. We find that the melting temperatures of the various reentrant integer states violate the particle-hole symmetry. We also report that as the temperature is lowered the magnetoresistance deviates from an activated dependence.

12:03PM Q11.00005 The even denominator fractional quantum Hall states at large Landau level mixing , NODAR SAMKHARADZE, MICHAEL MANFRA, GABOR CSATHY, Purdue University, LOREN PFEIFFER, KEN WEST, Princeton University — We present a study of the energy gaps of the even denominator fractional quantum Hall states of the second Landau level in a two-dimensional electron gas with a record low density of n = 8.2x10^{10} cm^{-2}. These measurements are motivated by the expectation that Landau level mixing present in samples of low densities breaks the degeneracy of the Pfaffian and its particle-hole conjugate anti-Pfaffian. Cooling the electron gas in our Helium-3 immersion cell to 5mK reveals at filling factor 5/2 a fully quantized Hall plateau and a vanishingly small magnetoresistance. Because of the low density of our sample, the 5/2 fractional state is observed at the highest degree of Landau level mixing reported to date. We have measured the energy gaps of the 5/2 and 7/2 fractional quantum Hall states. The intrinsic gap deduced in the limit of no disorder will be compared to previously reported values for samples with higher densities.

12:15PM Q11.00006 Nonconventional odd denominator fractional quantum Hall states in the second Landau level , GABOR CSATHY, ASHWANI KUMAR, MICHAEL MANFRA, Purdue University, LOREN PFEIFFER, KEN WEST, Princeton University — The odd denominator fractional quantum Hall states in the second Landau level of a two-dimensional electron gas are believed to be different from those of the lowest Landau level. While at first sight these states could be part of the composite fermion hierarchy, several recent theoretical works suggest that some might be supporting generalized Pfaffian-like correlations. Recent progress in cooling electrons allowed us to observe a new fractional quantum Hall state at the filling factor 2+6/13. By assuming that the effective mass of the composite fermions does not explicitly depend on the Landau level index we find that energy gaps of the prominent 2+1/3 and 2+2/3 states are consistent with the values predicted by the free composite fermion model. However, the weaker 2+2/5 and 2+6/13 states deviate significantly from the prediction of this model. This deviation constitutes a first demonstration of the nonconventional nature of the latter two odd denominator fractional quantum Hall states.

12:27PM Q11.00007 Tunneling experiments in the lowest Landau level[1] , C. DILLARD, XI LIN, M.A. KASTNER, MIT, L.N. PFEIFFER, K.W. WEST, Princeton University — Recently, a quasiparticle-tunneling experiment on the 5/2 state [1] led to the unintentional discovery of a process we term annealing. In this experiment top gates are used to bring counter-propagating edge states close enough together for tunneling to occur. By keeping the quantum point contact (QPC) top gates energized for a few days at 4 Kelvin, one can create equal electron densities in the QPC region and the bulk of a GaAs heterostructure. This is a great advantage for studying quasiparticle tunneling in QPCs. Conditions under which annealing has proved effective are presented. In addition, in order to better understand and control quasiparticle tunneling in QPCs, further tunneling experiments have been performed in the lowest Landau level.

[1] Iuliana P. Radu, J. B. Miller, C. M. Marcus, M. A. Kastner, L. N. Pfeiffer, and K. W. West, Science 320, 899 (2008).

[1]This work is supported by NSF under grant number DMR-0701386.

12:39PM Q11.00008 Haldane Statistics in the Finite Size Entanglement Spectra of Laughlin States , MARIA HERMANNS, ANUSHYA CHANDRAN, Princeton University, NICOLAS REGNAULT, ENS Paris, BOGDAN ANDREI BERNEVIG, Princeton University — We conjecture that the counting of the levels in the orbital entanglement spectra (OES) of finite-sized Laughlin Fractional Quantum Hall (FQH) droplets at filling $1/m$ is described by the Haldane statistics of particles in a box of finite size. This principle explains the observed deviations of the OES counting from the edge-mode conformal field theory counting and directly provides us with a topological number of the FQH states inaccessible in the thermodynamic limit- the boson compactification radius. It also suggests that the entanglement gap in the Coulomb spectrum in the conformal limit protects a universal quantity- the statistics of the state.

12:51PM Q11.00009 Polarized Fractional Quantum Hall States at 1/3 and 5/2 Filling: a Density-Matrix Renormalization Group Calculation , JIZE ZHAO, DONNA SHENG, Department of Physics and Astronomy, California State University, Northridge, California 91330, USA, F. DUNCAN M. HALDANE, Department of Physics, Princeton University, Princeton, NJ 08544 — In this talk, the density-matrix renormalization group method is employed to investigate the fractional quantum Hall effect (FQHE) at filling numbers $\nu = 1/3$ and $5/2$. We present benchmark results for both filling numbers for larger system sizes to show the accuracy as well as the capacity of our numerical algorithm. Furthermore, we demonstrate that by keeping a large number of states, one can also obtain reliable entanglement spectrum at $\nu = 5/2$, which characterizes the topological properties of FQHE states. Based on a finite-size scaling analysis, we also confirm that the entanglement gap defined by Li and Haldane for $\nu = 5/2$ state with Coulomb interaction remains finite in the thermodynamic limit.

1:03PM Q11.00010 Paired composite fermion wavefunctions for excitations at 5/2 , SREEJITH GANESH JAYA, The Pennsylvania State University, CSABA TOKE, Institute of Physics, University of Pecs, Hungary, ARKADIUSZ WOJS, Institute of Physics, Wroclaw University of Technology, JAINENDRA JAIN, The Pennsylvania State University — The Pfaffian wave function, which is thought to be relevant for the ground state at filling fraction $\frac{5}{2}$, represents a paired state of composite fermions. It can be expressed as an antisymmetrized bilayer (331) wave function. This formulation can be extended to construct wave functions for neutral as well as charged excitations of the Pfaffian. The space spanned by the quasihole excitations exactly matches that of the previously known quasihole wave functions. By comparison to exact results with up to 14 particles, we find that our neutral excitations and also the quasiparticle excitations describe well the actual excitations of the model three body interaction for which the Pfaffian ground state wave function is exact. The relevance to the solutions of the second Landau level Coulomb interaction is less conclusive. Also, the counting of states on the quasihole and quasiparticle sides is significantly different. Relation of our wave functions to other ansatz wave functions in the literature will be discussed.

1:15PM Q11.00011 Suppression of Interlayer Phase Coherence by Gauge Fluctuations in Bilayer Composite Fermi Liquids , ROBERT CIPRI, YAFIS BARLAS, N.E. BONESTEEL, Dept. of Physics and NHMFL, Florida State University — The ν =1/2+1/2 bilayer quantum Hall system exhibits at least two phases as a function of layer spacing, d. For $d/l \gg 1$, (l is magnetic length), the system decouples into two $\nu = 1/2$ composite fermion (CF) liquids. For d/l sufficiently small, the system enters an incompressible bilayer quantum Hall state. Recently, Alicea et al. [1] have proposed a state which might exist for intermediate layer spacing ($d \sim l$). In this "interlayer phase coherent" state, CFs tunnel coherently between layers forming well-defined bonding and antibonding Fermi seas, though there is no actual tunneling of physical electrons. Here we show that scattering from gauge fields in the CF liquids leads to strong layer-dependent fluctuations in the Aharonov-Bohm phases seen by CFs which suppress interlayer phase coherence. This suppression appears as a singular contribution to the correlation energy which inhibits any T=0 phase transition into an interlayer phase coherent state, and drives any such transition first order. Work supported by US DOE.

[1] J. Alicea, O.I. Motrunich, G. Refael, M.P.A. Fisher, PRL 103, 256403 (2009).

1:27PM Q11.00012 Pinning mode of 2D electron system with short-range alloy disorder , B.H. MOON, B.A. MAGILL, L.W. ENGEL, NHMFL/FSU, D.C. TSUI, L.N. PFEIFFER, K.W. WEST, Princeton University — At the low Landau filling (ν) termination of the fractional quantum Hall effect (FQHE) series, a two-dimensional electron system (2DES) becomes an insulator, which is identified in sufficiently low-disorder samples as a form of pinned Wigner solid. The microwave conductivity spectrum of such a solid shows a striking resonance, which is understood as a pinning mode, in which pieces of solid oscillate within the disorder potential. We report on the observation of the pinning mode of a 2DES that resides within $Al_xGa_{1-x}As$ with x=0.85%. For a carrier density of n= 8.7 x10^{10} /cm^2, a resonance with a peak frequency (f_{pk}) of about 5 GHz appears as ν goes below the 2/3 FQHE. A local minimum in resonance amplitude vs. ν occurs around ν =1/2. We will discuss the contribution of the alloy disorder to f_{pk}.

1:39PM Q11.00013 Properties of the Composite Fermion Wigner Crystal , ALEX ARCHER, JAINENDRA JAIN, The Pennsylvania State University — In two dimensional electron systems at small filling factor the ground state is a Wigner crystal. Wigner crystals can also be observed for systems near integer fillings, where electrons or holes in the partially filled Landau Level form a Wigner crystal. Recent experimental evidence (PRL 105, 126803 (2010)) suggests that a Wigner crystal of composite fermions forms near the filling factor of $v = \frac{1}{3}$. Motivated by these results, we calculate the shear modulus of the composite fermion Wigner crystal in the vicinity of several fillings of the form $v = \frac{1}{3}, \frac{2}{5}, \frac{3}{7}$, following the procedure of Maki-Zotos, using the effective two-body real space interactions between composite fermions calculated by Lee, Scarola, and Jain. We discuss the differences from the electron Wigner crystal, and also the experimental implications of our results.

1:51PM Q11.00014 Fabry-Perot Interferometry in the Integer and Fractional Quantum Hall Regimes[1] , DOUGLAS MCCLURE, WILLY CHANG, ANGELA KOU, CHARLES MARCUS, Harvard University, LOREN PFEIFFER, KEN WEST, Princeton University — We present measurements of electronic Fabry-Perot interferometers in the integer and fractional quantum Hall regimes. Two classes of resistance oscillations may be seen as a function of magnetic field and gate voltage, as we have previously reported. In small interferometers in the integer regime, oscillations of the type associated with Coulomb interaction are ubiquitous, while those consistent with single-particle Aharonov-Bohm interference are seen to co-exist in some configurations. The amplitude scaling of both types with temperature and device size is consistent with a theoretical model. Oscillations are further observed in the fractional quantum Hall regime. Here the dependence of the period on the filling factors in the constrictions and bulk of the interferometer can shed light on the effective charge of the interfering quasiparticles, but care is needed to distinguish these oscillations from those associated with integer quantum Hall states.

[1]We acknowledge funding from Microsoft Project Q and IBM.

2:03PM Q11.00015 Topological screening and interference of fractionally charged quasi-particles , IVAN LEVKIVSKYI, University of Geneva, JUERG FROEHLICH, ETH Zurich, EUGENE SUKHORUKOV, University of Geneva — Interference of fractionally charged quasi-particles is expected to lead to Aharonov-Bohm oscillations with periods larger than the flux quantum Φ_0. However, according to the Byers-Yang theorem, observables of an electronic system are invariant under insertion of a quantum of singular flux. We resolve this paradox by considering a *microscopic* model of an electronic interferometer made from quantum Hall edges at filling factor $\nu = 1/m$. An approximate ground state of such an interferometer is described by a Laughlin type wave function, and low-energy excitations are incompressible deformations of this state. We construct a low-energy effective theory by projecting the state space onto the space of such deformations. Amplitudes of quasi-particle tunneling in this theory are found to be insensitive to the singular flux. This behavior is a consequence of *topological screening* of the flux by the quantum Hall liquid. We describe strong coupling of the edges to Ohmic contacts and the resulting quasi-particle current through the interferometer with the help of a master equation. As a function of the singular magnetic flux, the current oscillates with the period Φ_0. These oscillations are suppressed with increasing system size. When the magnetic flux is varied with a modulation gate, current oscillations have the quasi-particle period $m\Phi_0$ and survive in the thermodynamic limit.

Wednesday, March 23, 2011 11:15AM - 1:51PM –

Session Q12 DMP: Focus Session: Dopants and Defects in Semiconductors: Conducting Oxides

D223/224

11:15AM Q12.00001 Transparent Conductors: Understanding and Optimization[1] , JULIA MEDVEDEVA, Missouri University of Science and Technology — The unique combination of two mutually exclusive properties – optical transparency and electrical conductivity – is known to be a prerogative of only a few oxides of post-transition metals, namely, In_2O_3, ZnO, CdO and SnO_2. Advances in theoretical understanding of the underlying physical phenomena in conventional transparent conducting oxides (TCOs) and rapid development of the technologies for which TCO is a vital component, stimulate further research aimed at (i) broadening the range of the electronic and optical properties of application-specific transparent conductive materials in a controllable way; (ii) improving the functional capabilities and efficiency of TCOs in a device; and (iii) designing novel materials as a viable, inexpensive alternative to conventional TCOs. Here, we employ first-principles density-functional approach to investigate the structural, electronic and optical properties of several classes of transparent conductors including conventional single-cation main-group oxides, multi-component binary and ternary oxides, as well as several non-oxide materials. Systematic comparative investigations allow us to determine the role of the crystal structure, chemical composition and carrier generation mechanisms on the resulting optical and electronic properties and predict ways to optimize the properties.

[1]Supported by NSF grant DMR-0705626

11:51AM Q12.00002 Origins of superior symmetrical doping ability of monoclinic BiVO4 , YANFA YAN, WAN-JIAN YIN, SU-HUAI WEI, MOWAFAK AL-JASSIM, JOHN TURNER, National Renewable Energy Laboratory — Application of semiconductors for functional devices depends critically on their dopability. However, there are strong doping bottlenecks for wide-band-gap semiconductors – symmetrical doping is usually difficult, which severely restrict their potential applications. Here, we report superior symmetrical doping properties, i.e., n-type and p-type, of monoclinic $BiVO_4$ by first-principles density-functional theory calculation. Our results reveal that without external doping, $BiVO_4$ with moderate n-type and p-type conductivities can be obtained. However, doping of Sr, Ca, Na, and K atoms under oxygen-rich growth conditions can lead to outstanding p-type conductivity, whereas doping of Mo and W under oxygen-poor growth conditions can result in excellent n-type conductivity. We find that Bi 6s state is responsible for the good p-type doping and the presence of V 3d state is responsible for the good n-type doping. Furthermore, the Bi $6s$ and V $3d$ states are also responsible for producing very dispersive valence and conduction band edges, leading to small electron and hole effective masses. The superior symmetrical doping properties and high carrier mobility make $BiVO_4$ a promising candidate for electronic and optoelectronic device applications.

12:03PM Q12.00003 Donors and H impurities in SnO_2 studied by IR spectroscopy[1] , FIGEN BEKISLI, MICHAEL STAVOLA, W. BEALL FOWLER, Lehigh Univ, LYNN BOATNER, Oak Ridge National Lab, ERIK SPAHR, GUNTER LUEPKE, College of William and Mary — Theory predicts that SnO_2 is an attractive wide band gap candidate for achieving p-type conductivity. Interstitial H and H_O are suggested to be shallow donors in SnO_2 [1-3]. We have studied the properties of H in SnO_2 single crystals. An O-H line is observed at 3261 cm^{-1} that is polarized perpendicular to the c direction along with weaker features at 3258 and 3272 cm^{-1}. When D is introduced into SnO_2 by annealing in a D_2 ambient at 700 °C, a variety of new O-H and O-D lines is produced along with the low-frequency absorption that is characteristic of free carriers. To probe the relationship between H and the free carriers it introduces, we have examined the thermal stabilities of the O-H and O-D lines and their relationship to the thermal stability of the free-carrier absorption.

[1] A.K. Singh *et al.*, Phys. Rev. Lett. **101**, 055502 (2008).
[2] J.B. Varley *et al.,* Phys. Rev. B **79**, 245206 (2009).
[3] W.M. Hlaing Oo *et al.*, Phys. Rev. B **82**, 193201 (2010).

[1]Supported by NSF grant DMR-0802278.

12:15PM Q12.00004 ABSTRACT WITHDRAWN –

12:27PM Q12.00005 Asymmetric Cation stoichiometry in Spinels : Site occupancy in Co_2ZnO_4 and Rh_2ZnO_4[1] , TULA PAUDEL, S. LANY, A. ZUNGER, A. SIGDEL, A. ZAKUTAYEV, J. PERKINS, D. GINLEY, National Renewable Energy Laboratory, J. BETTINGER, Y. SHI, M. TONEY, SLAC National Accelerator Laboratory, A. NAGARAJA, N. PERRY, T. MASON, North Western University — Cations A and B in A_2BX_4 spinels normally appear in precise 2:1 Daltonian ratio only at low temperature. At finite temperature, they become either A-rich or B-rich, which control dopability of the compound. We survey the experimentally observed stoichiometry asymmetries and describe the first principles framework for calculating these. The results of the calculations compare well with the phase boundary determined from XRD and the site occupancy measured by anomalous-XRD on Co_2ZnO_4 and Rh_2ZnO_4 samples grown in thermodynamic equilibrium. Good comparison between theory and experiment allows us predict the co-existence line in composition range form first principle for other spinels, which in turn can be extended to predict the nature of electrical conductivity of a compound, while designing the material with the desired properties via principle of inverse design.

[1]This work was supported through the Center for Inverse Design, an EFRC funded by the U.S. DOE, Office of Science, Office of BES.

12:39PM Q12.00006 Dopants and defects in conductive oxide spinels[1] , ANDRIY ZAKUTAYEV, JOHN PERKINS, PHILLIP PARILLA, TULA PAUDEL, STAPHAN LANY, DAVID GINELY, ALEX ZUNGER, National Renewable Energy Laboratory — We will discuss the effects of extrinsic and intrinsic imperfections (dopants and defects) in a group of conductive oxide materials related to Co3O4. Co3O4 is a spinel with Co2+ and Co3+ on tetrahedral and octahedral sites, respectively. Doping of Co3O4 with Zn and Ni represent two limiting cases: Zn2+ ions have a preference to occupy tetrahedral (Co2+) sites and are predicted to be unable to dope effectively; Ni2+ ions have a preference to occupy octahedral (Co3+) sites, so these atoms are expected to be efficient dopants. We found that substitution of Co3O4 spinel with up to 33 percent of Zn and Ni results in formation of ZnCo2O4 normal spinel and NiCo2O4 inverse spinel, and causes 100-fold and 1000-fold increases in conductivity, respectively, matching the predicted trend. Increase in Zn and Ni concentraion up to 40 percent cause phase separation of ZnO and NiO and leveling out of the conductivity. The conductivity decreases sharply above 50-60 percent Zn and Ni substitution level. Small differences with the theoretical predictions may be explained by non-equilibrium character of the thin film deposition process.

[1]This work was supported by the "Center for Inverse Design" EFRC of the Department of Energy

12:51PM Q12.00007 Possible *n*-type carrier producers in $In_2O_3(ZnO)_k$ homologous compounds[1] , HAOWEI PENG, Northwestern University, JUNG-HWAN SONG, ARTHUR J. FREEMAN — $In_2O_3(ZnO)_k$ (k = integers) homologous compounds are promising intrinsic *n*-type transparent conducting semiconductors.[2] To find out the carrier producers, we investigated the energetics and thermodynamic properties of *n*-type defects and their complexes in $In_2O_3(ZnO)_k$, with the k=3 phase as prototype, using the first-princiles density functional method. We calculated the defect formation energies and defect transition energy levels of oxygen vacancies (V_O), substitutional indium on zinc sites (In_{Zn}), zinc and indium interstitials (Zn_i and In_i) on different atomic sites, and also some V_O–In_{Zn} and V_O–Zn_i defect complexes. We find, under the experimental growth condition of O-poor and $T = 1300°$C, that V_O, In_{Zn}, and V_O-In_{Zn} complexes have much lower formation energies than the others, among which V_O will stay in the neutral charged state and the latter two are the most possible *n*-type carrier producers. The V_O-In_{Zn} complex tends to form between V_O and In_{Zn} in the same atomic layer; thus its distribution should be affected by the site-preference of V_O.

[1]Supported by the NSF MRSEC at N.U. Materials Research Center
[2]T. Moriga, et.al., J. Am. Ceram. Soc. **81**, 1310 (1998).

1:03PM Q12.00008 Protonic motion in $Pr_{0.7}Ca_{0.3}MnO_3$ thin films and its implications on resistance change properties[1] , MIHIR TENDULKAR, NICHOLAS BREZNAY, YOSHIO NISHI, Stanford University — Thin films of $Pr_{0.7}Ca_{0.3}MnO_3$ (PCMO) exhibit resistance-change properties that are of acute interest for next-generation memory solutions. Recent work has demonstrated that oxidation / reduction of a reactive electrode is critical to the switching process, suggesting that interface engineering will solve the reliability issue. We show that an overlooked contributor to the process is hydrogen, which dopes the bulk film. Activated conduction and loss tangent measurements are correlated with FTIR spectra to demonstrate protonic motion through the repeated breaking and reforming of –OH bonds. SIMS and Hall measurements are presented in conjunction with UV-Vis spectroscopy to show that hydrogen also alters the electronic structure of the PCMO film. The implications of these effects on forming and switching are discussed.

[1]Financial support from the SRC / Intel Fellowship is gratefully acknowledged

1:15PM Q12.00009 Dynamics of Interstitial H in TiO_2[1] , W.B. FOWLER, A. MURPHY[2], M. STAVOLA, Lehigh Univ. — H transport in rutile TiO_2 is important because of the low energy barriers within the open lattice in the c-direction [1]. As part of a study of the dynamics of interstitial H, potential energy functions for the vibration of hydrogen between two cross-channel O were generated. Double-well functions were modeled using experimental data [2] for the fundamental stretching vibrational frequencies of the three isotopes of H along with theoretical information obtained from quantum-mechanical calculations using [3] CRYSTAL06. These functions were then used to predict where the first overtone may lie, and its relative transition probability. The unexpectedly large anharmonicity observed for the OH vibration is correlated with the hydrogen-bond nature of the O-H —-O potential.

[1] O. W. Johnson et al., J. Appl. Phys. 46, 1026 (1975); J. B. Bates et al., Phys. Rev. B 19, 4130 (1979); E. J. Spahr et al., Phys. Rev. Lett. 104, 205901 (2010).
[2] J. B. Bates and R. A. Perkins, Phys. Rev. B 16, 3713 (1977).
[3] R. Dovesi et al., Crystal06 User's Manual, Univ. of Torino, Torino, 2006.

[1]Supported by the NSF REU physics program at Lehigh University.
[2]Present address: California Univ. of Pennsylvania.

1:27PM Q12.00010 Interstitial and substitutional Zr in SrTiO3[1] , JOHN JAFFE, RENEE VAN GINHOVEN, WEILIN JIANG, Pacific Northwest National Lab — We investigate Zr in $SrTiO_3$ (STO) as an electronic dopant and as a model for nuclear waste forms in which radioactive Sr decays to Y and then to stable Zr through beta emission. Density functional theory (DFT) within the supercell model is used to predict the thermodynamic stability and electronic states of interstitial and Sr- or Ti-substituted Zr atoms in the STO lattice. Native point defects such as vacancies and antisites are also considered. When Zr replaces Sr, its most stable configuration is to simply occupy the Sr site (instead of, for example, replacing a Ti and displacing the Ti to the Sr site.) For Zr added to the lattice, its most stable configuration is to replace a Ti, making a Zr_{Ti} impurity plus a Ti interstitial (as opposed to the Zr just remaining as an interstitial atom.) Zr_{Sr} is predicted to be a double electron donor, Zr_{Ti} is electrically inactive and interstitial Zr and Ti are predicted to be quadruple donors, with all donor levels in the conduction band. Zr_{Sr} and the tetravalent interstitials are all predicted to increase the crystal volume, and the interstitials also are predicted to lead to a tetragonal distortion of the lattice. Experiments with injection of Zr atoms into STO qualitatively confirm these predictions of crystal structural changes.

[1]Supported by U.S. Department of Energy Waste Form Campaign.

1:39PM Q12.00011 ABSTRACT WITHDRAWN –

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q13 GSNP DFD: Glassy Systems and Jamming I D225/226

11:15AM Q13.00001 The Influence of Boundary Roughness on the Dynamics of Confined Colloidal Suspensions near the Glass Transition[1] , DANIEL J. REAL, KAZEM V. EDMOND, ERIC R. WEEKS, Emory University — We study the relationship between boundary conditions and particle motion in confined, concentrated colloidal suspensions. Studies of polymer fluids in confinement have shown that changes in mobility are strongly dependent upon the polymer/surface interaction. We model this interaction by observing the effects of textured surfaces on colloidal particle mobility in confined dense suspensions (near the glass transition). We use high-speed confocal microscopy to directly image and track the colloidal particles in thin, wedge-shaped sample chambers made from textured glass. We texture the glass in a controlled, reproducible manner by spincoating and sintering colloidal suspensions onto glass slides. We expect the texturing to frustrate the formation of layers seen in smooth-walled confinement, resulting in decreased translational diffusion as compared to the smooth wall case. By studying these dynamics we gain a better understanding of the glass transition and its dependence on interfacial dynamics versus finite size effects.

[1]Supported by NSF Grant No. DMR-0804174

11:27AM Q13.00002 Structural Rearrangements in Confined Colloidal Liquids under Oscillatory Shear , PRASAD SARANGAPANI, University of Notre Dame, ANDREW SCHOFIELD, University of Edinburgh, Y. ELAINE ZHU, University of Notre Dame — We have investigated the dynamics of confined suspensions under oscillatory shear using a micron-gap rheometer interfaced with confocal microscopy. Our system consists of sterically stabilized poly-(methyl methacrylate) (PMMA) particles suspended in density and refractive index matched solvents at particle volume fractions, ϕ = 0.40-0.43, confined between two solid surfaces with gaps ranging from ∼10-30 particle layers. Above a threshold strain of ∼6% where an applied deformation is sufficient to induce plastic behavior, we find that structural rearrangements are highly anisotropic. Non-affine motion, determined by subtracting the globally uniform strain from the bare particle coordinates, reveals that particles move as cooperatively rearranging groups with a preferred orientation transverse to the flow direction. Measures which probe cooperative dynamics all reveal a strong amplitude, thickness, and directional dependence on the characteristic sizes of cooperatively rearranging regions. Interestingly, we find that medium range orientational order has a significant influence on shear-induced dynamics, particularly the shapes of rearranging regions.

11:39AM Q13.00003 Application of Edwards' statistical mechanics to polydisperse and high-dimensional jammed sphere packings , MAXIMILIEN DANISCH, Ecole Normale Superieure de Cachan, YULIANG JIN, HERNAN MAKSE, The City College of New York, PATRICK CHARBONNEAU, Duke University, SAM MEYER, Université de Lyon, CHAOMING SONG, Northeastern University, FRANCESCO ZAMPONI, Ecole Normale Supérieure — The Edward's statistical mechanics of jammed sphere packings [Song et al., Nature (London) 453, 629 (2008)] is generalized to different systems: polydisperse sphere packings in three dimensions, and high-dimensional monodisperse sphere packings. The theory predicts the density of random close packing and random loose packing of polydisperse systems for a given distribution of particle size and describes packings for any interparticle friction coefficient. In the high-dimensional limit, an asymptotic solution of the self-consistent relation is obtained by saddle-point evaluation and checked numerically. The resulting random close packing density scaling is consistent with that of other approaches, such as replica theory and density-functional theory. The theory could serve as a starting point to solve more difficult problems: such as predicting the optimal density of non-spherical packings, and understanding the higher-order correlations present in amorphous jammed packings.

11:51AM Q13.00004 Cyclic simple shear in a two-dimensional granular system[1] , JIE REN, JOSHUA DIJKSMAN, ROBERT BEHRINGER, Department of Physics, Duke University — We study the evolution of a 2D granular system consisting of frictional photo-elastic disks under large numbers of small-amplitude cyclic shear cycles. We are particularly interested in the reversibility of the system under cyclic shear. The experiments are carried out on a specially designed apparatus which can create quasi-static, nearly uniform simple shear. By using photo-elastic particles and a fluorescent labelling technique, we obtain information about displacement, rotation and contact forces for each particle following each small strain. We also obtain the system-level behaviour over many shear cycles. To better understand the nature of jamming, we have carried out shearing runs that explore various initial states which are initially unjammed, isotropically jammed or anisotropically jammed, and we compare the results for different initial states.

[1]This work is supported by grants DMR09-06908, NSF 0835742, and ARO W911NF-07-1-1031

12:03PM Q13.00005 Microscopic Dynamics of Quasi-2D Dense Colloidal Gels[1] , MATTHEW LOHR, ARJUN YODH, University of Pennsylvania — In this work, we investigate the microscopic dynamics of quasi-2D dense attractive colloidal systems. We confine bidisperse polystyrene spheres between glass coverslips in a suspension of water and 2,6-lutidine; as we increase the temperature of the sample into a critical regime, lutidine wets the colloids, creating a strong attractive interaction ($>$ 4kT). We specifically study suspensions in the "dense gel" regime, i.e., at a volume fraction high enough that the attractive particles form a spanning cluster, yet just low enough that there exists some structural heterogeneity larger than the individual particle size. We track the particle locations via bright-field video microscopy and analyze the dynamics of the system in order to compare them to lower-volume-fraction gel states and higher-volume-fraction glassy states. In doing so, we pinpoint the similarities and differences in the mechanisms for dynamic arrest in low-density colloidal gels and high-density colloidal glasses.

[1] Supported by NSF Grant DMR-0804881, MRSEC Grant DMR-0520020 and NASA Grant NNX08AO0G.

12:15PM Q13.00006 Structural Correlations in Glass-Forming Hard Spheres Fluids , PATRICK CHARBONNEAU, Duke University, BENOIT CHARBONNEAU, St. Jerome's University and University of Waterloo — Recent studies have detected the presence of a growing static length scale associated with the glassy dynamical slowdown. Yet no fully satisfying microscopic description of such a length scale has yet been formulated. We critically evaluate the hypothesis that correlated structural defects could underlie the growing relaxation time in deeply supersaturated fluid. Though a clear structural signature of a developing order in these systems is found, the resulting defect geometry does not lead quite match the Frank- Kasper defect scenario. The dimensionally generalizable nature of the defects, however, make them promising options for defining static observables.

12:27PM Q13.00007 Study of experimental protocols for producing random close packed colloids , KELSEY HATTAM, ERIC R. WEEKS — A collection of spheres can be packed tightly into an amorphous state known as "random close packing." In our experiment, colloidal particles are allowed to slowly sediment forming a random close packed state. By adjusting the solvent's density we finely control the rate at which the sedimentation occurs. We then use confocal microscopy to image the sample. By imaging overlapping regions we determine the positions of hundreds of thousands of particles. From this data, we measure the distribution of Voronoi volumes and the contact number distribution, and examine how these distributions depend on the sedimentation rate.

12:39PM Q13.00008 Rotational and Translational Phonon Modes in Glasses Composed of Ellipsoidal Particles[1] , PETER J. YUNKER, KE CHEN, University of Pennsylvania, ZEXIN ZHANG, Soochow University, WOUTER G. ELLENBROEK, Eindhoven University of Technology, ANDREA J. LIU, ARJUN G. YODH, University of Pennsylvania — The effects of particle shape on the vibrational properties of colloidal glasses are studied experimentally. 'Ellipsoidal glasses' are created by stretching polystyrene spheres to different aspect ratios and suspending the resulting ellipsoidal particles at high packing fraction. By measuring displacement correlations between particles, we extract vibrational properties of the ellipsoidal glass. Low frequency modes in glasses composed of ellipsoidal particles with major/minor axis aspect ratios $\sim$1.1 are observed to have predominantly rotational character. By contrast, low frequency modes in glasses of ellipsoidal particles with larger aspect ratios ($\sim$3.0) exhibit a mix of rotational and translational character. All glass samples were characterized by a distribution of particles with different aspect ratios. Interestingly, even within the same sample it was found that small- aspect-ratio particles participate relatively more in rotational modes, while large-aspect-ratio particles tend to participate relatively more in translational modes.

[1]We acknowledge financial support from the NSF through DMR-0804881, PENN MRSEC DMR-0520020, and NASA NNX08AO0G.

12:51PM Q13.00009 Dynamical heterogeneities and fluctuations of the time variables in structural glasses , KARINA E. AVILA, HORACIO E. CASTILLO, Ohio University, AZITA PARSAEIAN, Northwestern University — The existence of dynamical heterogeneities in disordered materials is considered now as a crucial element in explaining many observed features of their dynamical behavior. In this work, we investigate a possible hypothesis for their origin, which assumes that they emerge from soft (Goldstone) modes associated with a broken continuous symmetry under time reparametrizations. To test this hypothesis, we construct coarse grained observables from data obtained in simulations of four models of structural glasses. The fluctuations of these observables are decomposed into transverse components associated with the postulated time-fluctuation soft modes and a longitudinal component unrelated to them. We find that as temperature is lowered and timescales are increased, the time reparametrization fluctuations become increasingly dominant and their correlation volumes grow together with the correlation volumes of the dynamical heterogeneities, while the correlation volumes for longitudinal fluctuations remain small.

1:03PM Q13.00010 Experimental observation of deformation and structural defects in hard-sphere colloid glasses , KATHARINE JENSEN, Harvard University Department of Physics, NOBUTOMO NAKAMURA, Harvard University School of Engineering and Applied Sciences, DAVID WEITZ, Harvard University Department of Physics, Harvard University School of Engineering and Applied Sciences, FRANS SPAEPEN, Harvard University School of Engineering and Applied Sciences — We performed experiments on a 1.55-μm-diameter monodisperse, hard-sphere colloid glass under simple shear at various strain rates, while simultaneously tracking real-time individual positions of roughly 100,000 particles by confocal microscopy. We probe the elastic, anelastic, and plastic responses of the system to applied strain, with particular focus on identifying the local mechanisms of deformation. In plastic deformation, we observe thermally activated rearrangements of groups of particles, the nature and concentration of which are correlated with local parameters such as strain, Voronoi volume, and free volume.

1:15PM Q13.00011 Aging dynamics of a colloidal glass - time resolved viscoelastic properties and the role of flow history[1] , CHINEDUM OSUJI, AJAY NEGI, Yale University — Many colloidal suspensions are inherently out of equilibrium and display a slow evolution of their dynamics over time. However, many features of the glass transition as encountered in polymer and molecular glasses are not conserved. This phenomenon is still not completely understood and little is known of the connection between flow history, as a determinant of the initial system state, and subsequent aging dynamics. Further, the changes in the energy landscape during aging can be understood from the frequency and strain dependence of the shear modulus but the non-stationary nature of these systems frustrates investigation of their instantaneous underlying properties. Here we discuss the use of stress jump experiments that investigate the role of flow history on aging, and the systematic reconstruction of the frequency and strain dependence as a function of age for a repulsive colloidal glass undergoing structural arrest and aging. We uncover a connection between the aging behavior and the rate of flow cessation that is additionally reflected in the dynamics of residual stress relaxation. Strikingly, the frequency dependence at fixed times can be rescaled onto a master curve, implying a simple connection between the aging of the system and the change in the frequency dependent modulus.

[1]The authors acknowledge NSF funding under CBET-0828905.

1:27PM Q13.00012 Jamming, Clogging, and Fragility in Frictionless Disk Systems with Quenched Disorder , CHARLES REICHHARDT, Los Alamos National Laboratory, EVAN GROOPMAN, ZOHAR NUSSINOV, Washington University, CYNTHIA OLSON REICHHARDT, Los Alamos National Laboratory — We consider a two-dimensional simulation model of binary frictionless disks which have a well defined jamming density of $\phi_j \approx 0.84$ in the absence of quenched disorder. When quenched disorder is added in the form of impenetrable immobile disks, the jamming density is reduced. As the density of the quenched disorder sites increases, we observe a crossover from a jamming transition to a clogging transition. The clogged state is defined as a highly heterogeneous granular packing that resists shear along one direction and that is composed of a combination of high density patches at the clean jamming density and very low density patches or voids. These clogged states are fragile in the sense that they are only clogged in the direction of an externally applied drive. After a clogged state has formed, if a new drive is applied in a different direction the disks can flow freely for a period of time before reorganizing into a new clogged state. In contrast, jammed systems are jammed in all directions simultaneously.

1:39PM Q13.00013 Coupling Between Translational and Orientational Order in Fiber Suspensions[1] , ALEXANDRE FRANCESCHINI, EMMANOUELA FILIPPIDI, Center for Soft Matter Research, New York University, ELISABETH GUAZZELLI, IUSTI-CNRS UMR 6595 - Polytech Marseille - Aix-Marseille University, DAVID PINE, Center for Soft Matter Research, New York University — Suspensions of non-Brownian fibers under a small oscillatory shear flow find a random but completely reversible state, called "random organization": at each period, the non-hydrodynamic interactions modify both the orientation and positions of fibers, until a reversible configuration is found. As observed in sphere suspensions, there is a nonequilibrium absorbing phase transition when the strain is increased above a concentration-dependant threshold. The transient time, during which the activity decays algebraically, has a diverging duration; critical exponents are consistent with Manna universality class. Above the threshold, fibers get progressively aligned towards the vorticity and a reversible steady state is eventually found for a range of strain. This behavior is specific to fiber suspensions. We study whether or not these oriented reversible states are critical states. We experimentally evaluate the angles distribution of fibers in both vertical and horizontal planes and discuss the relation between these distributions and the existence of a reversible state.

[1]Primarily funded by the MRSEC Program of the NSF under Award Number DMR-0820341

1:51PM Q13.00014 Force correlations near point J in a lattice model of jamming , SCOTT MILNER, JILLIAN NEWHALL, Penn State University — We have constructed a lattice model of a jammed system in $d = 2$ dimensions near the isostatic point (Point J). Adapting the Tighe model, we represent a jammed pack of particles as a regular hexagonal array, with repulsive forces between nearest neighbors. We generate near-isostatic jammed configurations by carrying out a Monte Carlo simulation with Tighe "wheel moves", which rearrange forces locally while preserving force balance on every particle. (Wheel moves correspond to a small dilation of a given particle.) The MC simulation is progressively biased towards the creation of "missing contacts", bonds which bear zero force. We reveal long-range correlations in the force network near Point J by determining for each particle the smallest "collective move" — a set of wheel moves that taken together dilates the given particle, while preserving the existing missing contacts. The size of these collective moves diverges as Point J is approached.

2:03PM Q13.00015 Time and volume fraction dependence of dynamic heterogeneity in a glass-forming binary hard-sphere mixture , ELIJAH FLENNER, GRZEGORZ SZAMEL, Colorado State University - Chemistry Department — We examined dynamic heterogeneity in a glass-forming binary hard-sphere mixture for volume fractions up to and including the so-called mode-coupling transition. We calculated the dynamic susceptibility $\chi_4(t)$, the four-point structure factor $S_4(q;t)$ and the dynamic correlation length $\xi(t)$. We find that the correlation length increases with time as $\xi(t) \sim \ln(t)$ and is independent of ϕ for times approximately between the β and α relaxation time. The dynamic length plateaus at a ϕ dependent value $\xi_{\max}(\phi)$. We find that $\xi_{\max}(\phi)$ is proportional to the dynamic length at the α relaxation time, $\xi(\tau_\alpha)$. Finally, while for a limited range of volume fractions $\xi(\tau_\alpha) \sim \tau_\alpha^{1/z}$ with $1/z \approx 0.2$, we find that $\xi(\tau_\alpha) \sim \ln(\tau_\alpha)$ describes our data well for all ϕ.

Wednesday, March 23, 2011 11:15AM - 2:15PM –
Session Q14 GSNP: Focus Session: Extreme Mechanics: Elasticity and Deformation I D227

11:15AM Q14.00001 Geometric Nonlinear Computation of Thin Rods and Shells[1] , EITAN GRINSPUN, Columbia University — We develop simple, fast numerical codes for the dynamics of thin elastic rods and shells, by exploiting the connection between physics, geometry, and computation. By building a discrete mechanical picture from the ground up, mimicking the axioms, structures, and symmetries of the smooth setting, we produce numerical codes that not only are consistent in a classical sense, but also reproduce qualitative, characteristic behavior of a physical system—-such as exact preservation of conservation laws—-even for very coarse discretizations. As two recent examples, we present discrete computational models of elastic rods and shells, with straightforward extensions to the viscous setting. Even at coarse discretizations, the resulting simulations capture characteristic geometric instabilities. The numerical codes we describe are used in experimental mechanics, cinema, and consumer software products.

[1]This is joint work with Miklós Bergou, Basile Audoly, Max Wardetzky, and Etienne Vouga. This research is supported in part by the Sloan Foundation, the NSF, Adobe, Autodesk, Intel, the Walt Disney Company, and Weta Digital.

11:51AM Q14.00002 Wrinkling of an Annulus , KAMIL TOGA, University of Massachusett, Amherst, BENOIT ROMAN, JOSE BICO, Laboratoire de Physique et Mecanique des Milieux Heterogenes, ESPCI Paris, France, THOMAS RUSSELL, NARAYANAN MENON, University of Massachusett, Amherst, UNIVERSITY OF MASSACHUSETT, AMHERST TEAM, LABORATOIRE DE PHYSIQUE ET MECANIQUE DES MILIEUX HETEROGENES, ESPCI PARIS, FRANCE TEAM — We report on an experiment in which we study the wrinkling of an annular elastic film subject to different radial tensions at the inner and outer diameter. The annuli were made from polystyrene films of thickness ranging from 62 to 180 nm, and floated on water. They were then transferred onto a Langmuir-Blodgett trough filled with acidic aqueous subphase. The surface tension on the inside of the annulus is held fixed, while the surface tension outside the annulus is continuously varied by compressing an insoluble surfactant. When the differential tension is increased beyond a threshold value, radial wrinkles form in the interior of the annulus and extend outwards. We studied the length of wrinkles formed as a function of the differential tension produced by the surfactant, and for a range of film thickness.

12:03PM Q14.00003 Dancing Discs: Bending and Twisting of Soft Materials by Anisotropic Swelling , DOUGLAS HOLMES, MATTHIEU ROCHÉ, TARUN SINHA, HOWARD STONE, Princeton University — Soft materials, e.g. biological tissues and gels, undergo morphological changes, motion, and instabilities when subjected to external stimuli. Tissues can exhibit residual internal stresses induced by growth, and generate elastic deformations to move in response to light or touch, curl articular cartilage, aid in seed dispersal, and actuate hygromorphs, such as pine cones. Understanding the dynamics of such osmotically driven movements, in the influence of geometry and boundary conditions, is crucial to the controlled deformation of soft materials. We examine how thin elastic plates undergo rapid bending and buckling instabilities after anisotropic exposure to a favorable solvent that swells the network. An unconstrained beam bends along its length, while a circular disc bends and buckles with multiple curvatures. In the case of a disc, a large-amplitude transverse travelling wave rotates azimuthally around the disc. Theoretical interpretations inspired by the complementary thermal expansion problem of transient shape changes triggered by time-dependent heating are presented and allow collapse of time-dependent data on universal curves. Understanding the dynamics of strain-driven shape changes provides new insight into natural systems and control of advanced functional materials.

12:15PM Q14.00004 Sinusoidal to helical buckling of a thin rod under a cylindrical constraint , JAMES MILLER, Massachusetts Institute of Technology, ARNAUD LAZARUS, MIT, NATHAN WICKS, JAHIR PABON, Schlumberger-Doll Research, PEDRO REIS, MIT — We investigate the buckling and post-buckling behavior of a thin, elastic rod loaded under cylindrical constraint. Our desktop experiments consist of compressing a hyper-elastic rod inside a transparent acrylic pipe with a motorized linear actuator. Under imposed displacement, the initially straight rod first buckles into a sinusoidal mode and eventually undergoes a secondary instability into helical buckling. This buckling and post-buckling behavior is found to be highly dependent on the systems' geometry, namely the rod length and the aspect ratio of the rod to pipe diameter. We quantify the wavelength and pitch of the period patterns through direct digital imaging and record the reaction forces at both end of the pipe. The observed behavior is rationalized through scaling arguments.

12:27PM Q14.00005 Shape evolution of a thin loop sedimenting in a viscous fluid , JAMES HANNA, CHRISTIAN SANTANGELO, Department of Physics, UMass-Amherst — We consider the non-local elastic problem of a closed thin filament settling under gravity in a fluid at zero Reynolds number. The filament is modeled as an inextensible chain, with no bending or twist rigidity. Although the equations admit rigid motions of the chain, there are no stable trajectories. We explore whether a stable envelope may exist around a recirculating blob and tail arrangement.

12:39PM Q14.00006 3D micro-modeling of wrinkling phenomena , DAMIEN EGGENSPIELER, GOZDE INCE, KAREN GLEASON, MARY BOYCE, MIT — Wrinkles, formed by the buckling of stiff layers adhering to soft substrates, are commonplace in nature. From wrinkles on smiling or aging faces to the wrinkled shape of pumpkins or the wrinkled electrospun nano-fibers due to the radial evaporation of the solvent used in the processing of these fibers, wrinkles have been found ranging from the nano- to the macroscopic scales. More recently, studies have shown that this buckling phenomenon can be directed via a selective stiffening of either ones of the layers composing this composite system. We are introducing a 3D numerical model for the buckling of a shell on a soft layer. The selective stiffening of the shell can reproduce the "stiffness patterning" obtained experimentally by UV-Ozone treatment of a soft PDMS substrate through a photomask. This model can predict the final shape of the surface of this composite system for periodic photomasks and might be used in the design of specific micro-topographies.

12:51PM Q14.00007 Coiling Spaghetti: Deposition of a Thin Rod onto a Moving Substrate , PEDRO REIS, Massachusetts Institute of Technology, JUNGSEOCK JOO, UCLA, JOSEPHINE MANNENT, MIT, JOEL MARTHELOT, ESPCI, Paris, DANNY KAUFMAN, EITAN GRINSPUN, Columbia University — We investigate the oscillatory coiling patterns obtained when a thin elastic rod is deposited onto a moving solid boundary (conveyor belt). Through a combination of well controlled desktop experiments and numerics, we explore the phase diagram of this coiling process and identify the underlying physical ingredients. Our novel numerical method implements a discrete notion of bending and twist based on ideas ported from differential geometry, and exhibits excellent performance and robustness. This enables us to carry out predictive direct simulations of the large deformations of the thin elastic rod interacting with the moving substrate, that are in excellent agreement with our experiments. Applications of this coiling process range from the coiling of nanotubes to the laying down of transoceanic cable and pipelines in the ocean bed.

1:03PM Q14.00008 Geometry-ruled deformation of thin elastic shells , ARNAUD LAZARUS, Massachusetts Institute of Technology, PEDRO MIGUEL REIS, MIT — We study the mechanical response of thin elastic shells subject to point or plate load and in different mechanical environments (with or without an in-out pressure difference). The geometry and material properties of the ellipsoidal shells used in our experiments can be accurately controlled using digital fabrication techniques. The linear and nonlinear mechanical response of the shells is quantified through load-displacement compression tests and the post-buckling patterns are analyzed using digital imaging. In the linear regime, we explore the geometry-induced rigidity of shells with different shapes. In the nonlinear regime, we focus on the formation of structures with localized curvature, which we denote by s-cones (shell-cones) and examine their mechanical and morphological properties.

1:15PM Q14.00009 The Buckliball: Pressure Induced Pattern Transformation of a Structured Elastic Shell , JONGMIN SHIM, Harvard University, CLAUDE PERDIGOU, Massachusetts Institute of Technology, KATIA BERTOLDI, Harvard University, PEDRO REIS, Massachusetts Institute of Technology — We report an experimental and computational study of a patterned elastic shell which, under pressure loading, undergoes a transformation in its structural configuration. The geometry of the ball comprises of an elastomeric spherical shell patterned with a regular array of circular holes. These voids are covered with a thin membrane, thereby making the ball air tight. Upon reduction of the internal pressure, the thin membranes first invert their curvatures inward. Consequently, beyond the critical pressure, the thin ligaments between the holes buckle leading to a cooperative buckling cascade of the skeleton of the ball. During this process, the initially circular holes evolve into an elliptical shape, and eventually become fully closed. This pattern transformation is induced by mechanical instability that opens the possibility for reversible encapsulation, over a wide range of length scales.

1:27PM Q14.00010 Polymer Thin Film Buckling: Wrinkling and Strain Localizations[1] , YURI EBATA, University of Massachusetts, Amherst, ANDREW B. CROLL, North Dakota State University, ALFRED J. CROSBY, University of Massachusetts, Amherst — Out of plane deformations of thin films are observed in everyday life, e.g. wrinkled aging human skin or folded fabrics. Recently, these deformations are being pursued for fabricating unique patterned surfaces. In this study, the transition from wrinkling, a low-strain buckling behavior, to localized deformations such as fold and delamination, is investigated for polystyrene films with thickness ranging from 5nm to 180nm. The thin films are attached to a uniaxially strained polydimethysiloxane substrate and the strain is released incrementally to apply increasing compressive strain to the attached film. The wavelength and the amplitude of local out-of-plane deformation are measured as global compression is increased to distinguish between wrinkling, folding, and delamination. The transition from wrinkling to strain localizing events is observed by tracking the statistics of amplitude distribution sampled across a large lateral area. A critical strain map is constructed to denote the strain regimes at which wrinkle, fold, and delamination occur.

[1]NSF-DMR 0907219

1:39PM Q14.00011 Statistical Mechanics of Pressurized Shells , JAYSON PAULOSE, Harvard School of Engineering and Applied Sciences, Cambridge, MA 02138, GERRIT VLIEGENTHART, GERHARD GOMPPER, Institut fur Festkorperforschung, Forschungszentrum Juelich, Germany, DAVID NELSON, Physics Department, Harvard University, Cambridge, MA 02138 — It is well known that thermal fluctuations strongly modify the large length scale elastic behavior of flat solid membranes. A thin spherical shell may be considered a solid membrane with a uniform nonzero curvature. This curvature couples the in-plane stretching modes with the out-of-plane undulation modes, giving rise to qualitative differences in the fluctuations of spherical shells compared to flat membranes. In addition, a shell can support a pressure difference between its interior and exterior. We study the statistical mechanics of deformations of a spherical shell using perturbation theory and Monte Carlo simulations, explicitly including the effects of curvature and pressure. Thermal corrections to the predictions of classical shell theory for point indentation and pressure-induced buckling experiments on microscale shells diverge as the ratio of shell radius to thickness tends to infinity.

1:51PM Q14.00012 Complex Morphogenesis from Elastic Instability of Thin Sheets , PASCAL DAMMAN, Universite de Mons — Thin sheets are mechanically unstable to boundary or substrate-induced compressive loads. Moderate compression results in regular wrinkling while further confinement can lead to crumpling. In this communication, we will first show the emergence of a new morphological instability triggered by a period-doubling bifurcation observed for large compression ratio. A periodic self-organized focalization of the deformation energy is observed provided a symmetry breaking, induced by the elastic foundation, occurs. This effect will be explained by considering geometrical nonlinearities leading to a Euler-Lagrange equation similar to the equation of a parametric resonance in nonlinear oscillator. In the second part, we will show that thin sheets, from suspended graphene to ordinary hanging curtains, under boundary confinement spontaneously generate a universal self-similar cascade of wrinkled patterns. We develop a formalism based on *wrinklons*, a localized transition zone in the merging of two wrinkles, as building-blocks to describe the cascade morphology. These physical models based on elasticity and geometry constitutes a new theoretical toolkit to understand the morphology of various confined systems, such as coated materials or living tissues. Moreover, it also opens the way to new kind of microfabrication design of multiperiodic or chaotic (aperiodic) surface topography via self-organization.

2:03PM Q14.00013 Stability of a drop-strip system , MARCO RIVETTI, SÉBASTIEN NEUKIRCH, ARNAUD ANTKOWIAK, Institut d'Alembert, Paris, UPMC & CNRS — When a flexible material is placed in contact with a liquid-air interface, capillary forces may cause deformations and large displacements in the structure. Such kind of elastocapillary interactions play a crucial role in many technological applications, like deflection of nanotubes carpets or microscale self-assembly. We study the problem of a drop deposited on a thin and narrow strip. Using a simplified 2D model including surface tension interactions, elastic and gravitational energies, we are able to predict the shape of the equilibrium solutions, as well as the appearance of instability in the system. Theoretical predictions are confronted to experiments and a good agreement is obtained.

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q15 DMP GMAG FIAP: Focus Session: Spins in Semiconductors - Quantum Dots and Nuclear Spins D171

11:15AM Q15.00001 Protecting the electron spin coherence in a quantum dot with inhomogeneously polarized nuclear spins via dynamic nuclear polarization[1] , WENXIAN ZHANG, JUN ZHUANG, Department of Optical Science and Engineering, Fudan University, Shanghai 200433, China, J.Q. YOU, Department of Physics, Fudan University, Shanghai 200433, China — An electron spin in a quantum dot is decohered by its surrounding nuclear spins via hyperfine coupling. During the dynamic nuclear polarization process, when the nuclear spins are polarized inhomogeneously by repeatedly injected polarized electron spins, a fully polarized nuclear spin core is formed. As a consequence, the polarized nuclear spin core can be harnessed to protect the electron spin coherence. In this way, we find that the electron spin coherence time can be extended tens times with the total nuclear polarization as low as 20%, in contrast to the usual requirement of 90% polarization, in a quantum dot with 256 nuclear spins. The total nuclear polarization goes even lower for larger quantum dots. The effect of the dipolar interaction between nuclear spins is also discussed.

[1]Supported by the 973 Program under Grant No. 2009CB929300, NCET, Specialized Research Fund for the Doctoral Program of Higher Education of China under Grant No. 20090071120013, Shanghai Pujiang Program under Grant No. 10PJ1401300.

11:27AM Q15.00002 Electrically detected nuclear magnetic resonance in GaAs/AlGaAs-based quantum point contacts , ZACHARY KEANE, MATTHEW GODFREY, ADAM BURKE, JASON CHEN, SEBASTIAN FRICKE, OLEH KLOCHAN, ADAM MICOLICH, University of New South Wales, HARVEY BEERE, DAVE RITCHIE, University of Cambridge, KIRILL TRUNOV, DIRK REUTER, ANDREAS WIECK, Ruhr Universitaet Bochum, ALEX HAMILTON, University of New South Wales — Nuclear magnetic resonance (NMR) is a well-known technique with widespread applications in physics, chemistry and medicine. Conventional NMR studies use inductive coils to detect the magnetic field produced by precessing nuclear spins; this approach requires on the order of 10^{12} spins for detection. Recently, resistive detection of NMR through the hyperfine interaction has been demonstrated with electrons in mesoscopic 2- and 1-dimensional devices based on high-quality GaAs/AlGaAs heterostructures. These studies are typically sensitive to 10^8 spins, enabling NMR on much smaller sample volumes. Holes are predicted to have much weaker nuclear spin coupling than electrons, which could be relevant to the emerging fields of spintronics and quantum information processing. We present a preliminary comparison between the magnitude of the NMR signal in electron and hole quantum point contacts.

11:39AM Q15.00003 Enhancing 29Si Dynamic Nuclear Polarization Through Microwave Frequency Modulation[1] , MAJA CASSIDY, MEN YOUNG LEE, CHARLES MARCUS, Harvard University — We demonstrate up to a four-fold enhancement in the dynamic nuclear polarization (DNP) of silicon particles by applying an a.c. modulation to the microwave frequency used for irradiation of the electron spin system. The DNP enhancement is studied at temperatures ranging from 2-20 K and across a range of microwave powers. The total nuclear polarization is found to increase with decreasing temperature and increasing microwave power however, surprisingly, the polarization enhancement increases as the temperature is increased. The DNP enhancement is seen to increase with polarization time and is highest in spin-diffusion regime of polarization. By varying the frequency and amplitude of the applied modulation, dynamics of the electron spin system are probed. We find that the highest polarization enhancements are achieved with the frequency is modulated at a rate much greater than the electron spin lattice relaxation rate, where higher order electron spin processes can contribute to the polarization process.

[1]Supported by the NSF-BISF and the Harvard NSEC

11:51AM Q15.00004 Dynamic Nuclear Polarization in Double Quantum Dots , MICHAEL GULLANS, Department of Physics, Harvard University — We theoretically investigate the controlled dynamic polarization of lattice nuclear spins in GaAs double quantum dots containing two electrons.[1] Three regimes of long-term dynamics are identified, including the build up of a large difference in the Overhauser fields across the dots, the saturation of the nuclear polarization process associated with formation of so-called "dark states," and the elimination of the difference field. We show that in the case of unequal dots, build up of difference fields generally accompanies the nuclear polarization process, whereas for nearly identical dots, build up of difference fields competes with polarization saturation in dark states. The elimination of the difference field does not, in general, correspond to a stable steady state of the polarization process.

[1]M. Gullans, et. al., Phys. Rev. Lett. 104, 226807 (2010).

12:27PM Q15.00005 Spin-dependent tunneling into an empty lateral quantum dot , PETER STANO, PHILIPPE JACQUOD, Physics Department, University of Arizona, 1118 E 4th Street, Tucson, Arizona 85721, USA — In a recent experiment [Phys. Rev. B **78**, 041306(R) (2008)] Amasha *et al.* reported a strong spin dependence of the rate for electrons to tunnel into an empty quantum dot in a Zeeman field. Such dependence is intriguing, as one expects tunneling rates to depend on the orbital structure of the wavefunction, over which a Zeeman field has no effect. In search for an explanation, we find two mechanisms leading to a spin-dependent tunneling rate. The first originates from different electronic g-factors in the lead and in the dot, and favors the tunneling into the spin ground (excited) state when the g-factor magnitude is larger (smaller) in the lead. The second is triggered by spin-orbit interactions via the opening of off-diagonal spin-tunneling channels. It systematically favors the spin excited state. Numerically modeling the experimental setup, we find that in GaAs the spin-orbit interaction is unable to explain the experimental results, as it leads to no more than a $\sim$10% discrepancy in the spin up vs spin down tunneling rates. We conjecture that the significantly larger discrepancy observed experimentally originates from the enhancement of the g-factor in the laterally confined lead. Reference: P. Stano and Ph. Jacquod, Phys. Rev. **B** 82, 125309 (2010)

12:39PM Q15.00006 Theory of spin blockade in a triple quantum dots[1] , CHANG-YU HSIEH, Department of Physics, University of Ottawa, Ottawa, Ontario, Canada K1N 6N5, YUN-PIL SHIM, Department of Physics, University of Wisconsin-Madison, Madison WI 53706, PAWEL HAWRYLAK, Quantum Theory Group, Institute for Microstructural Sciences, National Research Council, Ottawa, Canada, K1A 0R6 — We present a theory of electronic properties and spin blockade in a linear triple quantum dots. We use micoroscopic LCHO-CI and double-band Hubbard model to analyze the electronic and spin properties of a triple quantum dots near a symmetrical quadruple point involving the (1,1,1) configuration which is essential for implementing quantum information processing with electron spin. We calculate spectral functions and relate them via the rate equation, including coupling with a phonon bath, to current as a function of applied bias. We show that the spin blockade in a triple quantum dots can serve as a spectroscopic tool to distinguish spin polarized states from spin depolarized states. We also show that a spin blockade is developed only at high bias when an onsite triplet state on the edge quantum dot connected to the source lead becomes accessible in the transport window. In contradiction to the case of double quantum dot molecule, the onsite triplet is not only essential for lifting spin blockade but also important for building up spin polarisation and spin blockade in the system.

[1]The authors would like to acknowledge financial support from NSERC, OGS, and QuantumWorks.

12:51PM Q15.00007 Spin-polarized current generation in multiterminal quantum dot in Kondo regime , MIKIO ETO, TOMOHIRO YOKOYAMA, Keio University — We theoretically study the generation of spin-polarized current in a quantum dot with strong spin-orbit interaction, such as InAs quantum dot. As a minimal model, we consider two energy levels in a quantum dot, which is connected to N leads through tunnel barriers. When an unpolarized current is injected from a lead, spin-polarized currents are ejected to other leads in the case of $N \geq 3$. First, we show that the spin polarization of the output currents is markedly enhanced by resonant tunneling, around current peaks of Coulomb oscillation, when the level spacing in the dot is smaller than the level broadening. Next, we examine the many-body resonance induced by the Kondo effect in the Coulomb blockade regime. A large spin current is created in the presence of the SU(4) Kondo effect when the level spacing is less than the Kondo temperature.[1]

[1]M. Eto and T. Yokoyama, J. Phys. Soc. Jpn., in press; arXiv:1010.5956.

1:03PM Q15.00008 Spin blockade in the optical response of a charged quantum dot , ELEFTHERIA KAVOUSANAKI, GUIDO BURKARD, University of Konstanz, Germany — We theoretically model the population dynamics in a semiconductor quantum dot charged with a single electron in an optical pump-probe setup when the two lowest quantum dot levels are photoexcited. We calculate the differential transmission spectrum as a function of the time delay between the two circularly polarized optical pulses by using a density matrix formalism and treating intraband relaxation with the Lindblad equation. Taking into account both spin conserving and spin-flip relaxation processes we investigate the possibility for spin-dependent blocking of intraband relaxation due to the presence of the ground state electron for zero and finite magnetic fields. We show that the differential transmission spectrum is initially dominated by the fast spin-conserving mechanism before the slower spin-flip processes start to contribute at longer time scales. As a consequence of spin conservation for short time scales, we find a spin blockade effect in the optical recombination process.

1:15PM Q15.00009 Simulating electron spin entanglement in a double quantum dot[1] , M.A. RODRIGUEZ-MORENO, A.D. HERNANDEZ DE LA LUZ, Centro de Investigaciones en Dispositivos Semiconductores, Instituto de Ciencias BUAP, LILIA MEZA-MONTES, Instituto de Fisica BUAP — One of the biggest advantages of having a working quantum-computing device when compared with a classical one, is the exponential speedup of calculations. This exponential increase is based on the ability of a quantum system to create and operate on entangled states. In order to study theoretically the entanglement between two electron spins, we simulate the dynamics of two electron spins in an electrostatically-defined double quantum dot with a finite barrier height between the dots. Electrons are initially confined to separated quantum dots. Barrier height is varied and the spin entanglement as a function of this variation is investigated. The evolution of the system is simulated by using a numerical approach for solving the time-dependent Schrödinger equation for two particles.

[1]Partially supported by VIEP-BUAP

1:27PM Q15.00010 Exchange coupling between hole qubits and between electron qubits in quantum dot molecules[1] , ALEX GREILICH[2], STEFAN C. BADESCU[3], DANNY KIM[4], ALLAN S. BRACKER, DANIEL GAMMON, NRL, Washington, DC — The exchange interaction between electron spins has been a paradigm for solid-state implementation of quantum gates. Holes are receiving an increasing attention for their reduced hyperfine coupling as compared to electrons in III-V semiconductors. Besides the isotropic exchange, both electrons and holes couple through spin-nonconserving interactions. Here we present detailed experimental evidence of these interactions for electrons and for holes in stacked InAs/GaAs quantum dots, achieved through electrical and magnetic fields that induce energy level resonances. Particularly large spin-mixing effects are found for holes, which involve their multi-band structure. We provide a theoretical understanding of the essential mixing mechanisms involved, tracing them down to system asymmetries and inhomogeneities.

[1]This work was supported in part by DARPA and ONR
[2]Currently at Univ. Dortmund, Dortmund, Germany
[3]Currently at AFRL, Dayton, OH
[4]Currently at Harvard Univ., Boston, MA

1:39PM Q15.00011 Chiral spin currents and spectroscopically addressable single merons in quantum dots , CATHERINE STEVENSON, JORDAN KYRIAKIDIS, Dalhousie University — We provide unambiguous theoretical evidence for the formation of correlation-induced isolated merons in rotationally-symmetric quantum dots beyond the lowest-Landau-level approximation. For experimentally accessible system parameters, unbound merons condense in the ground state at magnetic fields as low as B* = 0.3 T and for as few as N = 3 confined fermions. The four-fold degenerate ground-state at B* corresponds to four orthogonal merons characterised by their winding number ± 1 and topological charge ± 1. This degeneracy is completely lifted by the Rashba and Dresselhaus spin-orbit interactions, yielding spectroscopic accessability to individual merons. We further derive a closed-form expression for the topological chirality in the form of a chiral spin current and use it to both characterise our states and predict the existence of other topological textures in other regions of phase space.

1:51PM Q15.00012 Magnetoconductance of a Single-Electron Transistor in the Kondo Regime[1] , TAI-MIN LIU, BRYAN HEMINGWAY, ANDREI KOGAN, University of Cincinnati, STEVEN HERBERT, Xavier University, MICHAEL MELLOCH, Purdue University, THEO A. COSTI, Institut fur Festkorperforschung, Forschungszentrum Julich, 52425 Julich, Germany — We have measured the zero-bias conductance of a Single-Electron Transistor (SET) in the Kondo regime as a function of temperature, T, and magnetic field, B, oriented parallel to the plane of the device. Our SETs are fabricated on a GaAs/AlGaAs heterostructure with electron sheet density 4.8×10^{11} cm^{-2} and mobility 5×10^5 cm^{2}V^{-1}s^{-1}. Scaled plots of both the T and B-dependent data show universal behavior. At moderate and high B, the magnetoconductance data show good agreement with renormalization group calculations in the spin-1/2 Kondo regime. At very low B, we observe a non-monotonic behavior: as B increases, the conductance initially increases and only starts to decrease at a finite B. A possible explanation of this effect due to the presence of multiple orbital dot levels with similar energies will be discussed.

[1]Supported By: NSF DMR Grant No. 0804199

2:03PM Q15.00013 Measuring mesoscopic spin currents by spin-to-charge conversion , PHILIPPE JACQUOD, PETER STANO, Physics Department, University of Arizona, 1118 E 4th Street, Tucson, Arizona 85721, USA — A number of theoretical investigations show that spin currents can be magneto-electrically generated by passing electric currents through spin-orbit coupled quantum dots. Measuring these currents has however not been achieved to date. In this talk, we present a theoretical proposal for measuring such mesoscopic spin currents with a voltage probe connected to the quantum dot via a single channel quantum point contact. We demonstrate that a spin current flowing through the quantum point contact results in an odd dependence of the charge current $I_{\rm qpc}$ on an externally applied Zeeman field, while this response is even in the absence of the spin current. The magnitude of the spin current is proportional to the zero field derivative of $I_{\rm qpc}$, with a constant of proportionality depending weakly on the geometry of the point contact. Numerical estimates suggest that in this way, mesoscopic spin currents can successfully be measured in GaAs quantum dots.

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q16 DCOMP: Electronic Structure III D173

11:15AM Q16.00001 Oxides – a challenge for (theoretical) spectroscopy , P. RINKE, H. JIANG, M. SCHEFFLER, Fritz-Haber-Institut der MPG, 14195 Berlin, A. GREULING, M. ROHLFING, Universitaet Osnabrueck, 49069 Osnabrueck, A. JANOTTI, E. KIOUPAKIS, C. G. VAN DE WALLE, University of California at Santa Barbara, CA 93106 — Oxides are of tremendous technological importance, yet challenging materials to characterize. In many cases the agreement between experimental and theoretical spectroscopy observed for other material classes has not been attained. We use rutile TiO_2 as an example to illustrate some of the problems. Many-body perturbation theory in the G_0W_0 approach based on density-functional theory in the local-density approximation gives a fundamental band gap of 3.3 eV in seemingly good agreement with the 3.3±0.5 eV measured in direct and inverse photoemission [1]. However, the lowest exciton computed in Bethe-Salpeter calculations for the optical spectrum is found at an energy of 3.21 eV, while optical experiments only give 3.03 eV [2]. Polaronic effects, i.e. the renormalization of the band edges due to electron-phonon coupling, reduce the band gap, but it remains a challenge to include the ionic contribution to the dielectric function, which can be substantial in oxides, in the G_0W_0 calculations and to incorporate both effects consistently into Bethe-Salpeter calculations. Another aspect to consider is the role of electron correlations. [1] Y. Tezuka *et al.*, J. Phys. Soc. Jpn.**63**, 347 (1994). [2] J. Pascual *et al.*, Phys. Rev. B **18**, 5606 (1978).

11:27AM Q16.00002 Calculated Electronic Properties of Rutile TiO_2 and Cubic $SrTiO_3$, CHINEDU EKUMA, Louisiana State University, Baton Rouge, LA, DIOLA BAGAYOKO, Southern University and A&M College, Baton Rouge, LA — We present preliminary, calculated, electronic properties of rutile titanium dioxide (TiO_2) and of cubic strontium titanate ($SrTiO_3$). Our computations employed local density approximation (LDA) and generalized gradient Approximation (GGA) potentials for TiO_2 and $SrTiO_3$, respectively. We implemented the linear combination of atomic orbitals (LCAO) within the framework of the Bagayoko, Zhao, and Williams (BZW) method. In doing so, we solved, self-consistently, both the Kohn-Sham equation and the equation giving the ground state charge density in terms of the wave functions of the occupied states. Our preliminary findings indicate that TiO_2 has an indirect band gap of 2.95 eV, from Γ to R. The direct gap at Γ is 0.10 eV larger. The indirect band gap of $SrTiO_3$, from L to Γ or X, is 3.05 eV.

Work funded in part by the Louisiana Optical Network Initiative (LONI), the National Science Foundation (NSF) and the Louisiana Board of Regents [Award Nos. EPS-1003897 and NSF (2010-15)-RII-SUBR], and and Ebonyi State, Federal Republic of Nigeria [Award No: EBSG/SSB/FSA/040/VOL. VIII/039]

11:39AM Q16.00003 The confinement error corrections for the exchange energy in transition metal oxides , FENG HAO, Sandia National Laboratories, RICKARD ARMIENTO, MIT, ANN E. MATTSSON, Sandia National Laboratories — We present some recent advances towards a straightforward scheme to correct for the confinement errors of the exchange energy of the transition metal oxides (TMO). This approach includes two steps: (i) identifying the spatial regions where the confinement errors exist, using local density and kinetic energy density information, and (ii) mapping these spatial regions to harmonic-oscillator (HO) models [1], and quantifying and correcting the relative confinement errors based on the model system. The scheme has been applied to calculations with several local and semi-local functionals, and a trend of improvement for the equilibrium structure is obtained after applying these confinement error corrections. Sandia is a multiprogram laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Company, for the U.S. Department of Energy's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

[1] Hao et al, PRB **82**, 115103 (2010).

11:51AM Q16.00004 First principles study of electronic and structural properties of CuO , BURAK HIMMETOGLU, MATTEO COCOCCIONI, University of Minnesota — The ground state of CuO is particularly challenging to study with DFT-based computational techniques even below its Neel temperature. This situation is due to the inability of most approximate DFT energy functionals to describe electronic regimes hat are dominated by many-body effects. In this study, we show how a description of the ground state of this material in better agreement with observations can be obtained using extended Hubbard-based corrective energy functionals (DFT+U and DFT+U+V). In particular we uncover an orbitally ordered insulating ground state for the cubic phase of CuO (that was expected, but never reported before) whose appearance is determined by a fine interplay between correlation effects and magnetic interactions. Starting from this ground state we also study the tetrahedral distortion of the unit cell (recently reported in experiments), characterizing the reorganization of the electronic states and identifying all the equilibrium structures.

12:03PM Q16.00005 Transition metal dioxides: a case for the intersite term in Hubbard-model functionals , HEATHER KULIK, Stanford University, NICOLA MARZARI, Oxford University — Triatomic transition-metal oxides in the "inserted dioxide" (O-M-O) structure represent one of the simplest examples of systems that undergo qualitative geometrical changes via subtle electronic-structure modulation. We discuss three transition-metal dioxide molecules (MO_2 where M = Mn, Fe, or Co), for which equilibrium structural (eg bent or linear geometry) and electronic (eg spin or symmetry) properties have been challenging to assign both theoretically and experimentally. Augmenting a standard density-functional theory (DFT) approach with a Hubbard term (DFT+U) occasionally over-localizes the $3d$ manifold, leading to incorrect bond elongation and, in turn, poor equilibrium geometries for MO_2 molecules, while preserving good spin-state splittings. We recover a proper description of both geometry and energetics for these molecules through either calculating DFT+U relaxations at fixed M-O bond lengths or by inclusion of an inter-site interaction term V that favors M($3d$)-O($2p$) interactions. In the latter case, both U and V are calculated fully from first-principles and are not fitting parameters. Finally, we present an approach that more accurately determines the Hubbard U over a coordinate in which the character of bonding varies.

12:15PM Q16.00006 On the origins of the deficiencies of density functional theory exchange-correlation functionals for transition metal oxides , ANN E. MATTSSON, Sandia National Laboratories, RICKARD ARMIENTO, MIT, FENG HAO, Sandia National Laboratories — The transition metal oxides (TMO) are a class of compounds that are difficult to treat in density functional theory (DFT) with simple local and semi-local functionals. Especially for CuO, they failed to give the correct equilibrium monoclinic structure. The major source of the deficiency is attributed to the imperfect cancellation of the electronic self-interaction (SI) in the approximated exchange energy. Previous studies [1] show that a large part of the SI error is connected to the confinement error that can be modeled by harmonic-oscillator (HO) systems. We discuss recent advances towards a simple methodology to quantify the confinement errors in real TMO systems. Our results show that these confinement errors may account for the deficiencies of DFT functionals in obtaining the correct equilibrium structure of the TMO. Sandia is a multiprogram laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Company, for the U.S. Department of Energy's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

[1] Hao et al, PRB **82**, 115103 (2010).

12:27PM Q16.00007 Ab initio calculation of the orbital magnetization by Wannier interpolation , GRAHAM LOPEZ, Wake Forest University, DAVID VANDERBILT, Rutgers University, IVO SOUZA, University of California Berkeley, TIMO THONHAUSER, Wake Forest University — We present an analytic, first-principles scheme to efficiently calculate exactly the spontaneous orbital magnetization of ferromagnetic crystals [1,2]. This is in contrast to the standard method of integrating inside muffin-tin spheres which, while a good approximation in practice, is still an approximation. The method uses Wannier interpolation to perform the necessary Brillouin-zone integrals in a similar way as was done previously for the anomalous Hall conductivity [3]. The method has been implemented to work with a plane-wave density-functional code, and calculations were done on iron, cobalt and nickel. We compare our calculations of the orbital magnetization in these systems to recent ab initio and experimental results and find good agreement with both [4].

[1] T. Thonhauser et al., Phys. Rev. Lett. **95**, 137205 (2005).
[2] D. Xiao et al., Phys. Rev. Lett. **95**, 137204 (2005).
[3] X. Wang et al., Phys. Rev. B, **74**, 195118 (2006).
[4] D. Ceresoli et al., Phys. Rev. B **81**, 060409(R) (2010).

12:39PM Q16.00008 Origin for the disorder-induced quantum criticality in $NbFe_2$[1] , AFTAB ALAM, DUANE JOHNSON, Division of Materials Science and Engineering, Ames Laboratory, Ames, Iowa — Using KKR-CPA ab-initio electronic-structure method founded on an optimal site-centered basis-set, we investigate the key features giving rise to the quantum critical transitions observed in $NbFe_2$ upon doping with 1.75% Nb [1]. These phase transitions involve lowest-energy excitations at/near the Fermi surface. In particular, it is suggested to arise due to an accidental unconventional band critical point (uBCP) with vanishing quasi-particle velocity [2]. Moving off-stoichiometry by increasing Nb, or reducing electrons (e/a), we find the Fermi level E_f increases (rather than decreases based only on band-filling) and meet the uBCP to produce excitations driving the anomalies. We detail the concentration-dependence electronic dispersion, density of state, E_f shift, and energies for $NbFe_2$, and why disorder increase the E_f with electron loss. At stoichiometry all our results agree with those from full potential calculations, including itinerant magnetism.

[1] D. Moroni-Klementowicz et al., Phys. Rev B 79, 224410 (2009).
[2] Brian Neal, Erik R. Ylviskar, and Warren E. Pickett, private communication (2009).

[1]Work was supported by the Department of Energy, Office of Basic Energy Science under contracts DE-FG02-03ER46026, as well as DE-AC02-07CH11358 at the Ames Laboratory operated by Iowa State University.

12:51PM Q16.00009 Electronic structures of superionic conductor Li_3N , MASARU AOKI, Shizuoka Sangyo University, YOSHIYUKI ODE, KAZUO TSUMURAYA, Meiji University — Lithium nitride is a superionic conductor with high Li conductivity. The compound has been studied extensively because of its potential utility as electrolyte in solid-state batteries. Though the mobility of the cations within the crystalline solid is high comparable to that of molten salts, the mechanism of the high mobility of the cations remains unsolved. To clarify the origin of the mobility we investigate the electronic states of the Li cations in the Li_3N crystal with the first principles electronic structure analysis, focusing a correlation between the cations and the ionicities of the constituent atoms. We have found the existence of the covalent bonding between the Li atoms in the Li_3N crystal in spite of the ionized states of the constituent atoms.

1:03PM Q16.00010 Why are the copper cations superionic in the α-CuI crystal? , KAZUO TSUMURAYA, TAKAMITSU OHTSUKA, HIDEKAZU TOMONO, Meiji University — The mechanism of the superionic conduction is an unresolved issue in the solid-state physics. The cations are mobile species in α-CuI and α-AgI crystals. In these conductors, the constituent atoms are ionized. The clarification of the mechanism of the high mobility of the cations needs to investigate the electronic structures in the α-CuI crystal. We obtain the dynamically-averaged local (DAL) positions of the mobile copper cations in the crystal from the pair distribution function and the angle distribution functions, which we calculate from the first principles molecular dynamics simulations at 700 K. The positions predict the existence of a correlation among the cations in the α-CuI. The static electronic structure analysis, of the DAL structure, allows us to clarify the correlation. The correlation enables us to clarify the mechanism of the migration and the difference in the electronic structures between the conductors and the ionic crystals.

1:15PM Q16.00011 First-principles investigation of band offsets and dielectric properties of Silicon-Silicon Nitride interfaces[1] , TUAN ANH PHAM, Department of Chemistry, UC Davis, TIANSHU LI, Department of Chemistry, UC Davis and Department of Civil and Enviromental Engineering, The George Washington University, FRANCOIS GYGI, Department of Applied Science and Department of Computer Science, UC Davis, GIULIA GALLI, Department of Chemistry and Department of Physics, UC Davis — Silicon Nitride (Si3N4) is a possible candidate material to replace or be alloyed with SiO2 to form high-K dielectric films on Si substrates, so as to help prevent leakage currents in modern CMOS transistors. Building on our previous work on dielectric properties of crystalline and amorphous Si3N4 slabs [1], we present an analysis of the band offsets and dielectric properties of crystalline-Si/amorphous Si3N4 interfaces based on first principles calculations. We discuss shortcomings of the conventional bulk-plus line up approach in band offset calculations for systems with an amorphous component, and we present the results of band offsets obtained from calculations of local density of states. Finally, we describe the role of bonding configurations in determining band edges and dielectric constants at the interface.

[1] T. Anh Pham et al., Appl. Phys. Lett., 96, 062902 (2010).

[1]We acknowledge financial support from Intel Corporation.

1:27PM Q16.00012 STEM-EELS calculations including both fine structure and diffraction[1] , M.P. PRANGE, M.P. OXLEY, Vanderbilt University, S.J. PENNYCOOK, Oak Ridge National Lab, S.T. PANTELIDES, Vanderbilt University — Electron energy loss spectroscopy in scanning transmission electron microscopy (STEM-EELS) probes electronic excitations with high spatial and energy resolution. Interpretation of the spectra requires accurate treatment of both the diffraction of the electron probe and the electronic excitation of the sample. We present a theory of core loss STEM-EELS based on a detailed calculation of the mixed dynamic form factor (MDFF) using DFT which informs a Bloch wave treatment of the probe/sample interaction. No dipole approximation is made. The probe diffraction is computed using the Bloch wave method which includes the microscope geometry, multiple elastic, and thermal diffuse scattering. We illustrate the method with calculations of complex oxide materials.

[1]This work was supported by DOE grant DE-FG02-09ER46554 (M.P., M.P.O., S.T.P.) and by DOE BES Mater. Sci. and Eng. Div. (S.J.P.).

1:39PM Q16.00013 Extended Pi-Sigma tilde orbital model for CO adsorption on Pt and Ru[1] , THOMAS MION, NICHOLAS DIMAKIS, University of Texas Pan American, FAISAL ALAMGIR, National Institute of Standards and Technology, CHERNO JAYE, Hunter College of CUNY, DANIEL FISCHER, National Institute of Standards and Technology, PAUL MCGINN, JAMES COOPER, University of Notre Dame, STEVE GREENBAUM, Hunter College of CUNY, EUGENE SMOTKIN, Northeastern University — Several discrepencies between the predicted Blyholder-type adsobtion models and experimental, as well as DFT calculated infared spectra have been addressed for atop CO on Pt in contrast to Ru. This model correlates increased Near Edge X-Ray Absorbtion Fine Structure intensity as the result of a sub-eV downshift from CO on Ru compared to CO on Pt thereby forming a weaker C-O bond. The model accounts for the hybrid orbitals electron transfer between the CO - metal bonds while taking in to consideration the orbital polarization within the CO itself. The charge redistribution of the s-tilde orbitals and reduced charge donation from CO to the surface results in a weaker internal CO bond upon Ru relative to Pt. The extended Pi-Sigma model explains why atop C-O stretching frequencies do not correlate with carbon p-type vacancies.

[1]Calculations done on the High Performance Computing Cluster at UT-Pan American. NEXAFS was done on U7A NIST/DOW beamline at Brookheaven National Synchrotron Light Source with funding from the Army Research Office.

1:51PM Q16.00014 Chirality and Electronic Structure of the Thiolate-Protected Au_{38} Nanocluster , OLGA LOPEZ-ACEVEDO, Department of Physics and Chemistry, Nanoscience Center, University of Jyväskylä, Finland, HIRONORI TSUNOYAMA, TATSUYA TSUKUDA, Catalysis Research Center, Hokkaido University, Japan, HANNU HÄKKINEN, Department of Physics and Chemistry, Nanoscience Center, University of Jyväskylä, Finland, CHRISTINE M. AIKENS, Department of Chemistry, Kansas State University, US — Our joint computational and experimental investigation of the structural properties of the $Au_{38}(SR)_{24}$ gold protected nanocluster will be presented [1]. We have identified a new low-energy, chiral, D_3 symmetric structure that yields an excellent match between computed and measured powder XRD function. We have characterized the electronic shell structure of this nanocluster in terms of a particle-in-a-cylinder model. The CD response in the low-energy region (below 2.2 eV) of the new structure is very similar to the one reported several years ago from experiments for $Au_{38}(SG)_{24}$. The mechanism of the chiral response for low excitation energies is related to the chiral arrangement of the gold-thiolate ligand shell around the bi-icosahedral Au_{23} core. The determination of the total structure of $Au_{38}(SC_2H_4Ph)_{24}$ nanoparticles by single crystal X-ray crystallography confirmed our results [2].

[1] O. Lopez-Acevedo et al J. Am. Chem. Soc., 2010, 132 (23)
[2] Qian et al J. Am. Chem. Soc., 2010, 132 (24)

2:03PM Q16.00015 Pseudospectral Calculation of Helium Wave Functions, Expectation Values, and Oscillator Strength[1] , PAUL GRABOWSKI, Los Alamos National Laboratory, DAVID CHERNOFF, Cornell University — We extend the pseudospectral method from the solution of Schrödinger's equation for two-electron atom S states to arbitrary angular momentum states. We evaluate the oscillator strength for the helium $1^1S \rightarrow 2^1P$ transition. The result, 0.27616499(27), compares favorably to the best determination in the literature. The length, velocity, and acceleration expressions all have roughly the same accuracy in a pseudospectral treatment. We evaluate leading order finite-nuclear-mass and relativistic corrections for the helium ground state. The pseudospectral method achieves near state-of-the-art accuracy without requiring the implementation of any special-purpose numerical treatments. All the relevant quantities tested converge exponentially with increasing resolution and at roughly the same rate. Quantum mechanical matrix elements are directly and reliably calculable with pseudospectral methods. A general prescription is given for choosing coordinates and subdomains to achieve exponential convergence when two-particle Coulomb singularities are present.

[1]This material is based upon work supported by the National Science Foundation under Grant No. AST-0406635 and by NASA under Grant No. NNG-05GF79G.

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q17 DMP GMAG: Focus Session: Bulk Properties of Complex Oxides - Ruthenates

11:15AM Q17.00001 High-pressure Synthesis and Magnetic Properties of 4d and 5d Transition-metal Oxides[1]

, J.-G. CHENG, University of Texas at Austin — The pressure effect on synthesis of oxides with perovskite ABO_3 and perovskite-related structures has become more clear in recent years. The geometric tolerance factor t $\equiv$ (A-O)/$\sqrt{2}$(B-O) measures the structural stability. High-pressure synthesis enlarges the range of the t factor where the perovskite structure can be stabilized. For the ABO_3 compounds with t $>$ 1, high pressure reduces the t factor since the A-O bond is more compressible than the B-O bond. Therefore, perovskite would be the high-pressure phase for ambient-pressure polytype structures. However, the bonding compressibility argument is no longer valid for the ABO_3 with t $<$ 1. A dt/dP $>$ 0 is normally obtained for t less than but very close to 1, *i.e.* the orthorhombic distortion becomes smaller under pressure. For those highly distorted perovskites with t factor far less than one, pressure enlarges further the orthorhombic distortion and eventually leads to a phase transition to the post-perovskite phase. As for $PbRuO_3$, high pressure prefers the small-volume perovskite phase relative to a competitive pyrochlore phase $Pb_2Ru_2O_7$. Understanding the pressure effect and the new capacity provided by a Walker-type multianvil press enabled us to expand the perovskite family and to obtain new phases of 4d and 5d oxides. Studies of these new 4d and 5d oxides allow us not only to address long-standing problems, but also to explore exotic physical properties. (1) In the perovskite $ARuO_3$ (A= alkaline earth), we have completed the phase diagram from A= Ca to Sr and to Ba and also accounted for the A-cation size-variance effect. A systematic study of the Curie temperature T_c and the critical behavior as a function of the average A-site size and the size variance as well as external high pressures reveals explicitly the crucial role of the lattice strain on the ferromagnetism. The mean-field critical behaviour near T_c found previously in $SrRuO_3$ is not typical of these perovskite ruthenates. T_c is completely suppressed by Pb doping in $Sr_{1-x}Pb_xRuO_3$ not due to the steric effect, but to the orbital hybridization between Pb^{2+} 6s and Ru^{4+} 4d. As the end member, metallic $PbRuO_3$ undergoes a first-order phase transition to a metallic *Imma* phase at $T_t \approx 90$ K. (2) A new polytype phase 5H has been synthesized under a narrow pressure range, which fits the structural sequence along with other polytypes 9R, 6H and 3C of $BaIrO_3$. The ground states of these $BaIrO_3$ polytypes evolve from a ferromagnetic insulator with $T_c \approx 180$ K in the 9R phase to a ferromagnetic metal with $T_c \approx 50$ K in the 5H phase, and finally to an exchange-enhanced paramagnetic metal in the 6H phase, which may be close to a quantum critical point. (3) In the $Ca_{1-x}Sr_xIrO_3$ system, high pressure stabilizes the post-perovskite structure on the Ca side (x $<$ 0.3), but favors the perovskite structure on the Sr side (x $>$ 0.6). Refs. J.-G. Cheng, *et al.* PRB **80**, 104430(2009); **80**, 174426 (2009); **81**, 134412(2010); JACS **131**, 7461(2009).

[1]Supported by NSF-DMR-0904282. Work under the supervision of Profs. J.-S. Zhou and J. B. Goodenough.

11:51AM Q17.00002 Spectroscopic Imaging - Scanning Tunneling Microscopy studies of the Nematic Metamagnet $Sr_3Ru_2O_7$

, M.P. ALLAN, Cornell University, University of St. Andrews, T.-M. CHUANG, Cornell University, National High Magnetic Field Lab, Y. XIE, Cornell University, A.W. ROST, University of St. Andrews, R.S. PERRY, University of Edinburgh, J.-F. MERCURE, University of Bristol, A. GIBBS, A.P. MACKENZIE, University of St. Andrews, J.C. DAVIS, LASSP, Dep. of Physics, Cornell University, Ithaca NY; CMPMS, Brookhaven National Laboratory, Upton, NY; University of St. Andrews, Fife, Scotland — The metamagnetic perovskite $Sr_3Ru_2O_7$ can be tuned towards a putative quantum critical point in an external magnetic field, and in ultrapure samples, an electronic nematic forms in a small region of the phase diagram around this putative quantum critical point. Much insight about these phenomena in $Sr_3Ru_2O_7$ come from a wealth of high-quality thermodynamic experiments but little is known about the microscopic electronic origin of criticality and nematicity. We recently re-engineered our SI-STM to achieve sub-Kelvin temperatures and magnetic fields up to 9T, and are now imaging the local density of states in different regions of the $Sr_3Ru_2O_7$ phase diagram, including within the nematic phase.

12:03PM Q17.00003 Entropy Accumulation near Itinerant Magnetic Quantum Critical Points

, JIANDA WU, Rice University, LIJUN ZHU, LANL, QIMIAO SI, Rice University, ANDREAS ROST, ANDY MACKENZIE, University of St. Andrews — Quantum critical point (QCP) occurs at a continuous phase transition at zero temperature. It follows from general hyperscaling argument that, near a QCP, the Grüneisen ratio (ratio of thermal expansion coefficient to specific heat) diverges and entropy accumulates [1]. The enhanced entropy has been observed near the field-induced metamagnetic QCP in Sr3Ru2O7[2]. Here we present a detailed theoretical study of entropy across itinerant-magnetic QCPs, with a focus on the ferromagnetic cases. We propose a regularization scheme for the effect of a dangerously irrelevant quartic coupling on the free energy [3], and calculate the entropy using this scheme. While the entropy accumulation near the QCP basically follows the hyperscaling arguments, the correction to scaling is sizeable especially for the two-dimensional case. We compare the theoretical results with the experimental data for Sr3Ru2O7 [2], providing an entropic characterization of the degree to which the metamagnetic QCP in this system is described by the itinerant-magnetic quantum criticality.

[1] L. Zhu et al, PRL 91, 066404 (2003).
[2] A.W. Rost et al, Science 325, 1360 (2009).
[3] J. Wu, L. Zhu, and Q. Si, arXiv:1010.4593, to appear in J. Phys.: Conf. Series.

12:15PM Q17.00004 Thermodynamics of the critical fluctuations and nematic phase formation of $Sr_3Ru_2O_7$

, ANDREAS W. ROST, SUPA/Univ. of St Andrews, ROBIN S. PERRY, SUPA/Univ. of Edinburgh, JEAN-FRANCOIS MERCURE, Univ. of Bristol, SANTIAGO A. GRIGERA, SUPA/University of St Andrews; IFLYSIB, ANDREW P. MACKENZIE, SUPA/Univ. of St Andrews — The itinerant metamagnet $Sr_3Ru_2O_7$ has motivated a wide range of experimental and theoretical work in recent years because of the discovery of an unusual low temperature phase which is forming in the vicinity of a proposed quantum critical point. The transport properties of this phase which exhibit strong electron-nematic-like behaviour [1] have led to a range of theoretical proposals for the underlying physics [2]. A major challenge both experimentally and theoretically is the investigation of the thermodynamic properties of both this unusual phase and the fluctuations associated with the quantum critical point. Here I will report on recent thermodynamic measurements. I will concentrate on new specific heat measurements investigating the nature of the critical fluctuations of the system as well as the low energy excitations of the novel phase.

[1] R.A. Borzi, S.A. Grigera, J. Farrell, R.S. Perry, S. Lister, S.L. Lee, D.A. Tennant, Y. Maeno & A.P. Mackenzie, Science 315, 214 (2007).
[2] For a recent review, see E. Fradkin, S. A. Kivelson, M. J. Lawler, J. P. Eisenstein & A. P. Mackenzie, Annual Review of Condensed Matter Physics 1, 153 (2010)

12:27PM Q17.00005 ABSTRACT WITHDRAWN –

12:39PM Q17.00006 Magnetic and structural transitions tuned by non-magnetic Ti doping in Ca3Ru2O7

, JIN PENG, GAOCHAO WANG, Department of Physics and Engineering Physics, Tulane University, New Orleans, LEONARD SPINU, Advanced Material Research Institute and Physics Department, University of New Orleans, LA, XIANGLIN KE, TAO HONG, Scattering Science Division, Oak Ridge National Laboratory, Oak Ridge, TN, ZHIQIANG MAO, Department of Physics and Engineering Physics, Tulane University, New Orleans — We report the effect of Ti doping on the structural and magnetic transitions in the bilayer Ruthenate Ca3Ru2O7. Ca3Ru2O7 orders antiferromagnetically at 56 K followed by a simultaneous structural and metal-insulator transition at 48 K [1]. Ti doping in Ca3Ru2O7 causes dramatic changes in both antiferromagnetic and structural transitions. With the Ti doping concentration above 5%, both transitions move to much higher temperature and merge, e.g. TN 85 K for 5% Ti, 113 K for 10% Ti. For the latter sample, the structural parameters change much more remarkably through the transition compared to Ca3Ru2O7 [2]. Such structural and magnetic transitions tuned by Ti-doping highlight the strong spin-lattice coupling in Ca3Ru2O7. Neutron scattering measurement on these samples will also be discussed.

[1] Cao G et al; PRB 78, 1751 (1997)
[2] Yoshida Y et al; PRB 72, 054412 (2005)

12:51PM Q17.00007 Element-resolved electronic and magnetic properties of $Sr_3(Ru_{1-x}Mn_x)_2O_7$, V.B. NASCIMENTO, Louisiana State University, Baton Rouge LA, J.W. FREELAND, APS - Argonne National Laboratory, Argonne IL, BIAO HU, R. JIN, E.W. PLUMMER, Louisiana State University, Baton Rouge LA — Bulk $Sr_3Ru_2O_7$ is a metal with short-range antiferromagnetic correlation developed at low temperatures. In the $Sr_3(Ru_{1-x}Mn_x)_2O_7$ series, the partial substitution of Ru by Mn changes both electronic and magnetic correlations driven by the modification of lattice degree of freedom. We have employed polarized x-rays to perform an element-resolved study of electronic and magnetic properties of this system with $0 < x \leq 0.5$. Our results indicate that at low doping Mn goes in as an electron acceptor (i.e. Mn 3+) which effectively dopes holes into the Ru system in a systematic way with increasing x. Using x-ray magnetic circular dichroism we have extracted the Mn and Ru contributions to the total magnetic moment, which will be connected to measurements of the total moment.

1:03PM Q17.00008 Metastable Magnetic states in $Ca_3Ru_2O_7$, D. FOBES, J. PENG, Z.Q. MAO, Department of Physics and Engineering Physics, Tulane University, New Orleans, LA 70118 — We have performed systematic in-plane angle dependent c-axis transverse magnetotransport measurements on the double layered ruthenate $Ca_3Ru_2O_7$ throughout a broad field and temperature range. Our results reveal the magnetic states for $H \| b$ to be significantly more complex than for $H \| a$. When magnetic field is applied along the b-axis we probe several metastable magnetic states in close proximity to phase boundaries of long-range ordered antiferromagnetic (AFM) states previously revealed by neutron scattering, i.e. AFM states with magnetic moments oriented along the b-axis (AFM-b) and a-axis (AFM-a); canted AFM state (CAFM) (Wei Bao *et al.*, Phys. Rev. Lett. **100**, 247203 (2006)). These metastable states are characterized by magnetoresistivity anisotropy distinct from that seen in the AFM-a, AFM-b, or CAFM phases, and switch either to a weakly ferromagnetic or AFM-b state when the magnetic field is rotated toward the *a*-axis. Additionally, our results highlight the complex nature of the spin-charge coupling in $Ca_3Ru_2O_7$.

1:15PM Q17.00009 Interplay of oxygen octahedral rotations and electronic instabilities in strontium ruthenate Ruddlesden-Poppers from first principles , JOHANNES VOSS, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University, Ithaca, NY — The Ruddlesden-Popper ruthenates $Sr_{n+1}Ru_nO_{3n+1}$ display a broad range of electronic phases including p-wave superconductivity, electronic nematicity, and ferromagnetism. Elucidating the role of the number of perovskite blocks, n, in the realization of these differently ordered electronic states remains a challenge. Additionally dramatic experimental advances now enable the atomic scale growth of these complex oxide thin films on a variety of substrates coherently, allowing for the application of tunable epitaxial strain and subsequently the ability to control structural distortions such as oxygen octahedral rotations. Here we investigate from first principles the effect of oxygen octahedral rotations on the electronic structure of Sr_2RuO_4 and $Sr_3Ru_2O_7$. We discuss possible implications for the physics of the bulk systems and point towards new effects in thin films.

1:27PM Q17.00010 $Ca_2Ru_{1-x}Cr_xO_4(0 < x < 0.13)$: Negative volume thermal expansion via orbital and magnetic orders[1] , T.F. QI, O.B. KORNETA, M. GE[2], L.E. DE LONG, G. CAO, Department of Physics and Astronomy, University of Kentucky, S. PARKIN, Department of Chemistry, University of Kentucky, P. SCHLOTTMANN, Florida State University — Ca_2RuO_4 undergoes a metal-insulator transition at T_{MI}= 357 K, followed by a well-separated transition to antiferromagnetic order at T_N= 110 K. Dilute Cr doping for Ru reduces the temperature of the orthorhombic distortion at T_{MI} and induces ferromagnetic behavior at T_C. The lattice volume V of $Ca_2Ru_{1-x}Cr_xO_4$ ($0 < x < 0.13$) abruptly expands with cooling at both T_{MI} and T_C, giving rise to a total volume expansion $\Delta V/V \approx 1$ %, which sharply contrasts the smooth temperature dependence of the few known examples of negative volume thermal expansion driven by anharmonic phonon modes. In addition, the near absence of volume thermal expansion between T_C and T_{MI} represents an Invar effect. The two phase transitions, which surprisingly mimic the classic freezing transition of water, suggest an exotic ground state driven by an extraordinary coupling between spin, orbit and lattice degrees of freedom.

[1]This work was supported by NSF through grants DMR-0552267, DMR-0856234 (GC) and EPS-0814194 (GC, LED), and by DoE through grants DE-FG02-97ER45653 (LED) and DE-FG02-98ER45707 (PS).

[2]Department of Physics, University of Science and Technology of China

1:39PM Q17.00011 Correlation between Structural and Magnetic Properties in $Sr_3(Ru_{1-x}Mn_x)_2O_7$ Single Crystals , BIAO HU, Department of Physics and Astronomy, Louisiana State University, GREGORY T. MCCANDLESS, Department of Chemistry, Louisiana State University, O.V. GARLEA, Neutron Scattering Science Division, Oak Ridge National Laboratory, S. STADLER, E.W. PLUMMER, R. JIN, Department of Physics and Astronomy, Louisiana State University — We have studied the Mn-doping (x) dependence of structural and magnetic properties in $Sr_3(Ru_{1-x}Mn_x)_2O_7$. The system remains tetragonal as determined by single-crystal X-ray diffraction with the lattice parameters a and c varying with x. Correspondingly, the value of Jahn-Teller distortion (Δ_{JT}) of (Ru,Mn)O_6 octahedron decreases with increasing x with Δ_{JT}= 1.0 for x$\sim$0.5. At the same doping level, we note the sign change of Curie-Weiss temperature Θ_{CW} derived from high-temperature magnetic susceptibility. The correlation between structural and magnetic properties will be discussed.

1:51PM Q17.00012 Managing magnetization and antiferromagnetic coupling in epitaxially grown magnetic oxide heterostructures of (Ga,Fe)2O3 and SrRuO3[1] , JIHYE LEE, WILLIAM JO, Department of Physics, Ewha Womans University, CHRISTIAN MENY , FRANCOIS ROULLAND, NATHALIE VIART, Institute of Physics and Chemistry of Materials of Strasbourg — We have grown b-axis oriented epitaxial (Ga,Fe)2O3 (GFO) thin films on (111) oriented SrRuO3 (SRO) by pulsed laser deposition to know spin interaction in multilayer system. The easy axis of magnetization of the GFO is located on the plane of the thin films. On the other hand, SRO has unique anisotropic properties on various crystallographic directions in their structure. Magnetic properties of the films were measured as a function of temperature and external magnetic field by a superconducting quantum interference magnetometer. Curie temperature of SRO and GFO was measured at 150K and 370K, respectively. According to the direction of external magnetic field, the magnetic moment value of the GFO/SRO heterostructures show different behavior due to antiferromagnetic coupling.

[1]This research was supported by Leading Foreign Research Institute Recruitment Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education, Science and Technology(MEST) (2010-00453)

2:03PM Q17.00013 ARPES Studies of the Evolution of the Ruthenate Family with Dimensionality , JOHN HARTER, DAWEI SHEN, CAROLINA ADAMO, Cornell University, CHARLES BROOKS, Penn State University, DANIEL SHAI, ERIC MONKMAN, DARRELL SCHLOM, KYLE SHEN, Cornell University — The Ruddlesden-Popper homologous series of ruthenates exhibits a wide range of remarkable electronic phenomena coupled to dimensionality, from spin-triplet superconductivity in quasi-two-dimensional single-layer Sr_2RuO_4, to metamagnetism and nematicity in bilayer $Sr_3Ru_2O_7$, to ferromagnetism in the fully three-dimensional pseudocubic end-member $SrRuO_3$. We report high resolution angle-resolved photoemission spectroscopy measurements of the electronic structure of ruthenate films grown by molecular beam epitaxy, with particular interest in the evolution of the quasiparticle interactions with increasing dimensionality. We start by investigating the anisotropic renormalization of quasiparticles in $SrRuO_3$ by strong electron-boson coupling, and examine changes in the Fermi surface and associated quasiparticles as a function of temperature through the Fermi-liquid to non-Fermi-liquid crossover and above the ferromagnetic Curie temperature. We also investigate the strain dependence of the low-energy electronic structure and quasiparticle interactions of $Sr_3Ru_2O_7$.

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q18 DMP GMAG: Focus Session: Magnetic Oxide Thin Films - Multiferroic Thin Films

D172

11:15AM Q18.00001 Enhanced magnetoelectric effects via strain engineering and structural softness[1]

, JORGE INIGUEZ, ICMAB-CSIC — After describing a general theory of the magnetoelectric response, I will argue that inducing *structural softness* – i.e., tuning a material so that it takes a small amount of energy to distort its structure – constitutes a general and robust strategy to obtain very large effects. Further, I will argue that this design strategy will be effective at room temperature, and will not affect other desirable properties of the materials (i.e., their insulating character). I will illustrate this possibility with first-principles results for thin films of room-temperature multiferroic $BiFeO_3$, where the structural softness is induced by epitaxial strain. I will also present results for $BiFeO_3$-based solid solutions, discussing several alternative mechanisms by which their electromechanical and magnetoelectric responses can be enhanced. Finally, I will discuss the prospect of inducing in $BiFeO_3$ a so-called *morphotropic phase boundary*, where the material is expected to display very large functional responses in analogy to what occurs in strong piezoelectric $PbZr_{1-x}Ti_xO_3$.

[1]Work done in collaboration with J.C. Wojdel, O. Dieguez and O.E. Gonzalez-Vazquez (ICMAB-CSIC); financial support from the Spanish DGI and the FP7 program of the EU.

11:51AM Q18.00002 Electrically Controllable Magnetism in Strained $BiFeO_3$ Thin Films

, QING HE, University of California, Berkeley, W. LUO, R. RAMESH, UC Berkeley, J.-C. YANG, Y.-H. CHU, National Chiao Tung University, A. SCHOLL, LBNL — multiferroic $BiFeO_3$ (BFO) thin films epitaxial strain can lead to the formation of a mixed phase system – highly distorted rhombohedral (R') and distorted tetragonal (super-tetragonal) (T) phases. Interestingly, this R' phase has been observed to be with enhanced magnetization compare to bulk BFO. Then, in order to investigate the origin of the magnetism in R' phase, synchrotron x-ray absorption, and x-ray (magnetic) circular/linear dichroism have been employed with assistance of spectra simulation and the ferroelectric, antiferromagnetic and ferromagnetic properties of this magnetic R' films have been clearly identified. Surprisingly, enhanced magnetization emerges in (001) plane as soon as a critical DC field is applied to the film in $< 001 >$ direction. The key is that the movement of Fe^{3+} can be controlled by external electric field, which magnifies the effect of Dzyaloshinsky-Moriya interaction to the system, and enlarges the canting magnetic moment of Fe spins. Finally, the direction of the local magnetic moment can be deterministically by external electric field will be demonstrated.

12:03PM Q18.00003 Origin of Reversible Electric Exchange Bias Modulation in a Multiferroic Field Effect Device[1]

, STEPHEN WU, SHANE CYBART, PU YU, R. RAMESH, R.C. DYNES, Materials Sciences Division, Lawrence Berkeley National Lab — We report the fabrication and characterization of two different oxide heterostructure based electric field effect devices: the multiferroic/ferromagnet, $BiFeO_3$(BFO) / $La_{0.7}Sr_{0.3}MnO_3$(LSMO) and the ferroelectric/ferromagnet, $Pb(Zr_{0.2}Ti_{0.8})O_3$(PZT)/LSMO. By switching FE polarization of BFO in the multiferroic device we observe a change in conductivity in the channel of 50%, and a 55% change in magnetic coercivity at 5.5 K. Furthermore, we can reversibly switch between two distinct exchange bias states corresponding to the different FE polarizations without additional field cooling. The difference in exchange bias between the two states is approximately 20mT. We further characterize the device by performing Hall Effect and temperature dependent exchange bias modulation measurements. Finally, we compare this device to a similarly fabricated PZT/LSMO field effect device. We observe no exchange bias and significantly smaller coercivity. No change in magnetic coercivity is observed when ferroelectric polarization is switched in PZT. Models based on these results will be presented.

[1]This work was supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

12:15PM Q18.00004 Electrical Transport Measurements of a Manganite Multiferroic Field Effect Device[1]

, JAMES PARKER, SHANE CYBART, STEPHEN WU, PU YU, R. RAMESH, R.C. DYNES, Materials Sciences Division, Lawrence Berkeley National Laboratory — We report electrical transport measurements of multiferroic/ferromagnet, BiFeO3 (BFO) / La0.7Sr0.3MnO3 (LSMO), electric field effect devices. The antiferromagnetic (AFM) ordering of the BFO dielectric layer is coupled to the ferromagnetic (FM) ordering of the LSMO channel layer and is observed as exchange bias –a shift of the LSMO magnetic hysteresis curve along the applied field axis. We will present the temperature dependence of this exchange bias between 2K and 100K. Furthermore, we also investigate the exchange bias with respect to multiple gating variables, including channel current and gate pulsing patterns. We have observed that the current in the channel during gating plays an important role in setting the exchange bias.

[1]This work was supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

12:27PM Q18.00005 Magnetic Structure of Engineered Multiferroic Thin Films[1]

, XIANGLIN KE, Neutron Scattering Science Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — The intriguing properties of multiferroics, i.e., materials exhibiting the coexistence of magnetism and ferroelectricity, have stimulated intense research interest in recent years. From the viewpoint of practical applications, one needs to exploit the thin film architectures of multiferroic materials. However, fewer studies have addressed the magnetic structures of multiferroic thin films. I will present recent experimental works on two multiferroic films, $BiFeO_3$ and $EuTiO_3$, physical properties of which can be engineered via the epitaxial growth on appropriate substrates. Neutron diffraction studies on $BiFeO_3$ films deposited on vicinal $SrTiO_3$ substrates show that the magnetic structure of these films is closely correlated with the ferroelectric states that depend on the chosen substrate miscut [1]. Epitaxial $EuTiO_3$ grown on $DyScO_3$ susbtrate, which is a paraelectric antiferromagnet in its bulk form, is strain-tuned into multiferroics, displaying both ferroelectric and ferromagnetic characters [2]. The relationship between the strong magnetic anisotropy and the film microstructure will be discussed.

[1] X. Ke, P. P. Zhang, S. Baek, J. Zarestky, W. Tian, and C. B. Eom, Phys. Rev. B **82**, 134448 (2010).
[2] J. H. Lee, L. Fang, E. Vlahos, X. Ke, Y.W. Jung *et al.*, Nature **466**, 954 (2010).

[1]In collaboration with P.P. Zhang, S.Y Baek, C. B. Eom, J.H Lee, P. Ryan, J.W. Freeland, D.A. Muller, C.J. Fennie, V. Gopalan, P. Schiffer, E. Johnston-Halperin, and D.G. Schlom. This work was supported by the Clifford G. Shull Fellowship at ORNL.

1:03PM Q18.00006 Electric-field control of spin waves at room temperature in multiferroic $BiFeO_3$, MAXIMILIEN CAZAYOUS, PAULINE ROVILLAIN, YANN GALLAIS, ALAIN SACUTO, MARIE-AUDE MEASSON, Laboratoire Materiaux et Phenomenes Quantiques, Paris, France, ROGERIO DE SOUSA, Department of Physics and Astronomy, Victoria, Canada, DOROTHEE COLSON, ANNE FORGET, Service de Physique de l Etat Condense, CEA Saclay, France, MANUEL BIBES, AGNES BARTHELEMY, Unite Mixte de Physique CNRS/Thales, France — A particularly exciting prospect in the field of spintronics is to use the wave like excitations of a magnetic material as a means to transmit and process information. This technology named magnonics relies on the control of spin waves. The key goal of magnonics is to read/write non-volatile spin information with minimal energy consumption. Multiferroic materials have at least two coupled magnetic and ferroelectric orders leading to electrical control of magnetic effects and vice-versa. Multiferroic materials are thus potentially interesting as a medium for spin-wave-based information processing. Here we show that the spin wave excitations in $BiFeO_3$, a room temperature multiferroic can be controlled by an electric field at low power and in a non-volatile way. The present experiment clearly demonstrates spin waves can be tuned over 30% of their frequencies, several orders of magnitude larger than with previous methods. The switch and the control of the polarization is used to manage this tuning.

1:15PM Q18.00007 Electric-field control of spin waves in multiferroic BiFeO3: Theory[1] , ROGÉRIO DE SOUSA, Dept. of Physics and Astronomy, University of Victoria, BC Canada, P. ROVILLAIN, Y. GALLAIS, A. SACUTO, M.A. MÉASSON, Universite Paris Diderot-Paris 7, D. COLSON, A. FORGET, Service de Physique de l'Etat Condense, CEA Saclay, M. BIBES, A. BARTHÉLÉMY, Unite Mixte de Physique CNRS/Thales, France, M. CAZAYOUS, Universite Paris Diderot-Paris 7 — Our recent experiment [1] demonstrated gigantic (30%) electric-field tuning of magnon frequencies in multiferroic BiFeO3. We demonstrate that the origin of this effect is related to two linear magnetoelectric interactions that couple the component of electric field perpendicular to the ferroelectric vector to a quadratic form of the Néel vector. We calculate the magnon spectra due to each of these interactions and show that only one of them is consistent with experimental data. At high electric fields, this interaction induces a phase transition to a homogeneous state, and the multi-magnon spectra will fuse into two magnon frequencies. We discuss the possible microscopic mechanisms responsible for this novel interaction and the prospect for applications in magnonics.

[1] P. Rovillain, *et al.*, Nature Materials advance online publication Nov. 14 2010 (DOI 10.1038/nmat2899), http://dx.doi.org/10.1038/nmat2899

[1]We acknowledge support from NSERC-Discovery (Canada) and the Agence Nationale pour la Recherche (France).

1:27PM Q18.00008 Ultrafast dynamics in multiferroic $BiFeO_3$, YU-MIIN SHEU, ROHIT PRASANKUMAR, ANTOINETTE TAYLOR, Los Alamos National Laboratory — We report the ultrafast time-resolved optical measurements of multiferroic $BiFeO_3$, which exhibits both magnetic and ferroelectric ordering at room temperature. The coupling between these two orders makes it an attractive material for potential data-storage devices. However, a detailed understanding of this coupling is still under debate. Ultrafast optical spectroscopy can potentially shed light on magnetoelectric coupling in $BiFeO_3$ by unraveling the different contributions in the time domain. Here, we use degenerate 400 nm pump-probe spectroscopy to excite and probe a $BiFeO_3$ thin film above its bandgap. The measured relaxation consists of a fast decay ($\sim$1 ps) followed by a slow recovery ($\sim$150 ps). We attribute the fast component to the recovery of photoexcited carriers. The slow recovery may be due to spin-lattice relaxation.

1:39PM Q18.00009 Substrate induced strain effects on the multiferroism of $BiMnO_3$ thin films[1] , HYOUNG JEEN JEEN, PATRICK MICKEL, A.F. HEBARD, AMLAN BISWAS, Department of Physics, University of Florida, Gainesville, FL 32611, VALENTIN CRACIUN, Major Analytical Instrumentation Center University of Florida Gainesville, FL 32611 — $BiMnO_3$ is a single phase multiferroic material, which shows ferroelectricity and ferromagnetism at low temperature. However, it is difficult to grow $BiMnO_3$ either in bulk or thin film form, since it is metastable with substantial desorption of Bi ions at high growth temperature. Here we have used $SrTiO_3$ and $SrLaGaO_4$ substrates, which provide different degrees of compressive strain, to stabilize the $BiMnO_3$ phase and have introduced fast quenching after deposition in oxygen atmosphere to suppress re-evaporation of Bi-ions but retain film crystallinity. Surface morphology indicates island growth mode. X-ray diffraction (XRD) shows that the $BiMnO_3$ [111] is parallel with [001] $SrTiO_3$ and [001] $SrLaGaO_4$. XRD results confirm that the $BiMnO_3$ films on $SrTiO_3$substrates are epitaxial, with in-plane alignment. The films have a magnetization of 1 μ_B/Mn at 5 T and 10 K. We also observed ferroelectricity in our $BiMnO_3$ films. Based on these results, we will discuss the substrate induced strain effects on the multiferroic properties of $BiMnO_3$ thin films.

[1]NSF DMR-0804452 (AB) and NSF DMR-1005301 (AFH)

1:51PM Q18.00010 Room-Temperature Multiferroic Properties of Bismuth Manganite Thin Film , W.C. KUO, C.Y. KUO, H.J. LIU, H.J. LIN, Y.H. CHU, Y.C. CHEN, T.M. UEN, J.Y. JUANG — In multiferroic materials, low temperature multiferroic properties in perovskite type $BiMnO_3$ has been demonstrated. In this work, through epitaxial strains exerted by $LaAlO_3$ single crystal substrate, we successfully demonstrate the growth the c-axis oriented new phase in BMO thin film. After the deposition, HRXRD has been used to characterize the lattice structure, which show new fascinating phase that are different from the papers early reported. We further revealed manganese valence through the X-ray Magnetic Linear Dichroism measurement and exhibit the mixed +3 and +4 valence of manganese. With $LaNiO_3$ bottom electrode, room-temperature ferroelectricity is demonstrated by piezoelectric force microscopy, which revealed the reversible ferroelastic switching through the external electrical bias. M-H curves are measured by SQUID magnetometer as a function of temperatures. Ferromagnetic behaviors have been probed from room temperature (300K) to low temperature (10K), furthermore, ferromagnetic phenomenon has been observed at 300K. In our preliminary results, room temperature ferroelectric and ferromagnetic properties could be coexistent in single phase material through epitaxial strain, thus provide a modeling system to study the multiferroic material and a powerful candidate for the next- generation electronic devices.

2:03PM Q18.00011 Magnetic field dependence of the spin wave excitations in $Sr_2FeSi_2O_7$, KAZUKI IIDA, JOOSEOP LEE, NAOYUKI KATAYAMA, SUNGDAE JI, SEUNGHUN LEE, University of Virginia, DUC LE, Helmholtz Zentrum Berlin, SUNG CHANG, NIST Center for Neutron Research, TAEHWAN JANG, YOONHEE JEONG, SANGWOOK CHEONG, Pohang University of Science and Technology, UNIVERSITY OF VIRGINIA TEAM, HELMHOLTZ ZENTRUM BERLIN COLLABORATION, NIST CENTER FOR NEUTRON RESEARCH COLLABORATION, POHANG UNIVERSITY OF SCIENCE AND TECHNOLOGY COLLABORATION — Without field, the multiferroic $Sr_2FeSi_2O_2$ orders below 4.7 K into a simple square-lattice antiferromagnetic collinear structure. Application of a magnetic field at low temperatures induces four different magnetic phases with spontaneous electric polarization. We report inelastic neutron scattering measurements on a single crystal of $Sr_2FeSi_2O_7$ under magnetic fields to investigate how the magnetic fluctuations change with field. In zero field, no dispersion was observed in L-direction, indicating that $Sr_2FeSi_2O_7$ is a two dimensional magnet. The dispersion relation along (H 0 0.5) shows a Goldstone mode arising from the magnetic Bragg position at (1 0 0.5) with a periodicity of $2 \times 2\pi/a$, suggesting that the strongest magnetic interaction is between the nearest neighbor Fe^{2+} ions. Under the field, the magnetic fluctuations become more complex than the simple splitting of the doubly degenerate Goldstone mode into two gapped modes.

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q19 GMAG: Ising, Spin Glass, Frustrated Magnets D170

11:15AM Q19.00001 Thermodynamics of the two-dimensional random-bond Ising model , CREIGHTON K. THOMAS, Texas A&M University, HELMUT G. KATZGRABER, Texas A&M University and ETH Zurich — The two-dimensional Ising spin glass possesses the disorder and frustration necessary to describe the rich behavior found in glassy materials with complex free-energy landscapes. Recently-developed exact algorithms for this model with arbitrary quenched bond disorder have allowed for equilibrium simulations of systems far larger than those accessible by other methods. We use a Pfaffian technique to measure thermodynamic quantities such as the specific heat and the domain-wall free energy to characterize the phase transitions in this model as either temperature or disorder strength is varied. We also present precision measurements on the disorder-temperature phase diagram of this model, including a detailed study of the reentrance that has been seen for bimodal disorder.

11:27AM Q19.00002 Competing Low-Temperature Phases in a Dilute Ising Magnet , M.A. SCHMIDT, D.M. SILEVITCH, T.F. ROSENBAUM, University of Chicago, G. AEPPLI, University College, London — LiHo(x)Y(1-x)F4 serves as a physical manifestation of the Ising model in transverse field with controllable disorder. At dilute Ho3+ dipole concentration, the combination of ferromagnetic and antiferromagnetic couplings via the spatial anisotropy of the dipolar coupling, disorder, and random internal fields combine to produce a variety of possible ground states. We show for x = 0.045 the ability to choose between spin liquid and spin glass behavior with proper thermal preparation. We present both linear and nonlinear magnetic susceptibility data as well as magnetic pump/probe techniques to quantify the stability of the liquid, and to probe the coupling between the spin states and the nuclear spin bath.

11:39AM Q19.00003 The p, q-binomial distribution applied to the Ising model , PER HÅKAN LUNDOW, ANDERS ROSENGREN, KTH — Monte Carlo simulations have shown that the p, q-binomial distribution closely fits the magnetisation distribution for the d-dimensional Ising model at all temperatures when $d > 4$. It also fits well for some temperatures near T_c for $d = 2, 3$ and especially so for $d = 4$. At high and low temperatures, away from T_c, the p, q-distribution always fits extremely well. However, it appears very difficult to determine how the parameters p and q depend of the temperature. From high and low temperature series expansions we can get partial results on their temperature dependence. Near T_c for $d = 5$ we have approximately that $p = 1 - 0.0736/L^5$ and $q = 1 - 9.87/L^5$ whereas for $d < 5$ the linear coefficient of q grows logarithmically. We show numerically how the parameters behave near T_c with increasing d.

11:51AM Q19.00004 ABSTRACT WITHDRAWN –

12:03PM Q19.00005 An ab initio study of radiation damage effects on the magnetic structure of bulk Iron[1] , YANG WANG, Carnegie Mellon University, G. MALCOLM STOCKS, ROGER STOLLER, DON NICHOLSON, AURELIAN RUSANU, MARKUS EISENBACH, Oak Ridge National Laboratory — A fundamental understanding of radiation damage effects in solids is of great importance in assisting the development of structural materials with improved mechanical properties for nuclear energy applications. In this presentation, we discuss our recent theoretical investigation on the magnetic structure evolution in bulk Fe after an energetic particle has disturbed the lattice by a displacement cascade. We applied a linear scaling ab initio method to the study of magnetic moment distributions in a low energy cascade for a series of time steps. The primary damage state and the evolution of the defects were simulated using molecular dynamics with a Finnis-Sinclair interatomic potential. We will show the statistics of the magnetic moments in the sample and discuss its relationship with the atomic volume distribution.

[1]1This research is based upon work supported as part of the Center for Defect Physics in Structural Materials (CDP), an Energy Frontier Research Center funded by DOE, Office of Science, Office of Basic Energy Sciences.

12:15PM Q19.00006 Chaos, broken hyperscaling, and nonuniversality in a spin glass[1] , A. ALAN MIDDLETON, Syracuse University, CREIGHTON THOMAS, Texas A&M University, DAVID HUSE, Princeton University — Recently extended precise numerical methods and newly modified scaling arguments allow for a coherent picture of the glassy state in a two-dimensional spin glass to be assembled. This glassy state, where the correlation length is larger than the system size, is characterized by "chaos," the extreme sensitivity of the state to temperature. This chaos is shown to lead to a breakdown of hyperscaling in spin glasses. The length scale at which entropy becomes important is found to depend on the type of randomness, so that though there is a type of universality, the critical exponents depend on the distribution of disorder. The numerical simulations use multiprecision arithmetic to exactly compute the partition function in samples of sizes up to $L^2 = 512^2$ down to temperatures of less than $J/20$, where the typical strength of the disorder is J. These results can be used in support of studies of the non-equilibrium behavior of glassy models.

[1]NSF DMR-1006731

12:27PM Q19.00007 Disordered Pinned Anyons in Two Dimensions , CHRIS LAUMANN, Harvard University, DAVID HUSE, Princeton University, ANDREAS LUDWIG, UCSB, GIL REFAEL, Caltech, SIMON TREBST, UCSB, MATTHIAS TROYER, ETH Zurich — We consider the effect of disorder on the behavior of pinned anyons in two spatial dimensions. Within an approximate numerical strong disorder renormalization group (SDRG) treatment, we find that both Fibonacci and Majorana anyons exhibit flows back to weaker disorder rather than toward infinite randomness phases such as those they exhibit in d=1. Restricting to the technically simpler Majorana anyons, we map out the effects of sign and coupling strength disorder on the proposed translation invariant topological liquid found in the absence of disorder. In disordered Hall bars, the nature of this descendant phase, and in particular its localization properties, may be relevant to the interpretation of transport and non-Abelian interferometry.

12:39PM Q19.00008 Effective potential study of the Diluted Antiferromagnet in a Field , DAVID YLLANES, L.A. FERNANDEZ, V. MARTIN-MAYOR — We present a numerical study of the three-dimensional Diluted Antiferromagnet in a Field (DAFF), one of the experimental realizations of the Random Field Ising Model. We work in a constrained ensemble (tethered ensemble) where the Helmholtz effective potential is featured, rather than the free energy. Our method cures the problem of a strong violation of self-averaging, thus allowing us to compute the correlation length for systems sizes up to $L = 32$. This quantity, when measured in units of the lattice size, is independent of the system size at the critical point, a strong indication of a second-order phase transition. This scale invariance allows us to apply finite-size scaling in the form of Nightingale's phenomenological renormalization. We obtain accurate estimates of the critical exponents. Since our method reconstructs the effective potential, we can also compute accurately the hyperscaling violation exponent. We perform as well an investigation of the geometrical properties of the instanton-like configurations, namely, the minimal cost configurations joining the two ordered phases. This study sheds light on previous claims of a first-order phase transition in this system.

12:51PM Q19.00009 Quantum Fidelity Susceptibilities of the Anisotropic Triangular Antiferromagnet: Conjugate Field Fidelity Susceptibilities , MISCHA THESBERG, ERIK S. SORENSEN, McMaster University — The Heisenberg model of the Anisotropic Triangular Antiferromagnet(HATM) has seen a surge of interest owing to its relation to Cesium Copper Chloride, an inorganic salt with a potential spin-liquid phase. In this talk a new approach to quantum fidelity susceptibilities will be introduced and used to explore the phase diagram of the HATM. These fidelity susceptibilities are computable via exact diagonalization techniques and can be coupled to specific order parameters. We present results from such calculations shedding new light on the phase diagram of the Anisotropic Triangular Antiferromagnet.

1:03PM Q19.00010 Stabilization of surface spin glass behavior in core/shell-Fe67Co33/CoFe2O4 nanoparticles , GHULAM JAFFARI, Department of Physics and Astronomy, University of Delaware, Newark DE 19716, SYED ALI, Physikalisches Institut (IIA), RWTH Aachen University, 52056 Aachen, Germany, SYED HASANAIN, Department of Physics, Quaid-i-Azam University, Islamabad 45320, Pakistan, GERNOT GÜNTHERODT, Physikalisches Institut (IIA), RWTH Aachen University, 52056 Aachen, Germany, SYED SHAH, Department of Physics and Astronomy, University of Delaware, Newark DE 19716, Department of Materials Science and Engineering, University of Delaware — Magnetic properties of Co33Fe67–CoFe2O4 (core-shell) nanoparticles are presented. Both dc magnetization and ac susceptibility measurements indicate a spin glass (SG) like transition occurring at TF ∼175 K. The SG nature of the transition is also confirmed by the field dependence of the freezing temperature TF(H) following the well known Almeida–Thouless line, δTF∼H$^{2/3}$. Additionally, the particles exhibit a large exchange bias (HEB ∼ 1357 Oe) arising from the core-shell (ferromagnetic-SG) coupling. The unusually high SG transition temperature and large exchange bias effects are attributed to a combination of several factors including the thickness of the amorphous oxide shell and large values of the exchange and anisotropy constants associated with the CoFe2O4 shell.

1:15PM Q19.00011 Critical Behavior of Lévy Spin Glasses , JUAN CARLOS ANDRESEN, Department of Physics, ETH Zurich, HELMUT G. KATZGRABER, Department of Physics, Texas A&M University & ETH Zurich — Universality, one of the foundations of the theory of critical phenomena, is well established for many problems in statistical physics. However, there is still debate if changing the disorder between the spins-spin interactions in spin glasses can influence the universality class of the system. This apparent violation of universal behavior can be attributed to the numerical complexity of these systems which limits simulations to small systems sizes, typically paired with strong corrections to scaling. Although it is well established that universality is not violated for nearest-neighbor spin glasses with compact disorder distributions (e.g., Gaussian and bimodal), some studies suggest that this might not be the case when the disorder distributions are broad, as in the case of the Lévy distribution. Using large-scale Monte Carlo simulations that combine parallel tempering with specialized cluster moves, as well as innovative scaling techniques, we show that Lévy spin glasses do obey universality for the system sizes studied. Furthermore, we probe recent analytical predictions made for the critical temperature of Lévy spin glasses as a function of the disorder distribution width.

1:27PM Q19.00012 Spin glasses on scale-free networks: Simple models to describe opinion formation? , HELMUT G. KATZGRABER, Texas A&M University and ETH Zurich, CREIGHTON K. THOMAS, Texas A&M University — We study the critical behavior of Ising spin glasses on scale-free networks using large-scale Monte Carlo simulations. Our results show that when the exponent that describes the decay of the interaction degree in the scale-free graph is strictly larger than 3 the system undergoes a finite-temperature spin-glass transition. However, when the exponent is equal to or less than 3, the spin-glass phase is stable for all temperatures. This robustness to local (temperature) perturbations and global biases (field) is compared to experimental data from social networks.

1:39PM Q19.00013 Using Azimuthal Hysteresis for Determining the Anti-ferromagnet Moment Density at the Spin Glass Interface: The case of BFO , KHALID ASHRAF, SAYEEF SALAHUDDIN, UC Berkeley — We report a systematic procedure for extracting the anisotropies, exchange energies and the surface anti-ferromagnet (AFM) moment of AFM-ferromagnet (FM) systems that show spin glass (SG) behavior. In any SG system, the hysteresis characteristics at a critical angle combined with the azimuthal hysteresis properties give important information about the surface AFM moment density and the coupling energy. Using this scheme we report the interface magnetic energy parameters of the epitaxial BFO-FM system. We find a single value for the interface coupling energy that reproduces both the exchange bias and the enhancement. Our extracted surface AFM moment density is of the order of the FM moment density that is independent of the FM material used. The high moment density on the BFO surface indicates a significant magnetic property modification at the BFO-FM interface. The implication of the presence of this high AFM moment is discussed in the context of achieving deterministic electric field driven magnetic moment switching.

1:51PM Q19.00014 Study of the Grüneisen Parameters at a Field-induced Quantum Critical Point in NiCl2-SC(NH2)2[1] , FRANZISKA WEICKERT, Los Alamos National Laboratory, MPA-CMMS, Los Alamos, NM, 87545, USA, ROBERT KUECHLER, ALEXANDER STEPPKE, LUIS PEDRERO OJEDA, MICHAEL NICKLAS, MANUEL BRANDO, FRANK STEGLICH, Max Planck Institute for Chemical Physics of Solids, Dresden 01087, Germany, VIVIEN ZAPF, MARCELO JAIME, Los Alamos National Laboratory, MPA-CMMS, Los Alamos, NM, 87545, USA, A. PADUAN-FILHO, Univ. of Sao Paulo, Sao Paulo, Brazil — $NiCl_2$-SC(NH_2)$_2$, also known as DTN, is a quantum paramagnet, where the Ni^{2+} single ion anisotropy D = 8.9K opens an energy gap between the $S_z = 0$ ground state and the $S_z = \pm 1$ exited state. In this material an XY-antiferromagnetic ordered state is induced at low temperatures by applying magnetic fields between H_{c1} ≈ 2T and H_{c2} = 10.5T. At the phase boundaries critical exponents consistent with Bose-Einstein condensation of magnons are found. Here we present investigations of quantum criticality close to H_{c1} by thermal expansion, magnetization and specific heat measurements. Our data reveal a divergency for T→ 0 of the thermal and magnetic Grüneisen parameters as expected for a quantum critical point of a diluted Bose gas.

[1]Part of this work was carried out at the MPI for Chemical Physics of Solids in Dresden, Germany.

2:03PM Q19.00015 Characteristic time scales and overlap distributions in replica exchange Monte Carlo simulations of spin glasses[1] , BURCU YUCESOY, JON MACHTA, University of Massachusetts Amherst , HELMUT G. KATZGRABER, Department of Physics, Texas A & M University & ETH Zurich — We present a large-scale numerical study using replica exchange Monte Carlo (parallel tempering) of time scales of the three- dimensional Ising spin glass. We measure the integrated and exponential autocorrelation times for several observables, as well as the round-trip times for different disorder realizations in order to investigate the relationship between the characteristic time scales of a disorder realization and its overlap distribution.

[1]Supported in part by NSF DMR-0907235.

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q21 GIMS: THz and Impedance Spectroscopy D161

11:15AM Q21.00001 Bulk focused ion beam fabrication of nanoelectromechanical systems , WAYNE HIEBERT, DOUG VICK, National Institute for Nanotechnology, National Research Council of Canada, VINCE SAUER, Department of Electrical and Computer Engineering, University of Alberta, ALASTAIR FRASER, OLEKSIY SVITELSKIY, MARK FREEMAN, Department of Physics, University of Alberta — Focused ion beam (FIB) nanomilling of NEMS devices out of bulk material will be presented. Ion impingement from multiple directions allows sculpting with considerable 3-dimensional control of device shape, including tapering and notching. Finite element modeling of device frequencies agrees with interferometric measurements, including for the effect of a localized notch. The measurements are sensitive enough to determine the thermomechanical noise floor of a bulk FIBed NEMS device with displacement sensitivity of 166 fm per root Hz, limited only by a combination of optical shot noise and detector dark current. We envision that bulk FIB fabrication will be useful for NEMS prototyping, milling of tough-to- machine materials, and generalized nanostructure fabrication with 3-dimensional shape control.

11:27AM Q21.00002 Terahertz spectroscopy of ionized air and explosive vapor , BENJAMIN GRABER, US. Naval Research Laboratory / Temple University, RONGJIA TAO, Temple University, DONG HO WU, US. Naval Research Laboratory — In the past it has been demonstrated that terahertz spectroscopy could identify various chemical agents and explosives in solid and liquid phases. However peaks and dips in the terahertz spectra obtained from solid and liquid phases are not sharp and often ambiguous or ill-defined, as the interferences among the molecules in the solid or liquid obscure the molecule's characteristic resonances. Hence there has been considerable interest in obtaining terahertz spectrum of gas phase. Recently we have increased terahertz output power of our terahertz spectrometer, and measured terahertz spectra of gases, including water vapor, and ionized air produced by various ionization sources as well as explosive vapors. Our experiments revealed: (1) our terahertz spectrum of water vapor was highly consistent with other published data, (2) the spectra of ionized air produced by corona discharge and nuclear isotopes including Am-241, Bi-207, Ba-133, Co-60, Na-22 and Cs-137 were all different, and the characteristic spectrum changes largely depending on the type of ionization source, and (3) terahertz spectra of explosive vapor taken from TNT, PETN and RDX which were dissolved in acetonitrile or water exhibit very sharp resonance peaks and dips. We will present details of our experimental results.

11:39AM Q21.00003 Characterization of high power near THz radiation from CMOS circuits using a Michelson Interferometer[1] , DANIEL J. ARENAS, Department of Physics, University of North Florida, DONGHA SHIM, Department of Computer and Electrical Engineering, University of Florida, DIMITRIOS KOUKIS, Department of Physics, University of Florida, EUNYOUNG SEOK, Texas Instruments, Inc., DAVID B. TANNER, Department of Physics, University of Florida, KENNETH K. O, Texas Analog Center of Excellence, Department of Electrical and Computer Engineering, University of Texas, Dallas — Recently, a high frequency SiGe BiCMOS Colpitts oscillator circuit was reported capable of emitting a second, third and fourth harmonic signal at 295, 442 and 589 GHz, respectively. The operating frequencies of the circuit and the emission powers were characterized using a Fourier transform interferometric spectrometer. The results show that this optical technique is an efficient way to characterize high-frequency circuits. The power emitted from the circuit at each frequency was also compared to that emitted from conventional blackbody sources. The results show that the high power emission of these circuits makes them ideal candidates for future spectroscopic applications.

[1]Supported by the US DOE through contract DE-FG02-02ER45984 at UF.

11:51AM Q21.00004 CNT Quantum dots as Terahertz detectors[1] , MOHAMED RINZAN, Physics Department, Georgetown University, GREG JENKINS, DENNIS DREW, Department of Physics, University of Maryland, SERHII SHAFRANJUK, Department of Physics and Astronomy, Northwestern University, PAOLA BARBARA, Physics Department, Georgetown University — We study Carbon Nanotube (CNT) quantum dots as detectors of THz radiation via photon assisted single electron tunneling. Although successful detection was recently demonstrated [1], the coupling between the CNT and THz radiations was very weak. Here, we implement a novel device design where the radiation is effectively coupled to the CNT quantum dot through broad band on-chip antennas. We show that the enhanced coupling yields a highly sensitive broad band Terahertz sensor.

[1] Y. Kawano, S. Toyokawa, T. Uchida and K. Ishibashi, THz photon assisted tunneling in carbon-nanotube quantum dots, Journal of Applied Physics 103, 034307 (2008).

[1]Funded by Airforce office of Scientific Research, Grant #FA9550-09-1-0697.

12:03PM Q21.00005 Highly absorbing metal nanolaminates for THz bi-material detectors[1] , DRAGOSLAV GRBOVIC, FABIO ALVES, APOSTOLOS KARAMITROS, GAMANI KARUNASIRI, Naval Postgraduate School — Interest in THz-ray sensing has significantly increased in recent years. It has been demonstrated that bi-material MEMS detectors show a great potential to be used for THz imaging. Our work aims to identify metal nanolaminates to improve the detector absorption in the range of interest. Using a finite element simulation tools we demonstrate that Chromium and Nickel films can absorb up to 50 and 35%, respectively, between 1 and 5 THz, depending on the thickness of the layer. Different thickness of Cr and Ni layers were deposited on Si substrate using e-beam evaporation and the wafers were characterized using a FTIR expanded to THz range. The experimental results show excellent match with the simulations. Further analysis shows that by decreasing the surface filling fill-factor of Ni, it is possible to increase absorption closeup to the values obtained for the Cr films indicating that much lower stress Ni films can be used in bi-material MEMS detectors with absorption comparable with Cr films.

[1]Supported by ONR.

12:15PM Q21.00006 Nanocoax arrays via NIL for high resolution sensing applications[1] , BINOD RIZAL, PATRICK JAMIESON, SVET SIMIDJIYSKI, HUAIZHOU ZHAO, DONG CAI, STEPHEN SHEPARD, THOMAS C. CHILES, MICHAEL J. NAUGHTON, Boston College — We have used nanoimprint lithography to fabricate nanocoax array-based chemical sensors, starting from SU-8 polymer replicas of silicon nanopillars. Nanocoaxes are formed by metalizing the polymer pillars, followed by oxide dielectric coating and outer metal deposition, and a polymer filling for stabilization. Chemical mechanical polishing and reactive ion etching were then used to open the ends of the coaxes and form coaxial cavity (with a nanoporous component) structures, respectively. Adsorption of water and organic solvent molecules into the coax annuli caused significant changes to the complex impedance of the coaxial capacitor array ($\Delta C/C > 100\%$ for 50% relative humidity air). Impedance measurements with such coaxial nanocavity arrays thus provide highly sensitive and selective information for molecular detection, with ultimate sensitivity below 1 ppb, or $\sim$1 $\mu g/m^3$.

[1]Supported by the National Cancer Institute CA137681, the National Science Foundation PHY-0804718, and the Seaver Institute. Contact: naughton@bc.edu

12:27PM Q21.00007 A high performance humidity sensor based on dielectric detection with a novel coaxial nanostructure[1] , DONG CAI, HUAIZHOU ZHAO, BINOD RIZAL, TIMOTHY KIRKPATRICK, ZHIFENG REN, MICHAEL J. NAUGHTON, THOMAS C. CHILES, Boston College — High throughput coaxial nanocavity arrays are developed by overlaying porous Al_2O_3 and Al layers on vertically aligned carbon nanotube arrays. The porosity of Al_2O_3 was electrochemically characterized. The dielectric properties of the nanocoax structure were measured by impedance spectroscopy, from 10 mHz to 1 MHz. The capacitance of the sensor responded to humidity applied to the chip, *i.e.* soaking the array with water increased the capacitance by 130%. The detection mechanism was established for sensing changes to the dielectric constant due to adsorbed moisture in the porous Al_2O_3 coax annulus, with theoretical calculations based on the Clausius-Mossotti equation in agreement with the measurements. Highly sensitive humidity detection was demonstrated by applying relative humidity between 0.1% and 100%, with a power-law response, $RH \sim x^{\alpha}$. This nanocoaxial structure thus offers the possibility of unprecedented performance of porous Al_2O_3-mediated capacitancer sensing for humidity detection.

[1]The National Cancer Institute CA137681, the Department of Navy, the National Science Foundation PHY-0804718, and the Seaver Institute. Emails: caid@bc.edu; naughton@bc.edu

12:39PM Q21.00008 Capacitance response of porous and cavitized nanocoax arrays to various gases[1] , PATRICK JAMIESON[2], BINOD RIZAL, SVET SIMIDJIYSKI, HUAIZHOU ZHAO, DONG CAI, MARK HASENAUER, MICHELLE ARCHIBALD, STEPHEN SHEPARD, GREGORY MCMAHON, MICHAEL J. BURNS, THOMAS C. CHILES, MICHAEL J. NAUGHTON, Boston College — Arrays of nanoscale coaxial electrodes with hollow or porous annuli offer the potential of highly sensitive detection and identification of gases and molecules. We report on the response of a porous and a partially hollow (cavitized) array to the introduction of various vaporized laboratory solvents. The response is measured as the capacitance and loss changes due to the introduction of molecules into the annuli, associated with the dielectric constant of the solvents, as well as the quantity and pressure. A monotonic dependence on concentration in dry nitrogen was observed.

[1]Support provided by NIH-NCI and NSF.
[2]Supported by the URF (Undergraduate Research Fellowship) program at Boston College.

12:51PM Q21.00009 Damping effects of capacitive comb fingers on biomimetic MEMS directional microphone[1] , JOHN ROTH, MICHAEL TOUSE, JOSE SINIBALDI, GAMANI KARUNASIRI, Naval Postgraduate School — MEMS directional sound sensors that use two coupled wings moving in air are subjected to viscous damping. The amplitude of oscillation of the sensors is read out by measuring the capacitance of interdigitated comb fingers along the edges of the wings. In this presentation, effects of damping on MEMS sensors with and without comb fingers will be described. It was found that the sensors with comb fingers have a significantly larger damping indicating that the longer perimeter due to combs is responsible for the observed increase [1]. However, the increase in damping reduces the quality factor which improves the response time of the device.

[1] W. Zhang and K. Turner, *Sensors & Actuators: A.* **134** p.594 (2007).

[1]This work is supported by NSF.

1:03PM Q21.00010 Attofarad capacitance measurement on organic thin films using Scanning Microwave Microscopy , SHIJIE WU, Agilent Technologies, Inc, JING-JIANG YU, Agilent Technologies, Inc. — Scanning microwave microscopy (SMM) is a recent development in SPM technique that combines the lateral resolution of AFM and the measurement precision of microwave analysis. It consists of an AFM interfaced with a vector network analyzer (VAN). In the reflection mode (S11 measurement), the measured complex reflection coefficient of the microwave from the contact point directly correlates to the impedance of the sample under test. The maximum sensitivity of the measurement is obtained at the resonance where the impedance of the sample under test matches the characteristic impedance. Since the measured load impedance is largely determined by the impedance of the sample under test, SMM can be used to measure the capacitances over dielectric thin films. In this presentation, we report the calibration of SMM using a capacitance standard developed by NIST. Then SMM is used to measure the minute capacitance difference between decanethiol and octadecanthiol SAM layers. The coexistence of two different SAMs on the same substrate with a well-known height difference of 0.88 nm is achieved via an AFM-based nanolithography method known as Nanografting. The measured capacitance difference is about 24 attofarads under the condition that the effective tip/sample contact area was estimated to be about 60nm in diameter.

1:15PM Q21.00011 Intermodulation Spectral Analysis and The Intermodulation Lockin , DAVID HAVILAND, Royal Institute of Technology (KTH), ERIK THÖLEN, DANIEL PLATZ, DANIEL FORCHHEIMER, CARSTEN HUTTER — High quality factor oscillators are very useful for sensitive measurement. A weak perturbation to the oscillator gives a large change of response near resonance, which is typically analyzed to first order as change in the linear response (e.g. shift of resonance frequency). In many cases the measurement can be greatly enhanced by detecting higher order nonlinear response. With a single drive frequency, high order non-linearity gives response at high frequency harmonics, which are filtered out by the high Q oscillator. With two drive frequencies, high-order nonlinear response can be crowded near resonance by intermodulation, or frequency mixing. The intermodulation spectrum near resonance is highly correlated and from its analysis one can reconstruct high-order non-linearity[1] without high frequency spectral data. We developed a general-purpose lockin measurement instrument and software analysis algorithms for preforming this type of measurement. The instrument drives a system with two pure tones while simultaneously measuring both quadratures of response at 32 intermodulation product frequencies.[2]

[1]C. Hutter et al. Phys. Rev. Lett. **104**, 050801 (2010)
[2]E. A. Thölen et al. submitted to RSI, arXiv:1008.2722

1:27PM Q21.00012 A Study of Ionic Transport Through Randomly-Aligned Silica Nanospring Using Electrochemical Impedance Spectroscopy , YUKTA P. TIMALSINA, JOSHUA BRANEN, ERIC ASTON, KEN NOREN, DAVID N. MCILROY, University of Idaho, Moscow, ID 83844 — A study of ionic transport through randomly aligned (silica) nanospring (RANS) using electrochemical impedance spectroscopy is presented. The device used for this study is a parallel plate capacitor consisting of two conducting surfaces with RANS as the dielectric spacer layer. The device response is evaluated with test solutions consisting of sodium chloride in a phosphate buffer. The experimental impedance data is analyzed using a model equivalent resistor-inductor-capacitor (RLC) circuit. The solution resistance through RANS and electric double layer formed at solution- electrode interface are elements of equivalent circuit that are more responsive and are more likely to be affected by changes of ionic concentrations. From our analysis we have determined that an electric double layer forms at the solution- RANS interface, which acts as a barrier to diffusion of ions from the solution into the RANS, and vice versa. We have also determined that ion diffusion is impeded by the RANS, as illustrated by changes in the resistance of the element of the equivalent circuit that corresponds to diffusion of ions through the RANS. The linear response of the RANS-based device below 10 kHz is potentially useful for many sensing applications.

1:39PM Q21.00013 Gas Sensing Properties of Hybrid SnO_2/Carbon Nanotubes , AZLIN BIAGGI-LABIOSA, LAURA J. EVANS, JENNIFER C. XU, GARY W. HUNTER, NASA Glenn Research Center, GORDON BERGER, National Center for Space Exploration Research, FRANCISCO SOLA, NASA Glenn Research Center — Chemical sensors involving nanostructured materials can be developed into sensor systems with unique properties and improved performance. One approach is to combine different nanomaterials in order to form hybrid structures with properties different than that of the constituent materials. Hybrid nanostructures consisting of tin oxide (SnO_2) nanocrystals distributed on the surface of multiwalled carbon nanotubes (MWCNTs) and singlewalled carbon nanotubes (SWCNTs) were fabricated and incorporated on a sensor platform in a controlled and efficient manner with a novel approach that combines dielectrophoresis with standard microprocessing techniques. Current vs. voltage and current vs. temperature curves were taken at different concentrations of hydrogen (H_2), hydrocarbons and nitrogen oxides (NO_x) at various operating temperatures for the hybrid nanostructures and were compared with their counterparts without SnO_2 nanocrystals. The tests showed that the hybrid nanostructures exhibit room temperature sensing capability when exposed to low concentration gases in contrast to the high operating temperature typically required for SnO_2 nanocrystals alone. High resolution electron microscopy and electron energy-loss spectroscopy will also be presented.

1:51PM Q21.00014 Development of a Tunnel Diode Resonator technique for magnetic measurements in Electrostatic Levitation chamber[1] , N.S. SPYRISON, P. PROMMAPAN, H. KIM, J. MALONEY, G.E. RUSTAN, A. KREYSSIG, A.I. GOLDMAN, R. PROZOROV, Department of Physics and Astronomy, ISU, Ames, IA 50011, USA — The incorporation of the Tunnel Diode Resonator (TDR) technique into an ElectroStatic Levitation (ESL) apparatus was explored. The TDR technique is known to operate and behave well at low temperatures with careful attention to coil-sample positioning in a dark, shielded environment. With these specifications a frequency resolution of 10^{-9} in a few seconds counting time can be achieved.[2] Complications arise when this technique is applied in the ESL chamber where a sample of molten metal is levitating less then 10 mm from the coil in a large electrostatic field. We have tested a variety of coils unconventional to TDR; including Helmholtz pairs and Archimedean spiral coils.

[1]Work was supported by the Nation Science Foundation under grant DMR-08-17157

[2]C. V. Degrift, "Tunnel diode oscillator for 0.001 ppm measurements at low temperatures," Rev. Sci. Instrum. **46**, 599 (1975).

2:03PM Q21.00015 Microwave impedance imaging on semiconductor memory devices , WORASOM KUNDHIKANJANA, KEJI LAI, YONGLIANG YANG, MICHAEL KELLY, ZHI-XUN SHEN, Geballe Laboratory for Advanced Materials, Departments of Physics and Applied Physics, Stanford University, CA 94305 — Microwave impedance microscopy (MIM) maps out the real and imaginary components of the tip-sample impedance, from which the local conductivity and dielectric constant distribution can be derived. The stray field contribution is minimized in our shielded cantilever design, enabling quantitative analysis of nano-materials and device structures. We demonstrate here that the MIM can spatially resolve the conductivity variation in a dynamic random access memory (DRAM) sample. With DC or low-frequency AC bias applied to the tip, contrast between n-doped and p-doped regions in the dC/dV images is observed, and p-n junctions are highlighted in the dR/dV images. The results can be directly compared with data taken by scanning capacitance microscope (SCM), which uses unshielded cantilevers and resonant electronics, and the MIM reveals more information of the local dopant concentration than SCM.

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q22 DCMP: Metal-Insulator Phase Transitions II D163

11:15AM Q22.00001 Fast pulsed measurements of the electric-field-driven metal-insulator transition in magnetite[1] , J. SPENCER MORRIS, Rice University, Houston, TX, R.G. SUMESH SOFIN, IGOR V. SHVETS, Trinity College, Dublin, IE, DOUGLAS NATELSON, Rice University, Houston, TX — Magnetite, Fe3O4, is an example of a strongly correlated material in which strong electron-electron interactions lead to unusual magneto-electronic properties. In particular, it undergoes a first-order phase transition on cooling through TV∼122K in bulk, in which a structural transition is accompanied by a significant drop in electrical conductivity. Recent electronic transport measurements have shown an electric-field driven breakdown of the insulating state in large aspect-ratio nanogaps fabricated on magnetite thin-films. The mechanism of this breakdown is of great interest in understanding the Verwey transition, and probing the intrinsic speed of the breakdown may further constrain possible mechanisms. We investigate the kinetics of this nonequilibrium transition by employing a high-speed pulse generator to apply voltages approaching the nanosecond time scale that exceed the critical switching value, and measuring the transmitted pulse via a high-speed oscilloscope. A significant change in transmission is observed for pulses that exceed the critical amplitude necessary to initiate the transition. Our initial results include an evaluation of the material response as a function of temperature and amplitude of the applied voltage.

[1]This work is supported by DOE award DE-FG02-06ER46337.

11:27AM Q22.00002 Magnetic field dependence of the nonequilibrium metal-insulator transition in magnetite nanostructures[1] , DOUGLAS NATELSON, Department of Physics and Astronomy, Rice University, ALEXANDRA A. FURSINA, Department of Chemistry, Rice University, R. G. S. SOFIN, IGOR V. SHVETS, School of Physics, Trinity College, Dublin, IE — At low temperatures magnetite undergoes a Verwey transition from a comparatively conducting state to a strongly correlated, ordered, more insulating state, the detailed nature of which remains under active debate. Recent experiments using nanostructures based on epitaxial magnetite films have shown that an applied dc electric field can lead to a nonequilibrium transition out of the insulating state. The kinetics of this nonequilibrium transition are nontrivial, with switching taking place over a distribution of applied voltages in a particular device at a given temperature below the Verwey transition. An externally applied magnetic field is observed to alter the kinetics of the nonequilibrium transition as the magnetization of the magnetite film is coerced out of plane. We present this data and discuss what it implies about the nature of the ordered, insulating ground state.

[1]This work is supported by DOE award DE-FG02-06ER46337.

11:39AM Q22.00003 Mesoscopic transport in ultrathin films of $La_{0.67}Ca_{0.33}MnO_3$, C. BEEKMAN, J. ZAANEN, J. AARTS, University of Leiden — We investigate the electrical transport in mesoscopic structures of $La_{0.67}Ca_{0.33}MnO_3$ in the regime of the metal-insulator transition by fabricating microbridges from strained and unstrained thin films. We measure current-voltage characteristics as function of temperature and in high magnetic fields and with varying film thickness. For strained films, in warming from the metallic to the insulating state, we find non-linear effects in the steep part of the transition characterized by a differential resistance with a strong peak around zero applied current, and saturating at higher currents after resistance drops up to 60 %. We propose that this nonlinear behavior is associated with melting of the insulating state by injecting charge carriers, signalling the occurrence of an intervening phase which involves the formation of short range polaron correlations.

11:51AM Q22.00004 In-situ TEM Analysis and Transport in Manganites $La_{5/8-y}Pr_yCa_{3/8}MnO_3$ Exhibiting Phase Separation below Metal-Insulator Transition , V. VOLKOV, J. HE, T. OSAKA, Y. ZHU, Brookhaven National Laboratory, S. CHAUDHURI, R. BUDHANI, Indian Institute of Technology — Epitaxial films of doped $La_{5/8-y}Pr_yCa_{3/8}MnO_3$ (LPCMO: y = 0.275-0.375) manganites were examined by *in-situ* Lorentz microscopy and other TEM methods below the metal-insulator transition point T_{MI} ~164 K. Such films are known for colossal magneto-resistance effect (CMR). Clear evidences were obtained for mesoscale two-phase separation process involving antiferromagnetic charge-ordered (AFM/CO) and ferromagnetic (FM) phases, coexisting below T_{MI} in LPCMO films. The first-order CO-FM phase transition is accompanied by partial magnetic melting of the CO phase at CO/FM interfaces thereby creating charge-disordered spin-glass metastates. In contrast, FM phase shows specific "zig-zag" magnetic domains coupled with dense (101) crystal twins. This allows refining relations for charge-orbital and spin-ordering vectors in films. Transport resistance data show that T_{MI} point is decreased with Pr_y growth in LPCMO. On cooling films below T_{MI} their resistance drops by several orders in magnitude. The observed M-I transition shows striking linear relation for log-conductance curve versus FM fraction measured by TEM, which does not follow typical percolation equations, suggesting that percolation transport model in manganites needs further revisions.

12:03PM Q22.00005 First Order CMR Transitions and Spin-Charge Dynamics Above the Curie Temperature in the Two-Orbital Model for Manganites[1] , CENGIZ SEN, University of Tennessee, GONZALO ALVAREZ, Oak Ridge National Lab, ELBIO DAGOTTO, University of Tennessee — We study the two e_g-orbital model including Jahn-Teller lattice distortions and the superexchange interaction using exact diagonalization Monte Carlo techniques at various dopings, x. We report the presence of first order CMR transitions at the Curie temperature (T_C) for doping $x = 0.25$ for the clean system and with weak disorder [1], in qualitative agreement with several experiments. We also discuss spin and charge dynamics as a function of Monte Carlo time above T_C, addressing the properties that characterize the exotic CMR state. It is observed that in CMR regimes there are various quasidegenerate spin states that may play an important role in this phenomenon [2].

[1] C. Sen *et al.*, Phys. Rev. Lett. **105**, 097203 (2010).
[2] Shuhua Liang *et al.*, preprint, submitted to PRB. See also Hotta *et al.*, Phys. Rev. Lett. **86**, 4922 (2001).

[1]This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division

12:15PM Q22.00006 Spin frustration effect near the Mott transition in the pyrochlore-type molybdates , SATOSHI IGUCHI, YUTA KUMANO, KOJI OISHI, Univ. of Tokyo, YOSHINORI TOKURA, Univ. of Tokyo, Multiferroics Project ERATO, and CMRG-RIKEN — Spin frustration and nontrivial spin structures by antiferromagnetic spins on a frustrated lattice have been widely studied such as a spin ice system with the pyrochlore structure $Ho_2Ti_2O_7$. However, spin frustration effects on conduction electrons have been less studied so far. Here, we have investigated spin frustration effects near the insulator-metal (Mott) transition in pyrochlore molybdates, where a paramagnetic diffuse metal state with antiferromagnetic spins is characteristic. Hole carriers were introduced by doping of Cd ions into the spin glass (Mott) insulator $Y_2Mo_2O_7$. The insulator to metal transition occurs at around $x = 0.1$ in $(Y_{1-x}Cd_x)_2Mo_2O_7$ with magnetically spin glass ground state. With increasing in the hole concentration, the spin glass transition disappears at around $x = 0.30$ and the resistivity shows almost no temperature dependence. Such a paramagnetic diffusive metallic character has been widely observed in $R_2Mo_2O_7$ (R = rare-earth ion) under high pressures. We have also measured the heat capacity in the system and found the anomalous enhancement of effective electron mass at around the transition from the spin glass metal to the paramagnetic metal phase.

12:27PM Q22.00007 Mott transition in multi-orbital Hubbard models for iron pnictides , RONG YU, QIMIAO SI, Department of Physics and Astronomy, Rice University — The bad-metal behavior of the iron pnictides has motivated a theoretical description in terms of a proximity to Mott localization. Since the parent compounds of the iron pnictides contain an even number of 3d-electrons per Fe, it is important to determine whether a Mott transition robustly exists and the nature of the possible Mott insulating phases. We address these issues in multi-orbital Hubbard models for the parent iron pnictides using a slave-spin approach. We show a metal-to-Mott-insulator transition in xz and yz orbitals generally exists in these models [1]. The nature of the metal-to-insulator transition may be strongly affected by the Hund's couplings. For certain values of Hund's couplings, we show there is a orbitally selective metal-to-insulator transition: the transition to a Mott insulator in the xz and yz orbitals takes place at the same critical coupling as the transition to either an orbitally polarized insulator or a band insulator in the other orbitals. Implications for the electronic and magnetic properties of the iron pnictides are discussed.

[1] R. Yu and Q. Si, arXiv:1006.2337.

12:39PM Q22.00008 Transport and spectra in the half–filled Hubbard model , HIMADRI BARMAN, VIDHYADHIRAJA SUDHINDRA, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India — We study the issues of scaling and universality in spectral and transport properties of the infinite dimensional particle–hole symmetric Hubbard model within dynamical mean field theory. We have used and reformulated the iterated perturbation theory approach to avoid problems such as analytic continuation of Matsubara frequency quantities or calculating multi-dimensional integrals, while taking full account of the very sharp structures in the Green's functions that arise close to the Mott transitions. We find a "coherence peak" in the dc resistivity of the metallic regime, which appears to be a universal feature occurring at a temperature roughly equal to the low energy scale of the system and agrees qualitatively well with the pressure dependent dc resistivity experiments on Selenium doped NiS_2. Resistivity hysteresis across the Mott transition is found and a direct comparison of the thermal hysteresis observed in V_2O_3 with our theoretical results yields a value of the hopping integral, which we find to be in the range estimated through first-principle methods. Finally, a systematic study of optical conductivity is carried out and the changes in absorption as a result of varying interaction strength and temperature are identified.

12:51PM Q22.00009 Spectral function near the Mott transition in the one-dimensional Hubbard model , MASANORI KOHNO, National Institute for Materials Science, Japan — Spectral properties near the Mott transition are investigated in the one-dimensional Hubbard model. The single-particle spectral function is calculated using the dynamical density-matrix renormalization group method, and the dominant modes are identified using the Bethe ansatz. Characteristic features near the Mott transition, such as the pseudogap, hole-pocket behavior, spectral-weight transfer, and upper Hubbard band, are explained in a unified manner in terms of spinons, holons, antiholons, and doublons. From the insulating side, the Mott transition is characterized by the emergence of a gapless mode whose dispersion relation extends up to the order of hopping (spin exchange) in the weak (strong) interaction regime caused by infinitesimal doping. From the metallic side, the transition is characterized as a loss of charge character from the mode having both spin and charge characters, while the spin excitation remains gapless and dispersing. These features cannot be explained in either the rigid-band picture or the Fermi liquid theory. I expect that generic features near Mott transitions can be deduced from the present results.

1:03PM Q22.00010 ABSTRACT WITHDRAWN –

1:15PM Q22.00011 Localized states in Mott insulator κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl probed by photoluminescence[1] , NATALIA DRICHKO, Johns Hopkins University, RUDI HACKL, Walter Meissner Institute Garching Germany, JOHN SCHLUETER, Argonne National Laboratory — We present the luminescence spectra of a low-temperature Mott insulator (T_c=35 K) κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl and a metal with a superconductor transition κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br in the temperature range between 300 and 10 K. In the Mott insulating state we observe an appearance of a luminescence at 1.95 eV, which corresponds to a LUMO-HOMO transition in a BEDT-TTF molecule. This luminescence is quenched both in the higher-temperature semiconducting state of κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl and metallic κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br. To our knowledge, it is the first observation of luminescence driven by electronic correlations. This observation gives an evidence of the local character of BEDT-TTF energy levels in the Mott insulating state, in contrast to the band-character in the metallic and semiconducting states.

[1]Supported by Blewett Fellowship

1:27PM Q22.00012 Quantum electric dipoles in spin liquid dimer Mott insulator , CHISA HOTTA, Kyoto Sangyo University — We present an effective dipolar-spin model based on the strong coupling analysis, which may explain the possible origin of the "spin liquid Mott insulator" of the organic triangular lattice system, kappa-ET_2Cu_2 $(CN)_3$, whose gapless spin liquid state had been discussed in the context of geometrical frustration of exchange coupling, J, between spins on dimer orbitals. We find out that another degrees of freedom within the insulator, quantum electric-dipoles on dimers, interacts with each other by the Coulomb interaction and brings about a significant suppression of$J$ through the dipolar-spin coupling.

1:39PM Q22.00013 Numerical study on the ionic Hubbard model in one and two dimensions , JI-WOO LEE, YONG CHUL LEE, SOO HYUN CHO, Myongji University — We investigate the quantum phase transition of an ionic Hubbard model in one and two dimensions. There are three parameters in the ionic Hubbard model, one is the hopping term t, the other is the Coulomb term U between local spin-up and spin-down electrons, and another is the band energy Δ which corresponds to the difference in local chemical potentials of bipartite lattice. Via exact diagonalization and quantum Monte Carlo simulations, we obtained the phase boundary of Mott insulator, metal, and band insulator. We measure the ground state energy and the energy gap between the ground-state and the first excited-state energy, and also measure the order parameters such as Drude weight and double occupancy in the three phases to understand the nature of three phases.

1:51PM Q22.00014 Spectral properties of the one-dimensional Hubbard model: cluster dynamical mean-field approaches[1] , ARA GO, GUN SANG JEON, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea — We investigate static and dynamic properties of the one-dimensional Hubbard model using cluster extensions of the dynamical mean-field theory. It is shown that the two different extensions, the cellular dynamical mean-field theory and the dynamic cluster approximation, yield the ground-state properties which are qualitatively in good agreement with each other. We compare the results with the Bethe ansatz results to check the accuracy of the calculation with finite sizes of clusters. We also analyze the spectral properties of the model with the focus on the spin-charge separation and discuss the dependency on the cluster size in the two approaches.

[1]This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education, Science and Technology(2010-0010937).

2:03PM Q22.00015 Temperature Effects on Metal-Insulator Transitions in the Ionic Hubbard Model[1] , AARAM KIM, GUN SANG JEON, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea — The ionic Hubbard model is known to exhibit interesting transitions between metallic and insulating phases at zero temperature. We investigate finite-temperature phase transitions in the model. For an extensive finite-temperature study, we apply a dynamical mean- field theory with continuous-time quantum Monte Carlo method employed as an impurity solver. We examine how the transitions at zero temperature evolve as the temperature increases. We also discuss the effects of temperature on the nature of transitions and other properties of the system.

[1]This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education, Science and Technology(2010-0010937).

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q23 DMP DCOMP: Focus Session: Iron Based Superconductors – Fermi Topology

D165

11:15AM Q23.00001 Ab initio study of de Haas van Alphen effect in $BaRh_2P_2$ and $BaIr_2P_2$, SIMON BLACKBURN, MICHEL COTE, BOBBY PREVOST, ANDREA BIANCHI, Departement de physique, Universite de Montreal, QC, Canada, MAREK BARTKOWIAK, Paul Scherrer Institut-LDM, PSI, Switzerland, BEATE BERGK, OLEG IGNATCHIK, JOCHEN WOSNITZA, Dresden High Magnetic Field Laboratory, Forschungszentrum Dresden, Rossendorf, Germany, GABRIEL SEYFARTH, Univ Geneva, DPMC, CH-1211 Geneva, Switzerland, CIGDEM CAPAN, ZACHARY FISK, Department of Physics & Astronomy, University of California Irvine, Irvine, CA, USA — The de Haas-van Alphen (dHvA) effect is a powerful probe of the Fermi surface (FS) of a metal. Since it measures the area of a cross-section of the Fermi surface, a theoretical description of this surface complements well these experiments. However, a very accurate description of the FS is required from the ab initio calculations in order to calculate the dHvA frequencies. This is achieved using maximally localized Wannier functions (MLWF) (Marzari & Vanderbilt, *Phys. Rev. B*, 56, 12847)to interpolate the Hamiltonian on a dense k-point grid. In this work, we present a dHvA study of $BaRh_2P_2$ and of its isovalent material $BaIr_2P_2$, both structurally analog to the iron pnictide $BaFe_2As_2$. We also present results concerning $LaFe_2P_2$ and $CeFe_2P_2$ which are also related to $BaFe_2As_2$ by a rigid electronic band shift to account for the difference in the number of electrons.

11:27AM Q23.00002 ABSTRACT WITHDRAWN –

11:39AM Q23.00003 Transport properties of 3D extended s-wave states appropriate for iron-based superconductors[1]

, VIVEK MISHRA, University of Florida, SIEGFRIED GRASER, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, PETER HIRSCHFELD, University of Florida — The Fermi surfaces of Fe-pnictide superconductors are fairly two-dimensional (2D), and it has thus come as a surprise that recent penetration depth and thermal conductivity measurements on some systems have reported c-axis transport at low temperatures in the superconducting state comparable to or even larger than that in the ab plane. These results should provide important information on both the Fermi surface and the superconducting state. Here we consider the theory of the superfluid density and thermal conductivity in models of extended-s wave superconducting states expected to be appropriate for Fe-pnictide systems. We include both intra- and interband disorder and consider a range of different Fermi surfaces where gap nodes might exist. We show that qualitative fits can be obtained to match recent experiments on $Ba(Fe_{1-x}Co_x)_2As_2$, and discuss their implications.

[1]This work is supported by DOE DE-FG02-05ER46236 (PJH).

11:51AM Q23.00004 Fermi Surface of the Pnictide Superconductor $LaRu_2P_2$ studied by quantum oscillations

, PHILIP MOLL, Solid State Physics, ETH Zurich, FEDOR BALAKIREV, ROSS MCDONALD, NHMFL, LANL, Los Alamos, NM, JANUSZ KARPINSKI, ZBIGNIEW BUKOWSKI, Solid State Physics, ETH Zurich, PETER BLAHA, KARLHEINZ SCHWARZ, Computational Quantum Chemistry Group, TU Vienna, BERTRAM BATLOGG, Solid State Physics, ETH Zurich — $LaRu_2P_2$ is a stochiometric pnictide superconductor ($T_c \sim 4.1$K) and crystallizes in the $ThCr_2Si_2$ structure (the "122" pnictide family). We have mapped out its Fermi surface via the deHaas-vanAlphen effect in pulsed magnetic fields up to 60T (LANL/NHMFL). Pronounced oscillations were observed in the magnetic torque measured with a microcantilever setup. Two features are particularly noteworthy: The oscillations can be followed to surprisingly high temperatures beyond 20K, and the main frequency component at $\theta = 20^\circ$ ($\theta = 0^\circ$ at HIIc) is at 349T (α-peak), significantly lower than in the related compounds $LaFe_2P_2$. A second frequency originating from a larger Fermi surface cross-section at 1921 T (β-peak) is identified. The temperature dependence of the amplitudes is well described by the Lifshitz- Kosevich formalism and gives low effective masses $m^*/m = 0.80$ (α sheet) and 1.09 (β sheet). Therefore, most "122" metals appear to have similarly low effective masses.

12:03PM Q23.00005 Campbell penetration depth in stoichiometric LiFeAs - evidence for static fishtail effect

, PLENGCHART PROMMAPAN, HYUNSOO KIM, MAKARIY A. TANATAR, RUSLAN PROZOROV, Ames Laboratory, Ames, IA 50011, USA, BUMSUNG LEE, SEUNGHYUN KHIM, KEE HOON KIM, CeNSCMR & Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Republic of Korea — The "fishtail" or second magnetization peak is one of the most intriguing properties of high$-T_c$ cuprate superconductors. Now it has also been observed in iron-based materials and has been associated with weak collective pinning. To understand whether the fishtail effect has dynamic (due to field-dependent magnetic relaxation) or static behavior (due to actual non-monotonic field dependence of the true critical current) one needs to measure the clean system, which are rare in pnictide superconductors. A stoichiometric LiFeAs is one of the cleanest of the pnictides with RRR=65. We measured the Campbell penetration depth using a 10 MHz tunnel-diode resonator in DC magnetic fields of up to 9 T. As opposed to the "apparent" current density, estimated from the magnetization relaxed over tens of seconds, the Campbell penetration depth depends on the curvature of the pinning potential sampled at time intervals of 0.1 μsec, thus allowing one to estimate the unrelaxed, "true" $j_c(T, B)$. The obtained $j_c(T, B)$ shows a non-monotonic trend with a second peak shifting toward lower fields at higher temperatures implying a static origin of the fishtail effect in LiFeAs.

12:15PM Q23.00006 Measuring the Absolute Penetration Depth in Superconducting Materials.

, NICHOLAI SALOVICH, University of Illinois at Urbana-Champaign, RUSSELL GIANNETTA, University of Illinois at Urbana Champaign, RUSLAN PROZOROV, PAUL CANFIELD, Iowa State University, Ames Laboratory, SERGEY BUD'KO — The absolute penetration depths of a variety of superconductors were measured using a method involving a high precision tunnel diode oscillator and an Aluminum film coating method [1]. Variations of the Al film geometry (thickness, coverage area, etc) and microstructure (grain size, RRR, etc) were used to test the reliability and versatility of the coating technique. A variety of supplemental techniques (dual beam SEM, EBS, AFM, XRD, etc) were used to independently characterize the films and control their quality. Special emphasis was placed on measurements of cobalt doped iron pnictide samples given the well established quality of such samples now available. Work at UIUC supported by NSF DMR 10-05708, and Center for Emergent Superconductivity USDOE Award No. DE-AC02-98CH10886. Work at the Ames Laboratory was supported by the division of Materials Science and Engineering, Basic Energy Sciences, Department of Energy (US DOE), under Contract No. DEAC02-07Ch11358.

[1] R. Prozorov, et al, Appl. Phys. Lett 77,1202 (2000)

12:27PM Q23.00007 dHvA studies of the Fermi topology of Iron-based Superconductors and Metals[1]

, AMALIA COLDEA[2], University of Oxford — Quantum oscillations studies on various non-magnetic iron pnictides reveal a Fermi surface in broad agreement with the details of the band structure calculations and moderate enhancement of the electronic correlations [1,2,3,4]. Whether or not the nesting of the electron and hole bands are essential for explaining the superconducting behaviour in these materials is still under debate but it is becoming clear that structural alteration have a significant effect in determining their electronic properties. In this talk I will present quantum oscillations studies in materials in which the Fermi surface suffers major topological changes. I will discuss the effect of isoelectronic substitution and doping on the Fermi surface and the quasiparticle masses and their relevance for understanding the complex physics of these materials. This work is in collaboration with groups at Bristol University, Stanford University and Kyoto University [1,2,3,4] and experiments were performed at high magnetic field facilities in Tallahassee, Nijmegen and Toulouse.

[1] A. I. Coldea et al., Phys. Rev. Lett. 101, 216402 (2008);
[2] A. I. Coldea, et al., Phys. Rev. Lett. 103, 026404 (2009).
[3] J. G. Analytis, et al., Phys. Rev. Lett.103 076401 (2009).
[4] H. Shishido, et al., Phys. Rev. Lett.104, 057008 (2010).

[1]Acknowledge financial support from EPSRC and The Royal Society, UK
[2]United Kingdom

1:03PM Q23.00008 London penetration depth measurements in $Ba(Fe_{1-x}Ru_x)_2As_2$ single crystals

, RYAN GORDON, MAKARIY TANATAR, ALEXANDER THALER, RUSLAN PROZOROV, Department of Physics and Astronomy, Iowa State University and Ames Laboratory, Ames, IA — The variation of the in-plane London penetration depth with temperature, $\Delta\lambda_{ab}(T)$, has been measured in $Ba(Fe_{1-x}Ru_x)_2As_2$ single crystals by using a tunnel diode resonator (TDR). The crystals were grown out of self- flux, with superconductivity stabilized for $x > 0.2$ and the maximum $T_c \approx 16$ K corresponding to $x \approx 0.29$. The substitution of Ru for Fe in this compound is particularly interesting because it is isovalent, so that no additional charge carriers are added by the Ru. The low-temperature penetration depth has been found to exhibit a power law dependence, $\Delta\lambda_{ab}(T) \propto T^n$, with an x- dependent exponent, n. Using the penetration depth data, the superfluid density has been constructed and compared to known theoretical models for different superconducting pairing symmetries and impurity scattering limits. These results will be compared to previous measurements on different iron-based superconductors.

1:15PM Q23.00009 Superfluid Density Measurements of $Ba(Co_xFe_{1-x})_2As_2$ Films near Optimal Doping , JIE YONG, Dept. of physics, The Ohio State University, SANGHAN LEE, Dept. of M.S.E, University of Wisconsin, Madison, J. JIANG, Applied Superconductivity Center, National High Magnetic Field Laboratory, Florida State University, C.W. PARK, J.D. WEISS, E.E. HELLSTORM, D.C. LARBALESTIER, C.B. EOM, T.R. LEMBERGER — We report the first direct, low-frequency measurements of superfluid density, $n_s(T) \propto \lambda^{-2}(T)$, in $Ba(Co_xFe_{1-x})_2As_2$ thin films, near optimal doping. 100 nm thick films are fabricated by Pulsed Laser Deposition (PLD) in high vacuum and $SrTiO_3$ is used as template to match Ba layer in ba-122. Temperature dependence of superfluid density is measured by our two-coil mutual inductance apparatus down to 1.3K. The magnetic penetration depth, λ, at $T \approx 0$ is 350 to 430 nm. The T-dependence of λ^{-2} is well characterized by a small s-wave gap, $2\Delta(0)/k_BT_c = 2.2 \pm 0.1$. In detail, λ has power-law behavior at low T: $\lambda(T)/\lambda(0) - 1 = 0.60*(T/T_c)^{2.5\pm0.1}$. A tail of superfluid density near T_c is the only possible indication of a bigger gap. The small gap, together with power-law behavior at low-T, suggests strong intraband scattering on the larger-gap Fermi surface plus significant interband scattering between large-gap and small-gap Fermi surfaces.

1:27PM Q23.00010 Linear magnetoresistance in the underdoped iron pnictide $Ba(Fe_{1-x}Co_x)_2As_2$[1] , JIUN-HAW CHU, HSUEH-HUI KUO, SCOTT RIGGS, JAMES ANALYTIS, IAN FISHER, Stanford University — $BaFe_2As_2$ suffers an antiferromagnetic transition which has been described in terms of a nodal spin density wave. The material exhibits a striking linear magnetoresistance in the low temperature antiferromagnetic state, possibly related to the unique character of the reconstructed Fermi surface. Here we present data showing the evolution of the magnetoresistance as a function of both composition and temperature for the specific case of $Ba(Fe_{1-x}Co_x)_2As_2$, revealing a correlation with other transport properties, including the in-plane resistivity anisotropy.

[1]This work is supported by the DOE, Office of Basic Energy Sciences, under Contract No. DE-AC02-76SF00515.

1:39PM Q23.00011 Hall effect study of iron chalcogenide $Fe_{1+y}(Te_{1-x}Se_x)$, T.J. LIU, J. HU, B. QIAN, Z.Q. MAO, Department of Physics and Engineering Physics, Tulane University, New Orleans, LA 70118 — Our previous work reveals three composition regions with distinct physical properties in the phase diagram of $Fe_{1+y}(Te_{1-x}Se_x)$ (Liu *et al.*, Nature Materials **9**, 719 (2010)). Region I ($0 \leq x \leq 0.09$) exhibits long range $(\pi, 0)$ antiferromagnetic (AFM) order, while Region II ($0.09 < x < 0.29$) displays short range $(\pi, 0)$ magnetic correlations and is characterized by a weakly localized electronic state. Only in Region III ($x \geq 0.29$) do we find evidence of bulk superconductivity. In this talk, we will report Hall effect studies of this system. In the AFM state of Region I, we find that the inverse Hall angle (IHA) exhibits a quadratic temperature dependence, consistent with the Fermi liquid behavior probed by resistivity and specific heat measurements. In the weakly localized state of Region II, however, the IHA shows a linear temperature dependence, implying that the quasiparticle scattering rate in this region changes significantly compared with the AFM phase. We will discuss how quasiparticle scattering is associated with $(\pi, 0)$ magnetic fluctuations.

1:51PM Q23.00012 Upper Critical Field and the Fulde-Ferrel-Larkin-Ovchinnikov Transition in Multiband Superconductors , ALEX GUREVICH, National High Magnetic Field Laboratory, FSU, Tallahassee, FL 32303 — The effect of orbital and Zeeman pairbreaking on the upper critical field H_{c2} and the Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) transition in clean Fe-based superconductors is addressed using a multiband BCS theory. It is shown that the crystalline anisotropy and the $s^{\pm}$ pairing symmetry with the sign change of the order parameter on different sheets of the Fermi surface can significantly increase the orbitally-limited $H_{c2}(T)$ and facilitate the FFLO transition. Small pockets of the Fermi surface emerging upon doping can trigger the FFLO transition even for moderate values of the Maki parameter in the main bands.

2:03PM Q23.00013 Upper critical field study of a LiFeAs single crystal grown by Sn flux , SEUNGHYUN KHIM, BUMSUNG LEE, JAE WOOK KIM, Seoul National University, EUN SANG CHOI, Florida State University, G. R. STEWART, University of Florida, KEE HOON KIM, Seoul National University, SEOUL NATIONAL UNIVERSITY TEAM, FLORIDA STATE UNIVERSITY COLLABORATION, UNIVERSITY OF FLORIDA COLLABORATION — Temperaturedependence of the upper critical fields $H_{c2}(T)$ was investigated in a LiFeAs single crystal by measuring resistivity at a fixed magnetic field up to 36 T. $H_{c2}^{ab}(0)$ and H_{c2}^{ab} (0) values are obtained as 30 and 17.2 T respectively. $H_{c2}^{ab}(0)$ is lower than expected one from the orbital limiting field $H_{c2}^{orb}(0)$ because of the presence of a moderate Pauli limiting effect; upon fitting $H_{c2}^{ab}(T)$ with the WHH formula, the Maki parameter $\alpha = 0.65$. For $H_{c2}^{c}(T)$, rather a linearly increasing behavior of $H_{c2}(T)$ could be explained by a two-band model in a dirty limit. The anisotropy $H_{c2}^{ab}/H_{c2}^{c}(T)$ is ∼2.3 near $T_c$and decreases with temperature being lowered to reaches ∼1.3 at $T = 0$. We also compare H_{c2} (T) of this 111 system with those of other Fe-based superconductors and conclude that the moderateness of the spin-paramagnetic effect is related with rather a weak slope of $H_{c2}(T)$ near T_c, which is inversely proportional to the Fermi velocity and mean free path. Thus, the comparison of the slope of H_{c2} supports that LiFeAs is located in a rather clean limit among the Fe-based superconductors.

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q24 DCOMP DMP: Focus Session: Multiscale Modeling: Heterogeneous Systems and Interfaces D167

11:15AM Q24.00001 Kinetic Monte Carlo with fields: diffusion in heterogeneous systems , JOSE ALFREDO CARO, Los Alamos National Laboratory — It is commonly perceived that to achieve breakthrough scientific discoveries in the 21^{st} century an integration of world leading experimental capabilities with theory, computational modeling and high performance computer simulations is necessary. Lying between the atomic and the macro scales, the meso scale is crucial for advancing materials research. Deterministic methods result computationally too heavy to cover length and time scales relevant for this scale. Therefore, stochastic approaches are one of the options of choice. In this talk I will describe recent progress in efficient parallelization schemes for Metropolis and kinetic Monte Carlo [1-2], and the combination of these ideas into a new hybrid Molecular Dynamics-kinetic Monte Carlo algorithm developed to study the basic mechanisms taking place in diffusion in concentrated alloys under the action of chemical and stress fields, incorporating in this way the actual driving force emerging from chemical potential gradients. Applications are shown on precipitation and segregation in nanostructured materials. Work in collaboration with E. Martinez, LANL, and with B. Sadigh, P. Erhart and A. Stukowsky, LLNL. Supported by the Center for Materials at Irradiation and Mechanical Extremes, an Energy Frontier Research Center funded by the U.S. Department of Energy (Award # 2008LANL1026) at Los Alamos National Laboratory

[1] B. Sadigh et al. to be published
[2] E. Martinez et al. J. Comp. Phys. 227 (2008) 3804-3823

11:51AM Q24.00002 On the atomic-scale design of metal-metal heterointerfaces[1] , MICHAEL DEMKOWICZ, MIT Department of Materials Science and Engineering — I will describe a multiscale modeling effort to understand and control the properties of heterointerfaces in metal-metal nanocomposites, using their effect on radiation response as an example. For selected model interfaces, atomistic simulations are used to characterize interface structure and to determine the mechanisms of interface-point defects interactions, including trapping, diffusion, and defect reactions. This information is then incorporated into mesoscale dislocation-based and continuum approaches to investigate the steady-state interface response to radiation-induced defect fluxes. With insights gained from studying this "forward" problem of predicting radiation response of selected model interfaces, one may attempt to solve the "inverse" problem of determining what interfaces will yield desired radiation response.

[1]Center for Materials at Irradiation and Mechanical Extremes (CMIME), a DOE EFRC at LANL

12:27PM Q24.00003 Atomistic Mechanism of Kinking in the Vapor-Liquid-Solid Growth of Silicon Nanowires , SEUNGHWA RYU, WEI CAI, Stanford University — Understanding the atomistic growth mechanism of semiconductor nanowires from the catalytic droplet is important for better control of the shape and orientation of nanowires deposited through the Vapor-Liquid-Solid (VLS) process. Kinking is a frequently observed event, in which the nanowire suddenly changes the growth orientation. This behavior is usually undesirable, but can also be explored to grow nanowires of complex shapes if it can be controlled. Unfortunately, the atomistic origin of kinking is not well understood. We employ advanced sampling methods to compute the probability of the orientation change during VLS growth. Several growth directions and nanowire diameters are simulated at 1000 K. The simulation uses a recently developed Au-Si inter-atomic potential fitted to the experimental binary phase diagram.

12:39PM Q24.00004 Prediction of the anisotropic properties of energetic materials at elevated pressures and temperatures[1] , OSCAR OJEDA, TAHIR CAGIN, Texas A&M University — Localization of strain and changes under extreme conditions in energetic materials (EM) can cause runaway reactions and unexpected initiation. A clear understanding of the mechanical properties is a perquisite in understanding the interplay between mechanical, chemical and thermodynamic properties that relate sensitivity and EM's before they undergo initiation. We have conducted first principles ground state studies, complemented by atomistic calculations at elevated temperatures and pressures, for energetic commonly used secondary EM's with varying sensitivities. Chemical information found from ab intio methods, and from compression at elevated temperatures show that external conditions relevant to impact and shock behavior can have different effects on the studied systems. These range from changes in local conformation, changes in the hydrogen-bonding network, and more drastically to a full crystallographic transition in which the symmetry of the system undergoes a transformation. Due to the chemical, mechanical and thermodynamic level information that provides, multiscale modeling methods, can then be applied to the understanding of other type of systems and give a clearer understanding of the molecular processes that undergo energetic materials, prior to initiation.

[1]Laboratory of Computational Engineering of Nanomaterials

12:51PM Q24.00005 Migration energies of native defects and fission products in uranium dioxide[1] , ALEXANDER THOMPSON, CHRIS WOLVERTON, Northwestern University — Despite the importance of fission products like Xe in nuclear fuels, the mechanism of how these atoms diffuse in the lattice is not known. In an effort to identify this mechanism, we have used density functional theory as well as a variety of different classical potentials for to study the migration energies of a variety of atomic steps in UO2, with and without Xe impurities and native defects. We find that the classical potential of Basak gives results which compare favorably with density functional theory for the diffusion of a Schottky defect cluster. We observe a new path for xenon-tetravacancy (a UO2 Schottky defect plus an additional U vacancy) motion using molecular dynamics. This path has a lower energy barrier than previously reported xenon-tetravacancy paths. We examine the possibility of a uranium vacancy dissociating from the xenon-tetravacancy cluster and find that large barriers for this dissociation. We also calculate xenon-double Schottky defect migration and find it has a slightly larger barrier than xenon-tetravacancy motion with the oxygen vacancies being weakly bound to the defect.

[1]NERI-C 08-051

1:03PM Q24.00006 Interface Mediated Nucleation and Growth of Dislocations in fcc-bcc nanocomposite , RUIFENG ZHANG, JIAN WANG, IRENE J. BEYERLEIN, TIMOTHY C. GERMANN, Los Alamos National Laboratory — Heterophase interfaces play a crucial role in determining material strength for nanostructured materials because they can block, store, nucleate, and remove dislocations, the essential defects that enable plastic deformation. Much recent theoretical and experimental effort has been conducted on nanostructured Cu-Nb multilayer composites that exhibited extraordinarily high strength, ductility, and resistance to radiation and mechanical loading. In decreasing layer thicknesses to the order of a few tens of nanometers or less, the deformation behavior of such composites is mainly controlled by the Cu/Nb interface. In this work, we focus on the cooperative mechanisms of dislocation nucleation and growth from Cu/Nb interfaces, and their interaction with interface. Two types of experimentally observed Cu/Nb incoherent interfaces are comparatively studied. We found that the preferred dislocation nucleation sites are closely related to atomic interface structure, which in turn, depend on the orientation relationship. The activation stress and energies for an isolated Shockley dislocation loop of different sizes from specific interface sites depend strongly on dislocation size, atomic interface pattern, and loading conditions. Such findings provide important insight into the mechanical response of a wide range of fcc/bcc metallic nanocomposites via atomic interface design.

1:15PM Q24.00007 Atomic and Surface Interactions of Electrode Metals with a p-Type Organometallic Conductor[1] , BHASKAR CHILUKURI, THOMAS CUNDARI, Department of Chemistry, Center for Advanced Scientific Computing and Modeling (CASCaM), University of North Texas, Box 305070, Denton, TX 76203-5070 — A computational study of the interaction of high and low work function electrode metal atoms (M' = Al, Au, Cu, La, Ni, Pd, Pt, Ru, Ni) used in electronic devices with cyclo-[Au(μ-Pz)]$_3$ trimer (T) (Pz = pyrazolate ligand), a p-type organometallic semiconductor is presented. Metal (M'$_M$) and ligand (M'$_L$) sites of the gold trimer are investigated as the possible sites of deposition for the metal atoms. Examination of metal binding, geometric and electronic properties suggest that these metal-based, p-type conductors will form stable interfaces with good electron transfer with typical source/drain electrode metals. Encouraged by the molecular simulation results, we performed periodic interface calculations of metal (001) and (111) surfaces with a monolayer of cyclo-[Au(μ-Pz)]$_3$ trimer using a plane-wave DFT approach. Structural and electronic properties of metal-trimer interfaces and implications for interface stability and electron transfer will be discussed.

[1]This work was financially supported by the National Science Foundation (CHE-0911690, CHE-0741936) and the Texas Advanced Research Program (009741-0089-2007).

1:27PM Q24.00008 Structure of charge trapping in cerium-doped aluminophosphate and phosphosilicate glasses: combining molecular dynamics simulations and *ab initio* DFT calculations , LEOPOLD KOKOU, YUN LI, JINCHENG DU, University of North Texas, MSE TEAM — Cerium doping glasses find wide applications in optical and photonic devices. Both Ce^{3+} and Ce^{4+} can be present in oxide glasses, and their ratio depends on the glass composition, heat history and melting environment. In either oxidation state, the environments of cerium ions are important to the optical absorption and emission properties. In this paper, we present classical molecular dynamic simulations of cerium-containing aluminosilicate and phosphosilicate glasses using newly developed potential models containing cerium ions. The local environments around Ce^{3+} and Ce^{4+} are studied, and the bond length and coordination of cerium ions are determined. Small samples of the glasses are simulated using MD and then further relaxed with Density Functional Theory (DFT) calculations. Comparison of the structure of glasses from MD and after DFT relaxation is made, and the two are found to be in reasonable agreement. It is found that Ce^{3+} has a longer bond distance and higher coordination number of oxygen. Most interestingly, cerium ions are found to be preferentially coordinated by phosphorus ions in the second coordination shell in the glasses.

1:39PM Q24.00009 Surface Structure and Work Function of ZnO Based on First Principle DFT Calculations , YUN LI, JINCHENG DU, UNT — Zinc Oxide is a well known n-type wide band gap semiconductor material and remains actively as a strategic material for various photonic applications. The fabricate ZnO, is effectively used as a sensor in various applications, Because of its high infrared reflectance and high visible transmittance. Due to that fact, its electron property plays vital role and attract our attention. Via simulation method, their electron properties were studied through density function theory. Based on first principle theory, their structures with distinct cleaved planes were obtained and completed relaxed in DFT based methods. Depending on cleaved planes, there were Oxygen or Zinc atoms terminated along (001) direction and both of them locating on the cleaved surface (110). Work function and other electron properties will be discussed in detail for all of them and compared with the experimental values, the difference and prediction will be made.

1:51PM Q24.00010 Coupling Fluctuating Hydrodynamics with Molecular Dynamics at the Nanoscale , NIKOLAOS VOULGARAKIS, JHIH-WEI CHU, Department of Chemical and Biomolecular Engineering, University of California, Berkeley — Hydrodynamic fluctuations and solvation interactions are essential driving forces of transport phenomena in the micrometer to nanometer regime, including inter- and intra-cellular flows and flows in nanofabricated devices. Although all-atom molecular dynamics (MD) simulations can be used to model molecular fluids, the accessible time- and length-scales are severely limited. Since most of computational cost for MD simulations comes from the represetion of solvent molecules, a possible solution to this limitation is to model fluids with fluctuating hydrodynamics (FHD). While this approach reduces the computational time of MD simulations by three orders of magnitude, an accurate protocol to couple FHD with MD is still necessary. In this work we present a new methodology that couples FHD with MD by allowing the fluctuating fields to directly interact with particles through repulsive, attractive, and dissipating/fluctuating forces without introducing new degrees of freedom or boundary conditions. Numerical results show that solvation energy and diffusion dynamics are correctly described within our framework. Simulations on the collapse of two hydrophobic particles are also presented.

2:03PM Q24.00011 Multiscale Modeling of Solutions , OLAYINKA OLATUNJI-OJO, SANDRA BOETCHER, THOMAS CUNDARI, Center for Advanced Scientific and Computer Modeling, University of North Texas, Denton Tx 76203 — The sequestration of carbon dioxide is one proposed solution to alleviate the growing problem of increased atmospheric CO_2 concentration, and its resulting effect on global climate. However, the efficacy of such methods has yet to be demonstrated. Improved CO_2 sequestration methods are needed and this can be achieved through a better understanding of the chemical and physical consequences of CO_2 encapsulation through multiscale modeling. Multiscale modeling is an effective tool for combining different methods thereby creating an efficient way of modeling diverse chemical and physical phenomena. The goal of this research is to model carbon dioxide interactions in solutions from the quantum to continuum level. This is achieved through a combination of DFT calculations, molecular modeling (mesoscale) and computational fluid dynamics (continuum) simulations on CO_2 + H_2O. Interaction energies and interatomic distances are obtained from DFT calculations, which are used to derive a Lennard-Jones potential, from which one may obtain continuum properties such as viscosity via reverse non-equilibrium molecular dynamics (RNEMD) simulations.

Wednesday, March 23, 2011 11:15AM - 1:51PM –

Session Q25 DCMP: Superconductivity: Transport Properties D166

11:15AM Q25.00001 Networks of ultra-small MoGe nanowires: fabrication and properties[1] , ZHILI XIAO, Argonne National Laboratory, MICHAEL LATIMER, QIONG LUO, WAI-KWONG KWOK, Argonne National Laboratory — By developing a template-based method we were able to fabricate networks of MoGe nanowires with widths and thicknesses of few nanometers. Resistive measurements reveal magnetoresistance oscillations with a field period up to 2 Tesla. Detailed information on sample fabrication will be presented. Possible mechanisms on the observed magnetoresistance oscillations will be discussed.

[1]This work was supported by the Department of Energy Grant DE-FG02-06ER46334

11:27AM Q25.00002 Magnetization-dependent resistance of double ferromagnet-superconductor junctions , KUEI SUN, U. of Cincinnati & U. of Illinois at Urbana-Champaign, M. COLCI, U. of Illinois at Urbana-Champaign & Naval Research Laboratory, Washington DC, D.J. VAN HARLINGEN, U. of Illinois at Urbana-Champaign, NAYANA SHAH, U. of Cincinnati, SMITHA VISHVESHWARA, U. of Illinois at Urbana-Champaign — Studies of the crossed Andreev reflection (CAR) process in double ferromagnet-superconductor junctions have attracted a lot of attention as way of realizing solid-state entanglement. Here, we perform a theoretical analyses of such a system motivated by our surprising experimental findings that the resistance in the antiparallel alignment of the magnetization of ferromagnets is larger than that in the parallel state. We model the system using an extended Blonder-Tinkham-Klapwijk (BTK) treatment with spin-dependent interfacial barriers associated with the magnetization. We compute scattering amplitudes of CAR and other possible processes as well as the resistance as a function of interfacial parameters. Our results reveal significantly altered physics due to the magnetization-dependent scattering, such as a sign change in the relative resistance between the parallel and antiparallel cases. We can model the positive relative resistance corresponding to our experimental findings as well as the negative results observed in other experiments, both within sufficiently large parameter regions.

11:39AM Q25.00003 Measurements of the critical current of small Sr_2RuO_4 crystals , YIQUN YING, NEAL STALEY, YING LIU, Department of Physics, The Pennsylvania State University, YAN XIN, National High Magnetic Field Laboratory, Florida State University, DAVID FOBES, TIJIANG LIU, ZHIQIANG MAO, Department of Physics, Tulane University — We report critical current measurements of chiral p-wave superconductor Sr_2RuO_4. Because of the strong anisotropy possessed by Sr_2RuO_4, vortex lines along the in-plane direction are expected to be pinned more strongly than those along the c axis, resulting in anisotropic critical currents. We prepared small single crystals of Sr_2RuO_4 with a typical size of 50μm$\times$ 10μm$\times$1μm by mechanical exfoliation and characterized them by Raman spectroscopy and high-resolution transmission electron microscopy, showing that they were either pure Sr_2RuO_4 or eutectic phase containing one or more Ru microdomains. Four-point or Hall probes were prepared on the small crystals by photo lithography. While samples of pure Sr_2RuO_4 exhibited a typical transition temperature (T_c) of 1.2K, slightly lower than the optimal bulk T_c, 1.5K, those with Ru microdomains showed multiple resistive transitions with the highest T_c around 2K. The critical current and critical field phase diagrams were determined for these small crystals. Surprisingly, the in-plane critical current density, measured for the first time, was found to be significantly larger than that along c-axis of the bulk. The physical implications of these observations will be discussed. Supported by DOE.

11:51AM Q25.00004 Angle-dependent transport behavior near the magnetic-field tuned superconductor-insulator transition , MIN-SOO KIM, TAI-LUNG WU, Department of Physics, University at Buffalo-SUNY, L.W. ENGEL, National High Magnetic Field Laboratory, G. SAMBANDAMURTHY, Department of Physics, University at Buffalo-SUNY — Thin films of superconducting, amorphous indium oxide were driven insulating by the application of magnetic field and their transport behavior at different magnetic field values are studied. Well below the critical field of the transition, the current-voltage characteristics follow a power law V$\propto$ I^p, where p depends on the magnetic field. The dependence of the power p on magnetic field and the angle between the sample plane and the magnetic field direction will be presented. In particular, we find two distinct magnetic field values, well above the critical field, where the sample resistance is independent of the angle. Implications of these results in improving our current understanding of the transition will be presented.

12:03PM Q25.00005 T_c Enhancement in Electron-Doped Cuprate Heterostructures , P.L. BACH, K. JIN, X.H. ZHANG, Center for Nanophysics and Advanced Materials, University of Maryland, R.L. GREENE[1], University of Maryland, U. GRUPEL, E. ZOHAR, E. DIAMANT, Y. DAGAN, Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University, S. SMADICI, P. ABBAMONTE, Frederick Seitz Materials Research Laboratory, University of Illinois — Multilayer thin films of $La_{2-x}Ce_xCuO_4$ (LCCO) and $Pr_{2-x}Ce_xCuO_4$ (PCCO) were fabricated as superlattices of different dopings. Pairing over-doped and under-doped (or un-doped) layers is found to increase T_c significantly above that of the single-phase films corresponding to the under- or over-doped layers. We report transport measurements on these mulitlayer films and discuss possible mechanisms for the T_c enhancement. This work was supported by the US-Israel Binational Science Foundation Grant #2006385 and the Center for Nanophysics and Advanced Materials (CNAM).

[1]Center for Nanophysics and Advanced Materials, University of Maryland

12:15PM Q25.00006 Electronic Transport and Superconductivity in Bi Confined in a 200nm Opal Host[1] , MICHAEL NIESKOSKI, Fairfield University, RYAN JOHNSON, STEVEN DISSELER, MICHAEL GRAF, Boston College, TITO HUBER, Howard University, AUSTIN HOWARD, ANVAR ZAKHIDOV, University of Texas at Dallas — While bulk bismuth at ambient pressure is not a superconductor, changes in morphology are known to induce superconductivity in Bi at low temperatures. We present a study of bismuth nanoparticle arrays fabricated by confining bismuth into a porous opal host consisting of close-packed 200 nm silica spheres. Electrical transport was studied down to temperatures of 0.3K and magnetic fields up to 2T. We find the onset of superconductivity at 4.4K (confirmed by AC magnetic susceptibility) and global superconductivity at a temperature of 1.3K. This two step transition is typical for granular superconductors. Measurements of the critical temperature in magnetic field show that the higher temperature transition consists of at least two transitions. The low temperature upper critical field was calculated to be approximately 0.82T. These results are discussed in terms of the morphologies, namely amorphous and granular structure, that are known to make Bi a superconductor, and the three characteristic sizes for the nanoparticles in that has been used to describe superconductivity in lead imbedded in these host materials

[1]NSF REU grant DMR-0649169

12:27PM Q25.00007 Electrostatic Modification of Properties of Ultrathin YBCO Films using an Electronic Double Layer Transistor , XIANG LENG, ALLEN GOLDMAN, University of Minnesota — We have modified the transport properties of ultrathin films of YBCO using an electronic double layer transistor configuration employing the ionic liquid DEME-TFSI [1]. The films were prepared on STO substrates using high pressure oxygen sputtering. The electronic double layer configuration permits extraordinarily large transfers either involving the accumulation or depletion of carriers, employing relatively low gate voltages. Thus far the transition temperature of a 10 unit cell thick film has been shifted by as much as 30K, and the insulating state has been induced in a 7 unit cell thick film. The latest results will be reported on the use of this technique as an alternative to chemical doping. This work was supported by the National Science Foundation under grant NSF/DMR-0709584.

[1] J.T. Ye et al., Nature Materials 9, 125(2010).

12:39PM Q25.00008 Phase-fluctuating superconductivity in overdoped $La_{2-x}Sr_xCuO_4$, P.M.C. ROURKE, I. MOUZOPOULOU, University of Bristol, X. XU, C. PANAGOPOULOS, Nanyang Technological University, Y. WANG, Peking University, B. VIGNOLLE, C. PROUST, LNCMI Toulouse, E.V. KURGANOVA, U. ZEITLER, HFML Nijmegen, Y. TANABE, T. ADACHI, Y. KOIKE, Tohoku University, N.E. HUSSEY, University of Bristol — In underdoped cuprates, an energy gap (pseudogap), appears in the electronic density of states well before superconductivity develops. Similarities between the pseudogap and superconducting gap have led to the idea that the pseudogap is a precursor superconducting state in which the superconducting order parameter is finite but the phase fluctuates. However, this picture of precursor pairing has been challenged by measurements indicating that the pseudogap itself closes at a critical doping concentration just beyond optimal doping. By tracking the restoration of the normal state magnetoresistance in overdoped $La_{2-x}Sr_xCuO_4$, we show that the phase fluctuation regime remains broad across the entire superconducting composition range, in contrast to the evolution of the pseudogap. The universal low phase stiffness is shown to be correlated with a low superfluid density, a characteristic of both underdoped and overdoped cuprates. The formation of the pseudogap, by inference, is therefore both independent of and distinct from superconductivity.

12:51PM Q25.00009 Voltage Oscillations in Silver Doped $YBa_2Cu_3O_{7-x}$, ATILGAN ALTINKOK, MURAT OLUTAS, KIVILCIM KILIC, ATILLA KILIC, Abant Izzet Baysal University — Nonlinear transport phenomena and time effects were investigated by the time evolution of sample voltage ($V - t$ curves) on long time scales in Ag-doped $YBa_2Cu_3O_{7-x}$ sample (YBCO/Ag). We also investigated influence of bidirectional square wave current with various periods (P) and dc currents (I) on the evolution of $V - t$ curves in YBCO/Ag sample material at different temperatures (T) and external magnetic (H) fields. It was observed that a non-linear response seen in $V - t$ curves to bidirectional square wave (BSW) current with sufficiently short periods or sufficiently low amplitude reflects itself as regular sinusoidal- type voltage oscillations. The observed oscillating mode was correlated to the dynamic competition between pinning and depinning. Further, the similarity between the flux dynamics and the charge density waves is considered as a possible explanation of voltage oscillations in YBCO/Ag. Detailed analysis of $V - t$ curves and voltage oscillations reveals that adding of Ag causes degradation in both intergranular and surface pinning of YBCO material.

1:03PM Q25.00010 Andreev and Single-Particle Tunneling Spectra of Underdoped Cuprate Superconductors , KUN HUANG, Department of Physics, The University of Hong Kong, Hong Kong, KAI-YU YANG, Institut fuer Theoretische Physik, ETH Zrich, WEI-QIANG CHEN, Department of Physics, The University of Hong Kong, Hong Kong, T.M. RICE, Institut fr Theoretische Physik, ETH Zrich, FU-CHUN ZHANG, Department of Physics, The University of Hong Kong, Hong Kong — We study tunneling spectroscopy between a normal metal and an underdoped cuprate superconductor modeled by a phenomenological theory in which the pseudogap is a precursor to the undoped Mott insulator. In the low barrier tunneling limit, the spectra are enhanced by Andreev reflection only within a voltage region of the small superconducting energy gap. In the high barrier tunneling limit, the spectra show a large energy pseudogap associated with single particle tunneling. Our theory semi- quantitatively describes the two gap behavior observed in tunneling experiments.

1:15PM Q25.00011 Doping evolution of nodal quasiparticles in the cuprate superconductor YBCO via low-temperature thermal conductivity , SAMUEL RENE DE COTRET, J.-PH. REID, N. DOIRON-LEYRAUD, L. TAILLEFER, University of Sherbrooke, Sherbrooke, Canada, B.J. RAMSHAW, R. LIANG, D.A. BONN, W.N. HARDY, University of British Columbia, Vancouver, Canada — The thermal conductivity of the cuprate superconductor $YBa_2Cu_3O_y$ was measured at temperatures down to $T \sim 50$ mK in magnetic fields up to $H = 15$ T on high-quality single crystals with a hole doping ranging from $p = 0.08$ to $p = 0.18$. The residual linear term at $T \to 0$, a direct measure of the nodal quasiparticle velocities [1], is tracked as a function of doping, and compared to recent, high-resolution ARPES measurements of the Fermi velocity and gap magnitude as a function of doping, in the related cuprate superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ [2].

[1] D.G. Hawthorn *et al.*, Phys. Rev. B **75**, 104518 (2007).
[2] I.M. Vishik *et al.*, Phys. Rev. Lett. **104**, 207002 (2010).

1:27PM Q25.00012 Correlation Strength, Optical Conductivity and d-d excitons in high T_c cuprates[1] , ANDREW MILLIS, Columbia University, XIN WANG, University of Maryland, LUCA DEMEDICI, CNRS-Universite de Paris Sud — A single site dynamical mean field analysis is presented of models of high T_c copper-oxide superconductors, including oxygen orbitals and both $x^2 - y^2$ and $3z^2 - r^2$ Cu d-orbitals. The optical conductivity, doping dependent effective mass and the e_g portion of the d-d exciton spectrum are determined. The details of the oxygen-oxygen hopping are shown to be unimportant. A general connection between d valence and the metal/charge transfer insulator phase boundary is outlined.

[1]Funded by the US-NSF under grant DMR -0705847

1:39PM Q25.00013 Determining Transport Parameters for Superconductor/Normal Metal Point Contacts in an Applied Magnetic Field from Conductance versus Field Data at Fixed Temperature , PAUL J. DOLAN, JR., Northeastern Illinois University, CHARLES W. SMITH, University of Maine — Superconductor/normal metal point contact transport data often consists of normalized conductance as a function of reduced temperature, from which the elastic scattering parameter and the inelastic scattering parameter for the contact can be determined, in addition to other features of interest. We show a strategy for determining these parameters from normalized conductance as a function of reduced applied magnetic field, at fixed temperature, even when conductance versus variable temperature data is absent. This analysis strategy will be demonstrated for several point contacts, over a wide range of parameter values.

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q26 DMP DCOMP: Focus Session: Iron Based Superconductors – Optics, Heat Capacity, Thermopower D162/164

11:15AM Q26.00001 Optical Investigation of the Charge Dynamics in $Ba(Co_xFe_{1-x})_2As_2$[1] , L. DEGIORGI, ETH-Zurich — We report on a thorough optical investigation over a broad spectral range and as a function of temperature of the charge dynamics in $Ba(Co_xFe_{1-x})_2As_2$ compounds for Co-doping ranging between 0 and 18%. For the parent compound as well as for x=0.025 we observe the opening of a pseudogap, due to the spin-density-wave phase transition and inducing a reshuffling of spectral weight from low to high frequencies. For compounds with $0.051 \leq x \leq 0.11$ we detect the superconducting gap, while at x=0.18 the material stays metallic at all temperatures. We describe the effective metallic contribution to the optical conductivity with two Drude terms, representing the coherent components, and extract the respective scattering rates. Finally through spectral weight arguments, we give clear-cut evidence for moderate electronic correlations for $0 \leq x \leq 0.061$, which then crossover to values appropriate for a regime of weak interacting and nearly-free electron metals for $x \geq 0.11$. We also investigate the optical conductivity with light polarized along the in-plane orthorhombic a- and b-axes of $Ba(Co_xFe_{1-x})_2As_2$ for x=0 and 2.5% under uniaxial pressure across their structural and magnetic transitions. The charge dynamics at low frequencies and temperatures on these detwinned, single domain samples reveals an enhancement of both the scattering rate and Drude weight of the charge carriers along the antiferromagnetic a-axis with respect to the ferromagnetic b-axis. Our findings also allow us to estimate the dichroism, which extends to high frequencies. These results demonstrate the electronic nature of the structural transition found in underdoped Fe-pnictides. Co-authors: A. Dusza, A. Lucarelli, F. Pfuner, J.-H. Chu, I.R. Fischer.

[1]This work has been supported by the Swiss National Foundation for the Scientific Research within the NCCR MaNEP pool. This work is also supported by the Department of Energy, Office of Basic Energy Sciences under contract DE-AC02-76SF00515.

11:51AM Q26.00002 In-plane and c-axis optical spectroscopy study on 122 Fe-pnictides , NAN LIN WANG, Institute of Physics, Chinese Academy of Sciences — I present the in-plane and the c-axis optical spectroscopy investigations on 122 Fe-pnictides. For the parent compound $BaFe_2As_2$, the in-plane measurement revealed two different energy gaps in the SDW state, whereas for the c-axis polarized measurement only the energy gap at smaller energy scale could be clearly observed. We suggest different driving mechanisms for the formation of the two energy gaps. The large energy gap is caused by the nesting between disconnected 2D cylinder-like electron and hole Fermi surfaces. It is the main driving force for the SDW instability. The small energy gap is the one formed on the 3D Fermi surface due to the presence of reduced magnetic Brillouin zone which crosses the 3D Fermi surface. It is the consequence of the establishment of the magnetic order. For the doped superconducting 122 samples, the in-plane optical measurement revealed a formation of full superconducting energy gap, whereas the c-axis optical measurement indicated a large residual quasiparticle population down to very low temperature. Those quasiparticles contribute specifically to the c-axis transport. We suggest that there exist horizontal nodes in the superconducting gap in regions of the 3D Fermi surface that contribute dominantly to the c-axis optical conductivity. Work done with Z. G. Chen, W. Z. Hu, B. Cheng, G. Li, J. Dong, T. Dong, R. H. Yuan, P. Zheng, G. F. Chen, J. L. Luo, Z. Fang, X. Dai, C. L. Zhang and P. Dai.

12:03PM Q26.00003 Optical signature of sub-gap absorption in the superconducting state of $Ba(Fe_{1-x}Co_x)_2As_2$[1] , URMAS NAGEL, T. RÕÕM, Nat.-l Inst. of Chem. Phys. & Biophys., Tallinn, Estonia, R.P.S.M. LOBO, Y.M. DAI, LPEM, CNRS, UPMC, ESPCI-ParisTech, Paris, France, J. CARBOTTE, T. TIMUSK, McMaster Univ., Hamilton, Canada, D. COLSON, CEA, IRAMIS, SPEC, Gif sur Yvette, France — The optical conductivity of $Ba(Fe_{0.92}Co_{0.08})_2As_2$ shows a clear signature of the superconducting gap, but a simple s-wave description fails in accounting for the low frequency response. This task is achieved by introducing an extra Drude peak in the superconducting state representing sub-gap absorption, other than thermally broken pairs. This extra peak and the coexisting s-wave response respect the total sum rule indicating a common origin for the carriers. We discuss the possible origins for this absorption as (i) quasiparticles due to pair-breaking from interband impurity scattering in a two band $s_\pm$ gap symmetry model, which includes (ii) the possible existence of impurity levels within an isotropic gap model; or (iii) an indication that one of the bands in is highly anisotropic. The results are published in Phys. Rev B vol 82, 100506(R) (2010).

[1]Work in Tallinn was supported by the Estonian Ministry of Education and Research (SF0690029s09) and Estonian Science Foundation (ETF7011, ETF8170).

12:15PM Q26.00004 Femtosecond low-energy dynamics of superconducting and spin-density wave gaps in pnictides , K.W. KIM, A. PASHKIN, M. BEYER, H. SCHÄFER, M. PORER, T. WOLF, C. BERNHARD, J. DEMSAR, R. HUBER, A. LEITENSTORFER — Magnetism and superconductivity (SC) in pnictides as well as a possible link between them are subjects of intense studies. The infrared spectral regime plays a pivotal role en route to a microscopic understanding since it provides direct access to the fundamental low-energy excitations, such as spin-density waves (SDW) and SC-induced energy gaps. We investigate Ba(Fe,Co)2As2 by combining ellipsometry and ultrabroadband terahertz (THz) pump-probe experiments. Following a femtosecond near-infrared excitation, the spectral hallmark of SDW located in the 10 - 30 THz window disappears with a characteristic saturation fluence of $\Phi_s \approx 50$ J/cm^2 and recovers fast ($\tau < 1$ ps), while the SC gaps below 3 THz are fully closed at a much smaller fluence $\Phi_s \approx 3$ J/cm^2 and exhibit a slower relaxation behavior ($\tau > 10$ ps). The distinct spectral, temporal and saturation behavior provide a unique environment to monitor the interplay of the two order parameters. Furthermore we observe coherent oscillation at 5.5 THz which corresponds to an Arsenic vibration. Our results may add new aspects toward an understanding of interactions between fundamental excitations in pnictides.

12:27PM Q26.00005 Optical properties of $BaFe_{1.85}Co_{0.15}As_2$[1] , J.J. TU, Dept. of Physics, CCNY/CUNY, New York, L.J. LI, G.H. CAO, Z.A. XU, Dept. of Physics, Zhejiang University, Hangzhou 310027, China, C.C. HOMES, Condensed Matter Physics and Materials Science Dept., Brookhaven National Laboratory, Upton, New York — The detailed in-plane optical properties of the electron-doped iron-arsenic superconductor $BaFe_{1.85}Co_{0.15}As_2$ have been determined over a wide frequency range above and below $T_c = 25$ K. Despite being a multiband system, the normal state reveals that a single (electron) band dominates the low-frequency conductivity, which can be modeled by a single Drude component with plasma frequency $\omega_{p,D} \simeq 7840$ cm^{-1} and scattering rate $1/\tau_D \simeq 126$ cm^{-1}, determined just above T_c. For $T \ll T_c$ the superconducting plasma frequency is $\omega_{p,S} \simeq 5200$ cm^{-1} ($\lambda_{eff} \simeq 3000$ Å), indicating that less than half the free carriers in the normal state have collapsed into the condensate, suggesting that this material is not in the clean limit. There are two energy scales for the superconductivity, $\Delta_1(0) = 3.1 \pm 0.2$ meV and $\Delta_2(0) = 7.4 \pm 0.3$ meV. This corresponds to either the gapping of the electron and hole pockets, respectively, or an anisitropic *s*-wave gap on the electron pocket; both views are consistent with the $s^\pm$ model.[2]

[1]Supported by the DOE under Contract No. DE-AC02-98CH10886.
[2]J. J. Tu *et al.*, Phys. Rev. B **82**, 174509 (2010).

12:39PM Q26.00006 Raman investigation of the magneto-structural transition in electron doped $Ba(FeAs)_2$[1] , YANN GALLAIS, LUDIVINE CHAUVIERE, MAXIMILIEN CAZAYOUS, MARIE-AUDE MEASSON, ALAIN SACUTO, Universite Paris Diderot, DOROTHEE COLSON, ANNE FORGET, SPEC CEA Saclay — We report a doping dependent Raman scattering study of the magneto-structural transition in Co doped Ba(FeAs)2. Several zone centered phonons display significant anomalies at the tetragonal to orthorhombic transition. In particular, the doubly degenerate in-plane Eg phonon shows an enhanced splitting in the ortho phase. The splitting weakens considerably with doping and gives evidence for strong spin-phonon coupling in iron-pnictides. The electronic Raman continuum displays a systematic upturn at low energy around the magneto-structural transition. This quasi-elastic scattering is similar to magnetic energy fluctuations usually observed in magnetic insulators. Interestingly significant fluctuations are observed at low temperature even for x=0.065 doping, where the Neel temperature goes to zero and optimal Tc is reached. At high energy and low doping, the electronic Raman continuum displays clear signatures Fermi surface reconstruction due to the opening of the spin density wave gap at the magnetic transition.

[1]Work funded by Agence Nationale de la Recherche (ANR).

12:51PM Q26.00007 Effect of annealing on the gap structure of $Ba(Fe_{1-x}Co_x)_2As_2$: low temperature specific heat studies , K. GOFRYK, F. RONNING, E.D. BAUER, J.D. THOMPSON, Los Alamos National Laboratory, A.B. VORONTSOV, Montana State University, I. VEKHTER, Louisiana State University, A.S. SEFAT, Oak Ridge National Laboratory, T. IMAI, McMaster University — We report on the effect of annealing on the temperature and field dependencies of the low temperature specific heat of the electron-doped $Ba(Fe_{1-x}Co_x)_2As_2$ for under- (x = 0.045), optimal- (x = 0.08) and over-doped (x = 0.105 and 0.14) regimes. We observed that annealing significantly improves some superconducting characteristics in $Ba(Fe_{1-x}Co_x)_2As_2$. It considerably increases T_c, decreases γ_0 in the superconducting state and suppresses the Schottky-like contribution at very low temperatures. The improved sample quality allows for a better identification of the superconducting gap structure of these materials. We examine the effects of doping and annealing within a self-consistent framework for an extended s-wave pairing scenario. At optimal doping our data indicates the sample is fully gapped, while for both under- and over-doped samples significant low-energy excitations remain, possibly consistent with a nodal structure. The difference of sample quality offers a natural explanation for the variation in low temperature power laws observed by many techniques.

1:03PM Q26.00008 The low-temperature specific heat of Co-doped $BaFe_2As_2$, JIUNN-YUAN LIN, Institute of Physics, National Chiao Tung University, Hsinchu 30010, Taiwan — We have measured the low-temperature specific heat of $Ba(Fe_{1-x}Co_x)_2As_2$ (x=0,0.08,0.2) single crystals. The electronic specific heat of $Ba(Fe_{0.92}Co_{0.08})_2As_2$ in the superconductiong state with T_c=21 K is revealed. A T^2 term was observed at low temperatures, providing the evidence of nodes in the gap. Furthermore, the data suggest a multi-gap feature for $Ba(Fe_{0.92}Co_{0.08})_2As_2$. The mixed state data will also be reported.

1:15PM Q26.00009 The Electronic Specific Heat of $Ba_{1-x}K_xFe_2As_2$ from 2K to 380K[1] , JAMES STOREY, JOHN LORAM, JOHN COOPER, University of Cambridge, ZBIGNIEW BUKOWSKI, JANUSZ KARPINSKI, ETH Zurich — Using a unique differential technique, we have measured the specific heat capacity of polycrystalline $Ba_{1-x}K_xFe_2As_2$ with x = 0, 0.1, 0.2, 0.3, 0.5 0.9 and 1.0, between 2K and 380K and in magnetic fields (H) from 0 – 13T. We determine the electronic specific heat coefficient γ ($\equiv C_{el}/T$) over the entire range of T, H and x and compare it with the magnetic susceptibility of the seven samples. We show that our results are consistent with single crystal studies but give further interesting information. For $x < 0.3$, γ is progressively reduced at low T by a SDW gap, but is only weakly doping and T-dependent above the structural/magnetic transition. For $x = 0.3$ the normal state γ_n is constant up to 380K, but as x increases from 0.3 to 1.0, γ_n becomes increasingly T-dependent, increasing by a factor two at low-T and decreasing by a factor 1.5 at 380K for $x = 1$. We consider possible explanations for this striking T-dependence in terms of a sharp peak in the electronic density of states, a strongly x- and T-dependent effective mass enhancement, or low energy magnetic excitations. The H-dependent measurements allow us to extract the critical fields, superfluid density and coherence length as functions of doping and temperature.

[1]Supported by EPSRC (UK) and MaNEP (Switzerland).

1:27PM Q26.00010 Specific Heat to 35 T in P-doped and Co-doped $BaFe_2As_2$: Evidence for Nodes or Not?[1] , G.R. STEWART, J.S. KIM, P.J. HIRSCHFELD, Physics, University of Florida, F. RONNING, K. GOFRYK, MPA-10, Los Alamos National Laboratory, A.S. SEFAT, MST Division, Oak Ridge National Laboratory, S. KASAHARA, T. SHIBAUCHI, T. TERASHIMA, Y. MATSUDA, Physics, Kyoto University — We have measured the low temperature specific heat of annealed single crystal $Ba(Fe_{0.955}Co_{0.045})_2As_2$, unannealed single crystal $BaFe_2(As_{0.7}P_{0.3})_2$, and other $BaFe_2As_2$ derivatives in fields to 35 T. We report contrasting behavior, with the underdoped Co sample exhibiting behavior (specific heat $\gamma \sim H^{0.7}$) essentially up to H_{c2} similar to the Volovik effect prediction ($\gamma \sim H^{**}0.5$) for nodal behavior for fields $H < 0.1H_{c2}$. In contrast, γ up to 35 T (2/3 of H_{c2}) in $BaFe_2(As_{0.7}P_{0.3})_2$ exhibits linear with field dependence, consistent with fully gapped behavior but inconsistent with indications of nodal behavior from other measurements. Possible explanations, and up-to-date measurements will be presented.

[1]Work at Florida supported by DE-FG02-86ER45268 (GRS, JSK), DE-FG02-05ER46236 (PJH).

1:39PM Q26.00011 Thermoelectric power of $Ba(Fe_{1-x}Ru_x)_2As_2$ and $Ba(Fe_{1-x}Co_x)_2As_2$: possible changes in Fermi surface with and without changes in electorn count[1] , HALYNA HODOVANETS, EUNDEOK MUN, ALEX N. THALER, SERGEY L. BUD'KO, PAUL C. CANFIELD, Ames Laboratoty/ Iowa State University, Ames, IA 50011, USA — Temperature-dependent, in-plane, thermoelectric power (TEP) data are presented for $Ba(Fe_{1-x}Ru_x)_2As_2$ ($0 \leq x \leq 0.36$) single crystals. The previously outlined by resistivity and susceptibility $x - T$ phase diagram for this system is confirmed. The analysis of TEP evolution with Ru-doping suggests two concentrations, $x \sim 7\%$ and $x \sim 30\%$ of Ru-doping levels, near which significant changes in the electronic structure, correlations and/or scattering occur. These results are compared with an extended set of TEP data for the electron doped $Ba(Fe_{1-x}Co_x)_2As_2$ ($0.13 \leq x \leq 0.42$) single crystals. An analysis of TEP data for Co-doping in the overdoped region suggests two more concentrations, $x \sim 11\%$ and $x \sim 22\%$, in addition to x$\sim$ 2% previously reported, where Lifshitz transition might occur. These data for Co-doping were recently confirmed by ARPES measurements.

[1]Work at the Ames Laboratory was supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

1:51PM Q26.00012 Nernst and Seebeck coefficients of the iron-pncitide superconductor $Ba_{1-x}K_xFe_2As_2$, XIGANG LUO, H. SHAKERIPOUR, J. CHANG, F. LALIBERTE, J. -PH. REID, N. DOIRON-LEYRAUD, L. TAILLEFER, Universite de Sherbrooke, M.A. TANATAR, R. PROZOROV, Ames Laboratory, H.Q. LUO, Z.S. WANG, H.-H. WEN, Institute of Physics, Beijing — The Nernst and Seebeck coefficients of the iron-pnictide superconductor $Ba_{1-x}K_xFe_2As_2$ were measured in single crystals for K concentrations ranging from the parent compound at x=0 to the optimally-doped superconductor at x=0.40, where Tc=38 K. Both coefficients show sharp anomalies at T_N, the onset temperature for antiferromagnetic order. This allows us to track the doping dependence of T_N and hence to map out the T-x phase diagram of $Ba_{1-x}K_xFe_2As_2$. The reconstruction of the Fermi surface by the antiferromagnetic order causes a huge enhancement of the quasiparticle Nernst signal, suggesting that carrier density and Fermi temperature are dramatically reduced in the magnetic phase. The Nernst signal due to superconducting fluctuations is small by comparison, and it remains detectable up to a temperature approximately 15% above T_c, in the optimally-doped sample.

2:03PM Q26.00013 Coherence peak and pair-breaking effects in the ac conductivity of $BaFe_{2-2x}Co_{2x}As_2$ epitaxial thin films , N.P. ARMITAGE, ROLANDO VALDÉS AGUILAR, L.S. BILBRO, The Johns Hopkins University, S. LEE, C.W. BARK, C.B. EOM, University of Wisconsin, THE JOHNS HOPKINS UNIVERSITY TEAM, UNIVERSITY OF WISCONSIN TEAM — We report a study of high quality pnictide superconductor $BaFe_{1.84}Co_{0.16}As_2$ epitaxial thin films using time-domain THz spectroscopy. Near T_c we find evidence for a coherence peak and qualitative agreement with the weak-coupling Mattis-Bardeen form of the conductivity. At low temperature, we find that the real part of the THz conductivity is not fully suppressed and σ_2 is significantly smaller than the Matthis-Bardeen expectation. The temperature dependence of the penetration depth λ follows a power law with an unusually high exponent of 3.1. We interpret these results as consistent with impurity scattering induced pair-breaking. Taken together our results are strong support for an extended s$\pm$ symmetry order parameter.

Wednesday, March 23, 2011 11:15AM - 2:15PM –
Session Q27 GQI: Focus Session: Semiconductor Qubits- Quantum Control C155

11:15AM Q27.00001 Control and Manipulation of Two-Electron Spin Qubits in GaAs Quantum Dots[1] , AMIR YACOBY, Harvard University — We have developed means to both couple and decouple a two electron spin qubit from its environment. Using dynamic nuclear polarization we are able to suppress fluctuations in the nuclear environment and prolong T2* by nearly an order of magnitude reaching 150 nano seconds. Our polarization scheme employs a quantum feedback mechanism that directly conditions the rate at which the qubit polarizes its nuclear environment on a quantum limited measurement of the hyperfine field seen by the same qubit. In addition, the stabilized state of the nuclear environment allows us to perform controlled X rotations and thereby demonstrate full control over the entire Bloch sphere as well as full quantum state tomography. Using dynamic decoupling of the two electron spin qubit from its environment we are able to prolong T2 by nearly three orders of magnitude reaching nearly 300 micro seconds. Our results indicate that gate fidelities of up to 99.99% are within reach despite the fluctuating nuclear environment. Moreover, the demonstrated ultra long coherence time allows for more than 10^5 coherent gate operations which exceed the estimated threshold for quantum error corrections by a substantial margin.

[1]This work is supported by ARO and IARPA.

11:51AM Q27.00002 Quantum gates for the singlet-triplet T_+ qubit , HUGO RIBEIRO, University of Konstanz, J.R. PETTA, Princeton University, GUIDO BURKARD, University of Konstanz — We theoretically show that hyperfine interactions can be harnessed for quantum gate operations in GaAs semiconductor quantum dots [1]. In the presence of an external magnetic field B, which splits the triplet states, the hyperfine interaction results in an avoided crossing between the spin singlet S and spin triplet T_+, which form the basis of a new type of spin qubit. Coherent quantum control for this qubit is achieved through Landau-Zener-Stückelberg transitions at the S-T_+ avoided crossing [2]. A set of suitable transitions allows to build any single qubit gates on timescales shorter than the decoherence time $T_2^* \sim 16\mathrm{ns}$ [1]. We also show how to build a conditional two-qubit gate by capacitively coupling two S-T_+ qubits.

[1] H. Ribeiro, J. R. Petta, and G. Burkard, Phys. Rev. B 82, 115445 (2010).
[2] H. Ribeiro and G. Burkard, Phys. Rev. Lett. 102, 216802 (2009).

12:03PM Q27.00003 Coherent spin manipulation with a triple quantum dot , GHISLAIN GRANGER, Institute for Microstructural Sciences, National Research Council Canada, LOUIS GAUDREAU, National Research Council Canada and University of Sherbrooke, ALICIA KAM, SERGEI STUDENIKIN, PIOTR ZAWADZKI, GEOF AERS, Institute for Microstructural Sciences, National Research Council Canada, MICHEL PIORO-LADRIÈRE, University of Sherbrooke, ZBIGNIEW WASILEWSKI, ANDREW SACHRAJDA, Institute for Microstructural Sciences, National Research Council Canada — Recently, Landau-Zener-Stuckelberg (LZS) oscillations have been demonstrated in a double quantum dot device [1]. In this talk we demonstrate LZS oscillations in a triple quantum dot environment. Our triple quantum dot design allows us to tune to either the charge or spin qubit regimes. Using a pulsing technique in the spin qubit regime, we create a superposition of triple quantum dot states, allow for phase accumulation, and interfere. We demonstrate coherent LZS oscillations with three spins across the triple quantum dot structure. We investigate their dependence on pulse rise time, separation time, energy detuning, and magnetic field.

[1] J. R. Petta et al., Science 327, 669 (2010).

12:15PM Q27.00004 Novel Coherent Spin Oscillations in a Triple Quantum Dot Circuit , ANDREW SACHRAJDA, GHISLAIN GRANGER, LOUIS GAUDREAU, ALICIA KAM, SERGEI STUDENIKIN, PIOTR ZAWADZKI, GEOF AERS, National Research Council of Canada, MICHEL PIORO-LADRIERE, Sherbrooke University, ZBIG WASILEWSKI, National Research Council of Canada — We have demonstrated Landau-Zener-Stuckelberg oscillations in a triple quantum dot circuit related to pairs of triple quantum dot states. Different initialization schemes and pulse shapes involving all three dots will be discussed. However, the complexity of a triple quantum dot system suggests that in general coherent behaviour can be expected from interplays between various combinations of states. Here we demonstrate both experimentally and theoretically in a triple quantum circuit containing three spins, a coherent interplay between two coexisting qubits as a function of pulse amplitude and rise time. To further clarify the behaviour within the system we also observe and study coherent oscillations after a fourth spin has been added to the system in one of the relevant dots.

12:27PM Q27.00005 A Single Electron Charge Qubit in the Strong Driving Limit[1] , J. STEHLIK, Y. DOVZHENKO, J. R. PETTA, Department of Physics, Princeton University, H. LU, A. C. GOSSARD, Materials Department, University of California at Santa Barbara — The dynamics of strongly driven two-level systems in the presence of dissipation have been thoroughly studied using theoretical models.[1] We use a model system, a GaAs double quantum dot (DQD) containing a single electron, to experimentally explore the strong-driving regime. We measured the transport through the DQD as a function of detuning and applied microwave power and compare with the Tien-Gordon model. In contrast with previous experiments, we directly access the occupation of the DQD using a quantum point contact charge sensor. In the high frequency regime ($\hbar\omega_{driving} \gg \Delta$, where Δ is the tunnel coupling) we observe up to 9-photon transitions and clear Bessel function behavior of the DQD occupation with applied microwave power. We also studied the intermediate frequency regime, observing 18-photon transitions. The data are modeled using the time-dependent Schrodinger equation.[2] By comparing the data with the simulations, we estimate $T_1 \sim 15$ ns and $T_2 \sim 3$ ns.
[1] A. J. Leggett *et al.*, Rev. Mod. Phys. **59**, 1 (1987).
[2] S. N. Shevchenko, S. Ashhab, F. Nori, Phys. Rep. **492**, 1 (2010).

[1]Funded by the Sloan and Packard Foundations, NSF, and DARPA.

12:39PM Q27.00006 Non-adiabatic Quantum Control of a Semiconductor Charge Qubit[1] , YULIYA DOVZHENKO, JIRI STEHLIK, KARL PETERSSON, JASON PETTA, Princeton University, HONG LU, ARTHUR GOSSARD, University of California, Santa Barbara — A GaAs double quantum dot is configured in the single-electron regime and operated as a charge qubit. The two basis states correspond to the electron being in either the left or the right dot. Non-adiabatic voltage pulses are applied to the depletion gates to drive coherent rotations, and the double dot occupation is read out using a nearby quantum point contact charge sensor. In contrast with previous work, where a single non-adiabatic pulse was applied for quantum control, we apply multiple pulses working towards a charge echo.[1,2] Data for $\frac{\pi}{2}$ - τ - $\frac{\pi}{2}$ and the $\frac{\pi}{2}$ - τ_1 - π - τ_2 - $\frac{\pi}{2}$ "charge echo" pulse sequences are obtained and compared with numerical simulations of the charge qubit evolution. References:
[1] K. D. Petersson *et al.*, Phys. Rev. Lett. (in press).
[2] Y. Nakamura *et al.*, Phys. Rev. Lett. **88**, 047901 (2002).

[1]Funded by the Sloan and Packard Foundations, NSF, and DARPA.

12:51PM Q27.00007 Extended coherence of exchange operations in double quantum dot spin qubits using Hahn echo , MICHAEL SHULMAN, HENDRIK BLUHM, OLIVER DIAL, Harvard University, VLADIMIR UMANSKY, Weizmann Institute of Science, AMIR YACOBY, Harvard University — Semiconductor spin qubits are promising candidates for quantum computation because of their long coherence times and potential for scalability. The exchange interaction is a powerful resource in these qubits, as it can drive single qubit rotations and inter-qubit entanglement. However, spin qubits driven by exchange become sensitive to charge noise, which in free induction decay experiments has lead to dephasing after a few coherent exchange oscillations. We perform a Hahn echo measurement in two-electron spin qubits in GaAs quantum dots. The π-pulse is applied by means of a stabilized nuclear gradient in the quantum dots. We find an exponential dephasing with a time constant of up to 10μs, which is more than an order of magnitude larger than T_2^*, and corresponds to 500 coherent exchange operations within T_2. This increase in T_2 is expected to allow for several cPHASE operations between two charge coupled two-electron qubits within T_2.

1:03PM Q27.00008 Two-qubit operations of two-electron spin qubits in GaAs quantum dots , HENDRIK BLUHM, MICHAEL SHULMAN, OLIVER E. DIAL, Harvard University, VLADIMIR UMANSKY, Weizmann Institute, AMIR YACOBY, Harvard University — The realization of two-qubit entangling gates is one of the most important milestones for the development of quantum-dot based electron spin qubits. Our measurements and simulations of the coupling strength and the relevant coherence time indicate very favorable prospects for the realization of such gates using the Coulomb interaction between adjacent spin qubits. This operation can be protected against dephasing due to low frequency electric noise by simultaneously applying a π-pulse to both qubits, which is essential to achieve the required coherence time. We report the experimental realization of this echo operation in a two-qubit device, conditional evolution of one qubit depending on the charge state of the neighboring double dot, and further progress toward two-qubit entanglement.

1:15PM Q27.00009 Spin Manipulation in InAs Nanowire Double Quantum Dots[1] , M.D. SCHROER, M. JUNG, K.D. PETERSSON, C.M. QUINTANA, J.R. PETTA, Princeton University — Recently, much effort has been devoted to the development of physical qubits for integration into quantum computers. Qubits allowing control with electric fields are attractive, as ac magnetic fields are more difficult to generate and localize on the nanoscale. The material properties of InAs allow efficient driving of electron spin resonance via the spin–orbit interaction. Our work has focused on developing quantum dots in InAs nanowires as fully characterized and controllable qubits. We have optimized our nanowire growth to eliminate the presence of planar defects, which impede the predictable formation of quantum dots. Using a bottom–gated architecture [1], we demonstrate tunable InAs nanowire double quantum dots, with the occupation controllable to the last electron. Pauli blockade is observed in the two-electron regime, demonstrating spin-dependent transport. We are able to drive single spin rotations by applying microwaves to one of the local metallic gates; from the electron spin resonance condition we extract a g–factor of ∼9. Finally, we demonstrate full electrical control of the two-electron system and characterize gate fidelities.

[1] S. Nadj-Perge *et al.*, arXiv:1011.0064v1

[1]Funded by the Sloan and Packard Foundations, Army Research Office, and DARPA QuEST.

1:27PM Q27.00010 On-demand single-electron transfer between distant quantum dots with nanosecond pulses of surface acoustic waves , R.P.G. MCNEIL, M. KATAOKA[1], C.J.B. FORD, C.H.W. BARNES, J.P. GRIFFITHS, G.A.C. JONES, I. FARRER, D.A. RITCHIE, University of Cambridge — Quantum dots (QDs) provide a useful system for manipulating and storing quantum information. Methods for moving quantum information (spin) between processor and storage, or to a region of holes for conversion to photon qubits, will be required. Tunnelling of electrons over long distances between QDs is not viable. We show controlled long-range transfer of single electrons between QDs through a depleted 1D channel using pulses of surface acoustic waves (SAWs). In our device, two QDs are connected by a 4μm channel with QD occupancy monitored by 1D charge detectors. Electrons may be trapped and raised above the Fermi energy by stepping gate voltages. Having set the first QD to be 'full' and the other QD 'empty', a short SAW pulse is sent to transfer the electron to the opposite QD. This bi-directional process may be repeated over 100 times with the same electron. SAW power and pulse-width dependences suggest that transfer is achieved during the first few SAW cycles allowing sub-20ns pulses to be used.

[1]now at NPL Teddington

1:39PM Q27.00011 A proposed all-electrical spin qubit CNOT gate robust against charge noise[1] , SANKAR DAS SARMA, JASON KESTNER, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, MD — We shall propose an alternative to the Loss-DiVincenzo implementation of the CNOT gate in a quantum dot spin qubit system. Our all-electrical proposal has the advantage of being robust against uncertainties and fluctuations in the tunnel coupling, barrier gate voltage pulse area, and interwell detuning which typically arise due to charge noise. The core idea is to introduce an auxiliary dot and use an analog to the stimulated Raman adiabatic passage (STIRAP) pulse sequence in three-level atomic systems, often referred to in the context of electron transport in quantum dot systems as CTAP (Coherent Tunneling by Adiabatic Passage). Spin-dependent tunneling opens the possibility of performing entangling two-qubit gates by this method.

[1]Work supported by IARPA, LPS-CMTC, and CNAM.

1:51PM Q27.00012 Sensitivity to electronics error in coupled double quantum dot qubits , ERIK NIELSEN, RICHARD MULLER, MALCOLM CARROLL, Sandia National Laboratories — Reducing the effects of electronics control error in double quantum dot (DQD) quantum bits (qubit) is a central challenge to the creation of a solid-state quantum computing architecture. We investigate a system of capacitively coupled DQDs which implement a variant of the controlled phase gate when using each DQD as a singlet-triplet qubit. We identify regimes in which the gate action is more robust to sources of noise such as error around the applied bias point due to electronics or charge noise. Energy spectra are found using a configuration interaction (CI) method that accurately captures the (2,0) configuration of the DQD system, which is important for operating in these potentially low-noise regimes. This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

2:03PM Q27.00013 Gate Capacitance Reproducibility and Modeling in Silicon Double Quantum Dots , TED THORBECK, JQI: NIST & U. of Maryland, AKIRA FUJIWARA, NEIL ZIMMERMAN, NTT — For many applications the ability to design quantum dots with a specific set of gate capacitances and then rely on the reproducibility of those capacitances is crucial. For quantum computing, the ability to design our gate capacitances would help in reaching the few electron regime and in coupling multiple devices. For other applications the ability to design our gate capacitances would enable higher temperature operation. Our double quantum dots are formed by electrostatic gates on a silicon nanowire. We have measured 20 similar devices with 8 different sets of lithographic parameters. We will report on the reproducibility of the gate capacitances. For example, the range of capacitances is typically within 10% of the average. We will also compare our measured capacitances to simulations based on lithographic parameter. This simulation could then be used to design new devices.

Wednesday, March 23, 2011 11:15AM - 2:15PM –
Session Q28 DMP: Focus Session: Carbon Nanotubes and Related Materials: Devices II C156

11:15AM Q28.00001 Carbon nanotube based NEMS actuators and sensors , MICHAEL FORNEY, UNC Charlotte, JORDAN POLER — Single-walled carbon nanotubes (SWNTs) have been widely studied due to superior mechanical and electrical properties. We have grown vertically aligned SWNTs (VA-SWNTs) onto microcantilever (MC) arrays, which provides an architecture for novel actuators and sensors. Raman spectroscopy confirms that the CVD-grown nanotubes are SWNTs and SEM confirms aligned growth. As an actuator, this hybrid MC/VA-SWNT system can be electrostatically modulated. SWNTs are excellent electron acceptors, so we can charge up the VA-SWNT array by applying a voltage. The electrostatic repulsion among the charged SWNTs provides a surface stress that induces MC deflection. Simulation results show that a few electrons per SWNT are needed for measureable deflections, and experimental actuators are being characterized by SEM, Raman, and an AFM optical lever system. The applied voltage is sinusoidally modulated, and deflection is measured with a lock-in amplifier. These actuators could be used for nano-manipulation, release of drugs from a capsule, or nano-valves. As a sensor, this MC/VA-SWNT system offers an improved sensitivity for chemical and bio-sensing compared to surface functionalized MC-based sensors. Those sensors only have a 2D sensing surface, but a MC/VA-SWNT system has significantly more sensing surface because the VA-SWNTs extend microns off the MC surface.

11:27AM Q28.00002 High yield assembly and electron transport investigation of semiconducting-rich local-gated single-walled carbon nanotube field effect transistors , KRISTY KORMONDY, PAUL STOKES, SAIFUL KHONDAKER, Nanoscience Technology Center and Department of Physics, University of Central Florida, Orlando, Florida, 32826 — Single-walled carbon nanotubes (SWNTs) are ideal for use in nanoelectronic devices because of their high current density, mobility and subthreshold slope. Using individual local gates and scaling the gate oxide has shown faster switching behavior and lower power consumption. However, assembly methods must be developed to reproducibly align all-semiconducting SWNTs at specific locations with individually addressable gates for future integrated circuits. We show high yield assembly of local-gated semiconducting SWNTs assembled via AC-dielectrophoresis (DEP). Detailed electron transport investigations on the devices show that 98% display good FET behavior, with an average threshold voltage of 1V and subthreshold swing as low as 120 mV/dec.

11:39AM Q28.00003 Measurement of quantum capacitance in individual semiconducting single-walled[1] , YANFEI YANG, Physics Department, Georgetown University, GEORGY FEDOROV, RRC Kurchatov Institute, Russia, SERHII SHAFRANJUK, Physics and Astronomy Department, Northwestern University, PAOLA BARBARA, Physics Department, Georgetown University, PHYSICS DEPARTMENT, GEORGETOWN UNIVERSITY TEAM, SERHII SHAFRANJUK COLLABORATION, GEORGY FEDOROV COLLABORATION — The capacitance of a carbon nanotube consists of its geometrical capacitance and its quantum capacitance. The latter is determined by the electronic density of states of the nanotube and the electron interactions, therefore it is a tool for probing fundamental electronic properties in carbon nanotubes, as well as an important parameter to design carbon nanotube electronic devices. The quantum capacitance of a carbon nanotube was first measured by using a capacitance bridge at 77K [1]. Here we extract the quantum capacitance of a semiconducting single-walled carbon nanotube in two one-dimensional subbands from electronic transport measurements at 4.2 K. We compare our results to other experiments and predictions from theoretical models.

[1] S. Ilani, L. A. K. Donev, M. Kindermann, and P. L. McEuen, Nature Physics, 2, 687, (2006).

[1]Funded by NSF, DMR-0907220

11:51AM Q28.00004 Electronic transport in intermediate sized carbon nanotubes[1] , MARKUS AHLSKOG, University of Jyvaskyla, Department of Physics, DAVIE MTSUKO, ANTTI JUUTILAINEN, University of Jyvaskyla — We have measured low temperature transport properties of multiwalled carbon nanotubes (MWNT) of different diameters in the range 2-10 nm [1]. In nearly all samples the gate dependent conductance exhibits a gap whose size increases with decreasing tube diameter and increasing electrode separation. This so called transport gap is attributed, based on the experimental findings, on a combination of localization effects and narrow diameter induced gaps in the electronic band structure.

[1] M. Ahlskog, O. Herranen, A. Johansson, J. Leppäniemi, and D. Mtsuko, Phys. Rev. B **79**, 155408 (2009).

[1]This work was supported by the Academy of Finland.

12:03PM Q28.00005 Resistance of individual long suspended carbon nanotubes with known atomic structures , MITSUHIDE TAKEKOSHI, VIKRAM DESHPANDE, YUHEI MIYAUCHI, ZHENGYI ZHANG, CHENGUANG LU, TONY HEINZ, JAMES HONE, PHILIP KIM, Columbia University — We present electrical transport measurement on long individually suspended carbon nanotubes. Single walled carbon nanotubes (SWNTs) are grown by a chemical vapor deposition method across a slit made on silicon oxide/silicon substrate with pre-patterned platinum electrodes. Rayleigh spectroscopy allows us to determine atomic structure indices of individual SWNTs that connect the electrodes across the slit. We investigate the temperature dependent resistance of metallic SWNTs. The relation between electron-phonon interaction in SWNTs in the connection of the atomic structure will be discussed.

12:15PM Q28.00006 Electrical Resistance of Double-Wall Carbon Nanotubes with Determined Chiral Indices , LETIAN LIN, University of North Carolina at Chapel Hill, Curriculum in Applied Sciences and Engineering, TAORAN CUI, LU-CHANG QIN, SEAN WASHBURN, University of North Carolina at Chapel Hill, Department of Physics and Astronomy — The properties of carbon nanotubes (CNT), especially single-wall nanotubes (SWNT) and double-wall nanotubes (DWNT), are profoundly sensitive to the atomic structure described by its chirality. CNTs connected to sub-micron electrodes were suspended for transmission electron microscope (TEM) study. We determined the chiral indices of each individual CNT via its nano beam electron diffraction patterns and measured its electrical resistance by the four-probe method at room temperature. We studied the factor of different combinations of semiconducting/metallic shells on the electrical characterizations of DWNTs. The electrical properties were compared between DWNTs and SWNTs and the result show that the electrical transport of a DWNT is dominated by the chiral indices of outer shell.

12:27PM Q28.00007 Carbon nanotubes for interconnects in integrated circuits , JEAN DIJON, CEA/Liten — Carbon nanotubes are one of the materials that may be used for advanced interconnects beyond the 16nm node thanks to there extreme resistance to electro migration and to bottom up approach which allow to grow them in tiny holes with very high aspect ratio. The resistance of a via with area A and height h filled with CNT is expressed by $R_{via} = \frac{rq+rsh+rc}{Ad_t}$ where rq, rs, rc are respectively the 6.5kΩ quantum resistance, the scattering resistance and the contact resistances of one tube. To be competitive with copper via resistance, a large density d_t of carbon walls have to be paralleled. Following ITRS needs a density of 2 or 3 10^{13}cm^{-2} conducting CNT walls have to be obtained. This optimum wall density requests the growth of highly packed few nanometre diameter CNTs. Such density has been the main bottleneck for the development of CNT interconnects. Recently ultra high density integration scheme have been demonstrated and for the first time wall density close to the requested one have been integrated in devices. Such density comes from the development on conductive substrates of a CNT growth mode normally used to obtain forests of small tube diameter on insulating substrate like alumina. With this mode, CNTs are grown with base growth mode which is the mode requested for SWCNT or DWCNT thus by continuity it will be possible to increase the density still further by increasing the density of catalyst particles. Our bottom metal of choice is AlCu with iron as catalyst. With this system tube contact resistance between 10^4 to 10^6 Ohm have been measured on blanket AlCu substrates. This resistance must be decreased by one or two order of magnitude while increasing further CNT density. In this paper we will present our last integration developments and the role of plasma pre-treatment of the iron aluminium interface in order to decrease the contact resistance. We will show that the bottom profile of via has a major impact on the quality of CNT growing in the holes and discuss future evolutions of this technology.

1:03PM Q28.00008 Wide Contact Structures for Low-noise Nano-channel Devices based on Carbon Nanotube Network , HYUNGWOO LEE, MINBAEK LEE, SEON NAMGUNG, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea, SEUNGHUN HONG, Department of Physics and Astronomy; Department of Biophysics and Chemical Biology, Seoul National University, Seoul 151-747, Korea — We developed a wide-contact structure for low-noise devices based on carbon nanotube (CNT) networks. This wide-contact CNT network-based device has a dumbbell-shaped channel which is comprised of a narrow channel region and wide CNT/electrode contact regions. We showed that the wide-contact structure reduced 1/f noise which originated from CNT/electrode contact regions. We also systematically analyzed the noise characteristics of the structured CNT networks and established an empirical formula that can describe the noise behavior of CNT network-based devices including the effect of contact regions and CNT alignment. Interestingly, our noise analysis revealed that the noise amplitude of aligned CNT networks behaves quite differently compared with that of randomly-oriented CNT networks. These results would be an important guideline in designing low-noise nanoscale devices based on CNT networks for various applications such as a highly sensitive low-noise sensor.

1:15PM Q28.00009 Physics of aligned arrays of single-walled NTs: From transistor to diode applications , SLAVA V. ROTKIN, Department of Physics and Center for Advanced Materials and Nanotechnologies, Lehigh University, JOHN A. ROGERS, Beckman Institute and Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign — NTs have been originally proposed as a 1D high mobility semiconductor material for field-effect transistors (FET). This format is though appeared to be less practical due to low values of the currents through a single NT channel. On contrary, NT massive parallel arrays have already found implementation in flexible and RF electronics. Can we think of NT arrays being another semiconductor thin film materials? Where does the conventional knowledge apply for NT parallel array devices? This talk discusses specialized aspects of physics of electronic and optoelectronic device prototypes and presents recent results for NT FETs and LEDs (light-emitting diode) in parallel array geometries. Cross-talk between individual NTs in the array allows to beat the statistical "noise" in the device properties which appears due to randomized NT distribution in the array. Although, taking this into account, device-level characteristics should be used with a care to extract a single NT physical parameters.

1:27PM Q28.00010 ABSTRACT WITHDRAWN –

1:39PM Q28.00011 Macroelectronic Integrated Circuits Using High-Performance Separated Carbon Nanotube Thin-Film Transistors , CHUAN WANG, JIALU ZHANG, CHONGWU ZHOU, University of Southern California — Macroelectronic integrated circuits are widely used in applications such as flat panel display, transparent electronics, as well as flexible and stretchable electronics. However, the challenge is to find the channel material that can simultaneously offer low temperature processing, high mobility, transparency and flexibility. Here in this paper, we report the application of high-performance separated nanotube thin-film transistors (TFTs) for macroelectronic integrated circuits. We have systematically investigated the performance of TFTs using separated nanotubes with 95% and 98% semiconducting nanotubes, and high mobility transistors have been achieved. In addition, we observed that while 95% semiconducting nanotubes are ideal for applications requiring high mobility (up to 67 $cm^2V^{-1}s^{-1}$) such as analog and radio-frequency applications, 98% semiconducting nanotubes are ideal for applications requiring high on/off ratios ($>10^4$ with channel length down to 4 μm). Furthermore, integrated logic gates such as inverter, NAND and NOR have been designed and demonstrated using 98% semiconducting nanotube devices, and symmetric input/output behaviour is achieved, which is crucial for the cascading of multiple stages of logic blocks and larger scale integration. Our approach can serve as the critical foundation for future nanotube-based thin-film macroelectronics.

1:51PM Q28.00012 Anisotropic electronic transport in highly aligned carbon nanotube films , SEBASTIEN NANOT, XUAN WANG, JUNICHIRO KONO, ECE Dpt, Physics and Astronomy Dpt, Rice University, YANHUA DAI, RUI-RUI DU, Physics and Astronomy Dpt, Rice University, CARY PINT, ROBERT H. HAUGE, Smalley Institute for Nanoscale Science and Technology, Rice University — Electronic transport in carbon nanotube (CNT) networks has recently attracted much renewed interest due to the numerous advancements in controlling, sorting, and aligning CNTs. Understanding the roles of intra-tube and inter-tube transport in these systems is fundamentally important both from basic and applied points of view. We have studied samples of ultra-long and highly-aligned CNTs grown by CVD and laid down on Si/SiO2 substrates. We designed and fabricated a novel device structure in which we can separately study intra-tube and inter-tube transport. In the intra-tube configuration, ends of ultra-long CNTs were contacted and the current parallel to the alignment direction was measured, whereas, in the inter-tube configuration, transport perpendicular to the alignment direction was probed. We studied the magnetic field and temperature dependence of the resistance between 0.3 K and 300 K, revealing an interesting evolution of transport regimes as for the localization of charge carriers. Preliminary results of photoconductivity measurements will also be presented.

2:03PM Q28.00013 Air-Stable Conversion of Separated Carbon Nanotube Thin-Film Transistors from P-type to N-type Using Atomic Layer Deposition of High-κ Oxide and Its Application in CMOS Logic Circuits , JIALU ZHANG, CHUAN WANG, YUE FU, YUCHI CHE, CHONGWU ZHOU, University of Southern California — Pre-separated, high purity semiconducting carbon nanotubes hold great potential for thin-film transistors (TFTs) and integrated circuit applications. One of the main challenges it still faces is the fabrication of air-stable N-type nanotube TFTs with industry compatible techniques. Here in this paper, we report a novel and highly reliable method of converting the P-type TFTs using pre-separated semiconducting nanotubes into air-stable N-type transistors by adding a high-κ oxide passivation layer using atomic layer deposition (ALD). The N-type devices exhibit symmetric electrical performance compared with the P-type devices in terms of on-current, on/off ratio and mobility. Various factors affecting the conversion process including ALD temperature, metal contact material, channel length, have also been systematically studied. A complementary metal-oxide-semiconductor (CMOS) inverter with rail-to-rail output, symmetric input/output behavior and large noise margin has been further demonstrated. The excellent performance gives us the feasibility of cascading multiple stages of logic blocks and larger scale integration. Our approach can serve as the critical foundation for future nanotube-based thin-film macroelectronics.

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q29 GQI: Focus Session: Quantum Information for Quantum Foundations - Experiments and Tests C148

11:15AM Q29.00001 Foundational aspects of energy-time entanglement , JAN-ÅKE LARSSON, Linkoping University — This presentation will discuss whether energy-time entanglement is a properly Quantum Information representation, by considering its relation to Einstein-Podolsky-Rosen (EPR) elements of reality. The interferometric experiment proposed by J. D. Franson in 1989 provides the background, and the main issue here is whether a Local Realist model can give the Quantum-Mechanical predictions for this setup. The Franson interferometer gives the same interference pattern as the usual Bell experiment (modulo postselection). Even so, depending on the precise requirements made on the Local Realist model, this can imply a) no violation, b) smaller violation than usual, or c) full violation of the appropriate statistical bound. The discussion will include the nature of the requirements, the motivation for making them, and their effect. The alternatives include using a) only the measurement outcomes as EPR elements of reality, b) the emission time as EPR element of reality, and c) path realism. These subtle requirements need to be taken into account when designing and setting up future experiments of this kind, intended to test Local Realism, or indeed to do Quantum Information Processing.

11:27AM Q29.00002 Large violation of Bell's inequalities using both counting and homodyne measurements , VALERIO SCARANI, DANIEL CAVALCANTI, CQT, National University of Singapore, NICOLAS BRUNNER, PAUL SKRZYPCZYK, University of Bristol, ALEJO SALLES, Bohr Institute, Copenhagen — So far, all the optical demonstrations of violations of Bell's inequalities have involved discrete degrees of freedom (e.g. polarization, time-bins) and are plagued by the detection-efficiency loophole. Continuous degrees of freedom would be a very interesting alternative because of the efficiency of the homodyne measurement; but the feasible schemes proposed so far reach very weak violations. We show that large violations for easily-prepared states can be achieved if both photon counting and homodyne detections are used. Our simple scheme may lead to the first violation of Bell's inequalities with continuous variables and pave the way for a loophole-free Bell test.

11:39AM Q29.00003 A non-local quantum eraser[1] , X. MA, J. KOFLER, A. QARRY, N. TETIK, T. SCHEIDL, R. URSIN, S. RAMELOW, L. RATSCHBACHER, T. HERBST, A. FEDRIZZI, T. JENNEWEIN, A. ZEILINGER, Univ. of Vienna and OEAW — The complementarity behavior of quantum systems is strikingly illustrated by the quantum eraser, where one can actively choose whether or not to erase which-path information of one particle by performing suitable measurements on another particle entangled with it [1-2]. Quantum mechanics predicts that this choice can be arbitrarily delayed and spatially separated from interference [1-3]. We report the first quantum eraser experiment performed under Einstein locality, i.e. under relativistic space-like separation. We employ the hybrid entanglement between path and polarization of photon pairs and distribute the photons over an optical fibre link of 55 m and, in another experiment, over a free-space link of 144 km. A complementarity inequality is measured and well fits the predictions of quantum mechanics. Our experiment represents a conclusive demonstration of the quantum eraser concept.
[1] M. O. Scully, K. Drühl, Phys. Rev. A 25, 2208 (1982). [2] J. A. Wheeler, in Quantum Theory and Measurement (1984). [3] V. Jacques, *et al.*, Science 315, 966 (2007).

[1]Supported by the European Commission program (Q-ESSENCE, ERC Senior Grant QIT4QAD, Marie-Curie RTN EMALI) and the Austrian Scinece Fund (CoQuS and SFB-FoQuS).

11:51AM Q29.00004 On the Experimental Violation of Mermin's High-Spin Bell Inequalities in the Schwinger Representation , RUFFIN EVANS, OLIVIER PFISTER, University of Virginia — Since Bell's original paper in 1964, a wide variety of experimental tests have overwhelmingly supported the completeness of quantum mechanics over local hidden-variable theories. However, relatively little effort has focused on systems of spins larger than $\frac{1}{2}$; generalizing Bell's result to higher dimensions is difficult, and the experiments needed to test these high-spin Bell inequalities are exacting. New advances in high efficiency photon-number-resolving detectors suggest that experimental tests of these inequalities should be possible in the Schwinger representation, using the continuous-variable entangled (two-mode squeezed) fields produced by an optical parametric oscillator below threshold. In this paper, we explore the realistic experimental implementation of this proposal to violate Mermin's high-spin inequalities. We demonstrate that violation for spin values greater than 1 should be attainable under a range of feasible experimental conditions that include finite squeezing and nonideal detection efficiency.

12:03PM Q29.00005 Surface based detection schemes for molecular interferometry experiments - implications and possible applications , THOMAS JUFFMANN, ADRIANA MILIC, MICHAEL MUELLNERITSCH, MARKUS ARNDT, Univ. of Vienna - Faculty of Physics — Surface based detection schemes for molecular interferometry experiments [1] might be crucial in the search for the quantum properties of larger and larger objects [2] since they provide single particle sensitivity. Here we report on molecular interferograms of different biomolecules imaged using fluorescence microscopy. Being able to watch the build-up of an interferogram live and in situ reveals the matter-wave behavior of these complex molecules in an unprecedented way. We examine several problems encountered due to van-der-Waals forces between the molecules and the diffraction grating and discuss possible ways to circumvent these. Especially the advent of ultra-thin (1-100 atomic layers) diffraction masks might path the way towards molecular holography. We also discuss other possible applications such as coherent molecular microscopy.

[1] T. Juffmann, S. Truppe, P. Geyer, A.G. Major, S. Deachapunya, H. Ulbricht, M. Arndt, Phys. Rev. Lett. 103, 263601 (2009).
[2] T. Juffmann, S. Nimmrichter, M. Arndt, H. Gleiter, K.Hornberger, in print, Foundations of Physics.

12:15PM Q29.00006 Matter wave interferometry with large and complex molecules , STEFAN GERLICH, SANDRA EIBENBERGER, MATHIAS TOMANDL, University of Vienna, Faculty of Physics, JENS TÜXEN, MARCEL MAYOR, University of Basel, Department of Chemistry, MARKUS ARNDT, University of Vienna, Faculty of Physics — Matter wave interferometry with molecules of increasing size, mass and complexity explores the frontiers of quantum mechanics and it is a promising tool for determining molecular properties with high precision. The quantum wave nature of organic molecules is used in a Kapitza-Dirac-Talbot-Lau interferometer to generate a set of high-contrast interference fringes that are highly sensitive to external forces. This is exploited to access thermally averaged internal molecular properties, such as optical and static polarizabilities, static and thermally activated electric dipole moments, information about conformational differences and state changes, optical absorption spectra and more. The information about the internal states can be extracted through conservative interactions, i.e. allowing the persistence of full quantum delocalization in position space.

12:27PM Q29.00007 Violation of local realism with freedom of choice , JOHANNES KOFLER, THOMAS SCHEIDL, RUPERT URSIN, SVEN RAMELOW, XIAO-SONG MA, Institute for Quantum Optics and Quantum Information (IQOQI), Austrian Academy of Sciences, THOMAS HERBST, Faculty of Physics, University of Vienna, LOTHAR RATSCHBACHER, ALESSANDRO FEDRIZZI, NATHAN LANGFORD, THOMAS JENNEWEIN, ANTON ZEILINGER, Institute for Quantum Optics and Quantum Information (IQOQI), Austrian Academy of Sciences — Bell's theorem shows that local realistic theories place strong restrictions on observable correlations between different systems, giving rise to Bell's inequality which can be violated in experiments using entangled quantum states. Bell's theorem is based on the assumptions of realism, locality, and the freedom to choose between measurement settings. In experimental tests, "loopholes" arise which allow observed violations to still be explained by local realistic theories. Violating Bell's inequality while simultaneously closing all such loopholes is one of the most significant still open challenges in fundamental physics today. We present an experiment that violates Bell's inequality while simultaneously closing the locality loophole and addressing the freedom-of-choice loophole, also closing the latter within a reasonable set of assumptions. Reference: T. Scheidl et al., Proc. Natl. Acad. Sci. USA 107, 19708 (2010)

12:39PM Q29.00008 Experimental non-classicality of an indivisible system[1] , RADEK LAPKIEWICZ, PEIZHE LI, CHRISTOPH SCHAEFF, NATHAN LANGFORD, SVEN RAMELOW, MARCIN WIESNIAK, ANTON ZEILINGER, University of Vienna, Faculty of Physics, Vienna; Institute for Quantum Optics and Quantum Information, Austrian Academy of Sciences, Vienna — In Quantum Mechanics (QM) not all properties can be simultaneously well defined. An important question is whether a joint probability distribution can describe the outcomes of all possible measurements, allowing a quantum system to be mimicked by classical means. Klyachko et al. [PRL 101, 020403 (2008)] derived an inequality which allowed us to answer this question experimentally. The inequality involves only five measurements and QM predicts its violation for single spin-1 particles. This is the simplest system where such a contradiction is possible. It is also indivisible and as such cannot contain entanglement. In our experiment with single photons distributed among three modes (isomorphic to stationary spin-1 particles) we obtained a value of -3.893(9), which lies more than 90 standard deviations below the "classical" bound of -3.

[1]Supported by ERC (Advanced Grant QIT4QAD), the Austrian Science Fund (Grant F4007), the EU (Contract No. MRTN-CT-2006-035369 (EMALI)).

12:51PM Q29.00009 Testing spontaneous localization with ultra-massive cluster interferometry , STEFAN NIMMRICHTER, University of Vienna, KLAUS HORNBERGER, MPIPKS Dresden, MARKUS ARNDT, University of Vienna — Understanding the transition from the microscopic domain of quantum mechanics to our everyday classical world is still an open problem in modern physics. Collapse models are a possible way to resolve this issue by introducing mechanisms which break the quantum superposition principle above a certain mass and time scale. One of the best studied models is the theory of continuous spontaneous localization (CSL) by Ghirardi, Pearle and Rimini [1]. We show that it should be possible to test the predictions of the CSL model in the new matter-wave interferometer for heavy metal clusters that is currently built in Vienna. Extending the original Talbot-Lau setup for biomolecules, the new scheme will operate in the time-domain using three pulsed standing-wave gratings of UV laser light. We argue that this should enable us to see single-particle interference in an unprecedented mass range from 10^5 up to even 10^8 atomic mass units. Recent estimates of the strength of the CSL effect by Adler and Bassi [2,3] suggest that a breakdown of the quantum superposition principle would occur in precisely this mass regime.

[1] Phys. Rev. A 42, 78 (1990)
[2] J. Phys. A 40, 2935 (2007)
[3] arxiv eprint 1011.3767v1 (2010)

1:03PM Q29.00010 Hardy's paradox and a violation of a state-independent Bell inequality in time , ALESSANDRO FEDRIZZI, MARCELO P. ALMEIDA, MATTHEW A. BROOME, ANDREW G. WHITE, Department of Physics and Centre for Quantum Computer Technology, University of Queensland, Brisbane QLD 4072, Australia, MARCO BARBIERI, Groupe d'Optique Quantique, Laboratoire Charles Fabry, Institut d'Optique, CNRS, Universite Paris-Sud, France — Tests such as Bell's inequality and Hardy's paradox highlight the differences between local realistic theories and quantum predictions for measurement probabilities and correlations between distant particles. Transposing these tests to the temporal domain, i.e. making two measurements on the one quantum particle at different times, yield Hardy and Bell tests mathematically identical to their spatial counterparts, but give very different physical results. Here, we use a photonic entangling gate to implement non-destructive temporal measurements on a quantum system. We measure a much stronger form of Hardy's paradox and demonstrate violation of a Bell inequality in time independent of the quantum state, including for fully-mixed states. Our work yields interesting fundamental insights and opens up a path to more efficient quantum information processing protocols based on temporal quantum correlations.

1:15PM Q29.00011 Experimental Violation of Two-Party Leggett-Garg Inequalities with Semi-weak Measurements , JUSTIN DRESSEL, CURTIS BROADBENT, JOHN HOWELL, ANDREW JORDAN, University of Rochester — We generalize the derivation of Leggett-Garg inequalities to systematically treat a larger class of experimental situations by allowing multi-particle correlations, invasive detection, and ambiguous detector results. Furthermore, we show how many such inequalities may be tested simultaneously with a single setup. As a proof of principle, we violate several such two-particle inequalities with data obtained from a polarization-entangled biphoton state and a semi-weak polarization measurement based on Fresnel reflection. We also point out a non-trivial connection between specific two-party Leggett-Garg inequality violations and convex sums of strange weak values.

1:27PM Q29.00012 Causality, Bell's theorem, and Ontic Definiteness , JOE HENSON, Perimeter Institute — Bell's theorem shows that the reasonable relativistic causal principle known as "local causality" is not compatible with the predictions of quantum mechanics. It is not possible maintain a satisfying causal principle of this type while dropping any of the better-known assumptions of Bell's theorem. However, another assumption of Bell's theorem is the use of classical logic. One part of this assumption is the principle of *ontic definiteness*, that is, that it must in principle be possible to assign definite truth values to all propositions treated in the theory. Once the logical setting is clarified somewhat, it can be seen that rejecting this principle does not in any way undermine the type of causal principle used by Bell. Without ontic definiteness, the deterministic causal condition known as Einstein Locality succeeds in banning superluminal influence (including signalling) whilst allowing correlations that violate Bell's inequalities. Objections to altering logic, and the consequences for operational and realistic viewpoints, are also addressed.

1:39PM Q29.00013 On dipole anisotropy in spatial distribution of Plank's constant values , SIMON BERKOVICH, The George Washington University — The work relates to the remarkable fact discovered by John Webb et al. of angular variations of the fine structure constant $\alpha = e^2/hc$. We elaborate on this fact using our model of quantum mechanics (see [1] and references within). The peculiarity of quantum behavior stems from interactive holography appearing on top of the cellular automaton mechanism of the Universe. Nonlocality comes naturally from sliced holographic processing. As to the anisotropy of α, its is due to variations of h caused by different undulation control patterns in different positions with respect to the source of the holographic reference beam. The angular divergences in α are determined by the eccentric placement of the Solar system with respect to this reference holographic beam. This eccentricity factor imposes dipole structuring on several types of astrophysical observations. So, following [1], small opposite changes in h with respect to the eccentricity displacement of the Solar system could be anticipated. Before we have shown that the same eccentricity factor leads to the appearance of the "axis-of-evil" in CMB. Further, the recently discovered anisotropy in high-energy cosmic rays should be also determined by the eccentricity factor, i.e. it should adhere to the same dipole. [1] S. Berkovich, "A Comprehensive Explanation of Quantum Mechanics", http://www.bestthinking.com/topics/science/physics/ quantum_physics/a-comprehensive-explanation-of-quantum-mechanics

1:51PM Q29.00014 Scaling of quantum Zeno dynamics in thermodynamic systems , WING CHI YU, LI-GANG WANG, SHI-JIAN GU, Department of Physics, The Chinese University of Hong Kong, Hong Kong — Quantum Zeno effect (QZE) refers to the inhabitation of the unitary time evolution of a quantum system by repeated frequent measurements. It has been studied intensively within the content of quantum optics in recent decades. Among those analyses, the systems under consideration are only of a few levels. Little attention of QZE in thermodynamic systems has been paid so far. In this presentation, we will investigate the QZE in thermodynamic systems from the viewpoint of condensed matter physics. We take the one-dimensional transverse-field Ising model and the Lipkin-Meshkov-Glick (LMG) model as examples to illustrate analytically the criteria, in terms of the size dependence of the leading term of the survival probability in the short-time limit, for observing the QZE. Our analysis shows that in order to observe the QZE in the Ising model, the frequency of the projective measurement should be of comparable order to that of the system sizes. The same criterion also holds in the symmetry broken phase of the LMG model. However, in the polarized phase of the LMG model, the leading term of the survival probability is independent of the system size and the QZE can be easily observed.

2:03PM Q29.00015 Decoherence Free Neutron Interferometry , DMITRY A. PUSHIN, DAVID G. CORY, IQC, University of Waterloo, MICHAEL G. HUBER, NIST, MOHAMED ABUTALEB, MIT, MUHAMMAD ARIF, NIST, CHARLES W. CLARK, Joint Quantum Institute, NIST and the University of Maryland — A neutron interferometer (NI) is a unique example of the macroscopic quantum coherence and has been used to test fundamental principles of quantum mechanics. In practice, neutron interferometers are not widely used because of their extreme sensitivity to environmental noise which is in part due to the slow velocity (relative to light) of the neutron. We show that a neutron interferometer design can benefit from concepts of quantum information processing. We have machined a Decoherence Free (DF) neutron interferometer designed using a quantum error correction code,[1] and have shown it to be much less sensitive to mechanical vibrations than is the standard Mach-Zehnder (MZ) interferometer. Both the MZ and DF geometries are incorporated in one crystal, which allows direct comparisons to be made. We believe that our results and related quantum information approaches, such as "the power of one qubit,"[2] will enable a new series of compact neutron interferometers that can be tailored to specific applications in soft condensed matter and spintronics.

[1]D. A. Pushin, M. Arif, and D. G. Cory, Phys. Rev. A (http://pra.aps.org/abstract/PRA/v79/i5/e053635) 79, 053635 (2009)
[2]E. Knill and R. Laflamme, Phys. Rev. Lett. (http://prl.aps.org/abstract/PRL/v81/i25/p5672_1) 81, 5672 (1998)

Wednesday, March 23, 2011 11:15AM - 2:15PM –
Session Q30 DCMP: Graphene: Electron-Electron Interactions C147/154

11:15AM Q30.00001 The effective fine-structure constant of freestanding graphene measured in graphite[1] , YU GAN, JAMES REED, BRUNO UCHOA, YOUNG-IL JOE, University of Illinois at Urbana-Champaign, DIEGO CASA, Argonne National Laboratory, EDUARDO FRADKIN, PETER ABBAMONTE, University of Illinois at Urbana-Champaign — Electrons in graphene behave like Dirac fermions, permitting phenomena from high- energy physics to be studied in a solid-state setting. A key question is whether or not these fermions are critically influenced by Coulomb correlations. We performed inelastic x-ray scattering experiments on crystals of graphite and applied reconstruction algorithms to image the dynamical screening of charge in a freestanding graphene sheet. We found that the polarizability of the Dirac fermions is amplified by excitonic effects, improving screening of interactions between quasiparticles. The strength of interactions is characterized by a scale-dependent, effective fine-structure constant, $\alpha_g^*(\mathbf{k},\omega)$, the value of which approaches $1/7$ at low energy and large distances. This value is substantially smaller than the nominal $\alpha_g = 2.2$, suggesting that, on the whole, graphene is more weakly interacting than previously believed.

[1]Funding provided by DOE grants DE-FG02-07ER46459 and DE-FG02-07ER46453.

11:27AM Q30.00002 Excitonic Gap from Long-Range Coulomb Interaction in Graphene , JOSE GONZALEZ, Instituto de Estructura de la Materia (CSIC), Madrid, Spain — We apply renormalization group methods to analyze the development of an excitonic gap in the theory of Dirac fermions in graphene with long-range Coulomb interaction. In the large-N approximation, we show that the chiral symmetry is only broken below a critical number of two-component Dirac fermions $N_c = 32/\pi^2$, that is precisely half the value found in quantum electrodynamics. Adopting otherwise a ladder approximation, we give evidence of the existence of a critical coupling at which the order parameter of the transition to the gapped phase diverges. This result supports that the opening of an excitonic gap may be driven by a sufficiently strong Coulomb interaction, despite the divergence of the Fermi velocity at low energies in the Dirac theory of graphene.

11:39AM Q30.00003 Manifestation of explicit and spontaneous chiral symmetry breaking in graphene , SUNG-HOON LEE, HYUN-JONG CHUNG, JINSEONG HEO, HEEJUN YANG, SUNAE SEO, Samsung Advanced Institute of Technology, Korea — Using first-principles calculations of graphene having high- symmetry distortion or defects, we investigate the chiral symmetry breaking in graphene as the source of gap opening. We identify that the gap opening by the chiral symmetry breaking in the honeycomb lattice is an ideal two-dimensional (2D) extension of the Peierls metal-insulator transition in a linear lattice, the elemental 1D Dirac lattice, and find that the chiral symmetry breaking manifests itself in graphene by the formation of an internal structure of the lattice, which represents the intrinsic internal structure of massive Dirac fermions. We then show that the gap opening of many of previously reported structures of gapped graphene occurs by explicit breaking of the chiral symmetry, rather than by quantum confinement effects or others, and also show that spontaneous chiral symmetry breaking takes place via electron- phonon coupling at certain quasi-1D graphene structures and at 2D graphene under strain.

11:51AM Q30.00004 Theory of Kekule superconductor on graphene's honeycomb lattice[1] , BITAN ROY, IGOR HERBUT, Department of Physics, Simon Fraser University — A spatially non-uniform superconducting state is proposed as a variational ground state on honeycomb lattice, with the chemical potential close to and right at the Dirac point, when the nearest-neighbor attraction is the dominant component of the interaction. This state spontaneously breaks the translational invariance of the underlying lattice into the Kekule pattern of superconducting bond order parameters. Otherwise it is fully gapped, spin triplet, and odd under the exchange of two sublattices. Symmetries of the ground state for a range of nearest-neighbor interaction, the topological excitations of the Kekule superconductor, and its competition with other superconducting orders proposed in literature will also be discussed.

B. Roy and I. F. Herbut, Phys. Rev. B 82, 035429 (2010).

[1]This work has been supported by NSERC Canada.

12:03PM Q30.00005 Pairing in graphene: A Monte Carlo study , TIANXING MA, Department of Physics, Beijing Normal University, ZHONGBING HUANG, FEIMING HU, HAI-QING LIN — To address the issue of possibility of inducing superconductivity in graphene, we study the behavior of pairing correlation in the extended repulsive Hubbard model on a honeycomb lattice within both determinant quantum Monte Carlo and constrained path Monte Carlo method. We find that the system shows an antiferromagnetic correlation below Van Hove fillings. In the filling range of $<n>$=1.00 $\sim$ 1.20, pairing with $d+id$ symmetry is dominant over pairing with extent s symmetry, especially at low temperatures. The $d+id$-wave pairing susceptibility is enhanced as the electron filling increases, while the effective pairing interaction is suppressed. The summation of pairing correlation for long-range part is enhanced as the repulsion increases, however, for various lattice sizes and interactions, we find that the long-range part of $d+id$-wave pairing correlations both vanishes. Our results suggest that there maybe no superconductivity in pure and low doped graphene.

12:15PM Q30.00006 Interacting fermions on the honeycomb bilayer: From weak to strong coupling[1] , OSKAR VAFEK, National High Magnetic Field Lab/FSU — Many-body instabilities of the half-filled honeycomb bilayer are studied using weak-coupling renormalization group (RG) as well as strong-coupling expansion [1,2]. For spinless fermions, there are 4 independent four-fermion contact couplings. Generally, we find runaway RG flows which we associate with ordering tendencies. The broken symmetry state is typically a gapped insulator with either broken inversion or broken time-reversal symmetry, with a quantized anomalous Hall effect. Additionally, a tight-binding model with nearest-neighbor hopping and nearest-neighbor repulsion is studied in weak and strong couplings and in each regime a gapped phase with inversion symmetry breaking is found. In the strong-coupling limit, the ground-state wave function is constructed for vanishing in-plane hopping but finite interplane hopping, which explicitly displays the broken inversion symmetry and a finite difference between the number of particles on the two layers. In the spin-1/2 case we use Fierz identities to show that there are 9 independent four-fermion contact couplings[2]. The 9 RG equations in this case reduce to the 3 found in Ref.[1] under the assumptions stated in Ref.[1]. They are further used to show that, just as in strong coupling, the most dominant weak-coupling instability of the repulsive Hubbard model (at half filling) is an antiferromagnet. [1] O. Vafek and K. Yang, PRB **81**, 041401 (2010). [2] O. Vafek, PRB **82**, 205106 (2010)

[1]NSF CAREER award Grant No. DMR-0955561

12:27PM Q30.00007 Compressibility Instability of Interacting Electrons in Bilayer Graphene , XIN-ZHONG YAN, Institute of Physics, CAS, C.S. TING, Texas Center for Superconductivity/UH — Using the self-consistent Hartree-Fock approximation, we study the compressibility instability of the interacting electrons in bilayer grapheme at finite temperature. The chemical potential and the compressibility of the electrons can be significantly altered by an energy gap (tunable by external gate voltages) between the valence and conduction bands. For zero gap case, we show that the homogeneous system is stable. When the gap is finite, the compressibility of the electron system becomes negative at low carrier doping concentrations and low temperature. We also present the phase diagram distinguishing the stable and unstable regions of a typically gapped system in terms of temperature and doping.

12:39PM Q30.00008 Limits to universal conductance fluctuations of massless Dirac fermions[1] , MARIO BORUNDA, Harvard University, JESSE BEREZOVSKY, Case Western Reserve University and Harvard University, ROBERT WESTERVELT, ERIC HELLER, Harvard University — We study conductance fluctuations (CFs) and the sensitivity of the conductance to the motion of a single scatterer in two-dimensional massless Dirac systems. Our extensive numerical study finds limits to the predicted universal value of CFs. We find that CFs are suppressed for ballistic systems near the Dirac point and approach the universal value at sufficiently strong disorder. The conductance of massless Dirac fermions is sensitive to the motion of a single scatterer. CFs of order e^2/h result from the motion of a single impurity by a distance comparable to the Fermi wavelength. This result applies to graphene systems with a broad range of impurity strength and concentration while the dependence on the Fermi wavelength can be explored via gate voltages. Our prediction can be tested by comparing graphene samples with varying amounts of disorder and can be used to understand interference effects in graphene mesoscopic devices.

[1]Research supported by the U.S. Department of Energy under grants DE-FG02-08ER46513 and DE-FG02-07ER46422

12:51PM Q30.00009 Interplay between curvature and in-plane magnetic field in bilayer graphene , AVADH SAXENA, LANL, YOGESH JOGLEKAR, IUPUI — For a two-dimensional electron gas (2DEG) in a uniform magnetic field, the effect of the in-plane component on the orbital motion of carriers is ignored because "it can be gauged away." However, the effect of such a field on a massive quantum particle confined to a curved surface has been only recently explored [1]. We obtain the single-particle spectra for such a particle on a sphere, a cylinder, and a torus in the presence of a constant magnetic field. In addition to the geometric potential V_G that arises due to the confinement on a curved surface, we find that in-plane field leads to energy shifts $\Delta E \propto V_G(R/l_B)^4$ where R is the radius of curvature of the surface, and l_B is the magnetic length for the in-plane field. With bilayer graphene as a model for massive quantum particle on a curved surface, we estimate the energy shift for a cylindrical geometry, and show that it is significant for typical experimental parameters.

[1] G. Ferrari and G. Cuoghi, Phys. Rev. Lett. **100**, 230403 (2008).

1:03PM Q30.00010 Plasma Instability in Graphene Bilayers , ANTONIOS BALASSIS, Fordham University, GODFREY GUMBS, Hunter College of the City University of New York — The problem of plasma instability in a pair of coupled semiconductor layers when a dc current is passed through one of the layers has been vigorously investigated over the years. This may be carried out by solving for the real and imaginary parts of the frequency in the polarization function making the dielectric function vanish. We analyze the conditions for plasma instability in a graphene bilayer for various chemical potentials (doping) as well as layer separation.

1:15PM Q30.00011 Tight-binding theory of the spin-orbit coupling in graphene structures[1] , SERGEJ KONSCHUH, MARTIN GMITRA, JAROSLAV FABIAN, University of Regensburg, Germany — Spin-orbit coupling changes qualitatively the electronic band structure of graphene. Most important, the coupling induces spectral gaps at the K(K') points. Earlier theories estimated the *intrinsic* gap of 1 μeV for the single layer and several meVs for bi- and tri-layer graphene, based on σ-π coupling. Our first-principles calculations give the value of 24 μeV for all these systems, due to the presence of the orbitals of the d symmetry in the Bloch states of the π bands. A realistic multiband tight-binding model is presented to explain the effects the d orbitals play in the spin-orbit coupling of graphene and derive an effective single-orbital next-nearest-neighbor hopping model that accounts for the spin-orbit effects. We also study the *extrinsic* spin-orbit coupling, due to an applied transverse electric field. In a single layer the *extrinsic* effect is dominated by the π-σ hybridization. In contrast, in the multi-layer structures the *extrinsic* spin-orbit band splittings come from an interplay of the d-orbitals, the inter-layer hopping, and the electrostatic potential from the applied field.

[1]This work has been supported by SFB689.

1:27PM Q30.00012 Spin-orbit coupling in bi-layer and tri-layer graphene in transverse electric field: first-principles calculations[1] , MARTIN GMITRA, SERGEJ KONSCHUH, JAROSLAV FABIAN, University of Regensburg, Germany — Few-layer graphene structures may be potentially useful for optical and transport applications, due to the possibility of electrical control of the band gaps. Here we investigate the spin-orbit coupling of bilayer and tri-layer graphene around the Fermi level. We show, by performing first-principles full potential linearized augmented plane waves calculations that the spin-orbit physics in these structures derives essentially from monolayer graphene. In particular, the spin splitting of the bands is due to the spin-orbit coupling of the d-orbitals. These give a splitting of the order of 24 μeV at the K point, as in graphene. Breaking the spatial inversion symmetry by a transverse electric field does not change this (intrinsic) picture, unlike what we know from graphene.

[1]This work is supported by the DFG SFB 689.

1:39PM Q30.00013 Dynamical Jahn-Teller Effect at a Vacancy Center in Graphene[1] , SASHI SATPATHY, MOHAMMAD SHERAFATI, BIRABAR NANDA, University of Missouri, ZORAN POPOVIC, Institute for Nuclear Sciences, Belgrade — We study the substitutional vacancy center in graphene from density-functional LAPW calculations and show that it is magnetic and at the same time forms a dynamical Jahn-Teller center. A net magnetic moment of $2\mu_B$ is found, which is explained in terms of the occupation of the $sp^2\sigma$ dangling bond state and the zero-mode state derived from the π bands. The adiabatic potential surface resulting from the $E \otimes e$ vibronic coupling was computed and subsequently the Schrödinger equation was solved for the nuclear motion of the carbon atoms. Our calculations show the tunneling splitting 3Γ to be about 80 cm^{-1}, which is substantially larger than the typical strain fields, leading to a dynamical Jahn-Teller effect (JTE). This explains the puzzling behavior of why in the STM measurements a symmetric carbon triangle is observed around the vacancy, while at the same time we predict the splitting of the vacancy-induced electron states by the static JTE *in spite of* the triangular symmetry.

[1]Work supported by the US Department of Energy

1:51PM Q30.00014 Plasma Excitations in Graphene: Their Spectral Intensity and Temperature Dependence in Magnetic Field , JHAO-YING WU, SZU-CHAO CHEN, GODFREY GUMBS, MING-FA LIN — We calculated the dielectric function, the loss function, the magnetoplasmon dispersion relation and the temperature-induced transitions for graphene in a uniform perpendicular magnetic field. The calculations were performed using the Peierls tight-binding model to obtain the energy band structure and the random-phase approximation to determine the collective plasma excitation spectrum. The single-particle and collective excitations have been precisely identified based on the resonant peaks in the loss function. The critical wave vector at which plasmon damping takes place is clearly established. This critical wave vector depends on the magnetic field strength as well as the levels between which the transition takes place. The temperature effects were also investigated. At finite temperature, there are plasma resonances induced by the Fermi distribution function. Whether such plasmons exist is mainly determined by the field strength, temperature, and momentum.

2:03PM Q30.00015 Field Modulation on the Electronic Structure for the Bilayer and Trilayer Graphene[1] , BI-RU WU, Department of Nature Science, Center for General Education, Chang Gung University, Tao-Yuan, Taiwan — The electronic band gap plays a central role in modern device physics and a tunable band gap provides great flexibility in device design. I present the investigation of electric filed effect on the electronic structure of the bilayer and trilayer graphene. The hexagonal and Bernal type structures are studied for the bilayer and trilayer graphene, additionally, the rhombohedral type is also take into account for the trilayer one. It is found the band gaps of the Bernal type bilayer graphene and the Rhombohedral type trilayer graphene are tunable by a perpendicular electric field. The symmetry of the graphene plays a crucial role in the field modulation. The perpendicular electric field opens the band gap of the Bernal type bilayer graphene and the Rhombohedral type trilayer graphene by breaking the symmetry in z-direction.

[1]I would like to acknowledge NCTS and the financial support from NSC of Taiwan under Grant No.NSC96-2628-M-002-020-MY3 and NSC98-2112-M-004-003-MY3.

Wednesday, March 23, 2011 11:15AM - 2:03PM –

Session Q31 DMP GSCCM DCOMP: Focus Session: Materials at High Pressure V: Structure Prediction and Complex Materials C145

11:15AM Q31.00001 Crystal structure prediction using evolutionary algorithms: how to predict large and complex systems , ANDRIY LYAKHOV, Stony Brook University — Evolutionary crystal structure prediction proved to be a powerful approach in discovering new materials. Algorithm USPEX allows one to predict the most stable crystal structure for a given compound without requiring any experimental input. However, certain limitations are encountered for systems with a large number of degrees of freedom and complex energy landscapes. We explore the nature of these limitations and address them with a number of newly developed tools. For large systems a major problem is the lack of diversity. It is countered with modified variation operators that favor atoms with higher local order and a special initialization procedure for the first generation. For complex energy landscapes, the key problem is the possible existence of several energy funnels. To address this problem, we develop an algorithm incorporating the ideas of abstract "distance" between structures using the so called "fingerprint function." We will compare the efficiency of the old and new algorithm USPEX for different systems and show that the range of application for algorithm is increased. Some systems, where old algorithm couldn't find a solution are now solvable with the new algorithm. And the speed of finding the solutions for systems with the complicated energy landscape is substantially increased.

11:51AM Q31.00002 Prediction of complex high-pressure M-B crystal structures with an evolutionary algorithm , ALEKSEY KOLMOGOROV, SHEENA SHAH, ROXANA MARGINE, University of Oxford — We have carried out an ab initio ground state search in two binary metal-boron systems using an evolutionary algorithm [1] and identified remarkably complex configurations stabilized at high pressures [2,3]. An alkali-earth metal boride is shown to undergo a structural transformation from a semiconducting to a metallic state while a new semiconducting transition metal boride is stabilized at a composition known to have only metallic ground states. For the proposed candidate materials we calculate the electron-phonon coupling and demonstrate their potential to be phonon-mediated superconductors.

[1] A.N. Kolmogorov, http://maise-guide.org (MAISE)
[2] A. N. Kolmogorov, S. Shah, E. R. Margine, A. F. Bialon, T. Hammerschmidt, R. Drautz, Phys. Rev. Lett. 105, 217003 (2010).
[3] A. F. Bialon, T. Hammerschmidt, R. Drautz, S. Shah, E. R. Margine, A. N. Kolmogorov (submitted)

12:03PM Q31.00003 Structure prediction for molecular crystals using evolutionary algorithms: methodology and applications[1] , QIANG ZHU, Geosciences Department, Stony Brook University — Evolutionary crystal structure prediction proved to be a powerful approach in determining the atomic crystal structure of materials. Here, we present a specifically designed algorithm for the prediction of the structure of molecular crystals. The main feature of this new approach is that each molecule is treated as a whole body, which drastically reduces the search space and improves the efficiency, but necessitates the introduction of new variation operators described here. We illustrate the efficiency of this approach by a search for ice (H2O) structures at zero pressure and temperature, which easily finds the structures of ice Ih and Ic, as well as the thermodynamically stable at these conditions ice XI. We successfully apply this method to finding the hitherto unknown structures of plastic phases of methane at high pressure. These structures are distinguished by an icosahedral packing of the molecules, and are likely candidate solutions for methane A and B.

[1]The author thanks Intel Corporation, Research Foundation of Stony Brook University, Rosnauka (Russia,contract 02.740.11.5102), and DARPA (grant 54751) for funding.

12:15PM Q31.00004 Burnett-Cattaneo Continuum Theory for Shock Waves[1] , B.L. HOLIAN, Los Alamos National Laboratory, M. MARESCHAL, Universite Libre de Bruxelles, R. RAVELO, University of Texas-El Paso — We model strong shockwave propagation, both in the ideal gas and in the dense Lennard-Jones fluid, using a refinement of earlier work [2], which accounts for the cold compression by a nonlinear, Burnett-like, strain-rate dependence of the thermal conductivity, and relaxation of temperature components on the hot, compressed side of the shock front. The relaxation of the disequilibrium among the three components of the kinetic temperature, namely, the difference between the temperature in the direction of a planar shock wave and those in the transverse directions, particularly in the region near the shock front, is accomplished by a rigorous application of the Cattaneo-Maxwell relaxation equation to a reference state, namely, the steady shockwave solution of linear Navier-Stokes-Fourier theory, along with the nonlinear Burnett heat-flux term. Our new continuum theory is in nearly quantitative agreement with non-equilibrium molecular-dynamics simulations under strong shockwave conditions.

[1]Part of this work supported by the U.S. Department of Energy under contract DE-AC5206NA25396.
[2]B.L. Holian, M. Mareschal, and R. Ravelo, J. Chem. Phys. **133**, 114502 (2010)

12:27PM Q31.00005 High-pressure behavior of a novel, nitrogen-rich energetic material[1] , R. STEWART MCWILLIAMS, Howard University, JENNIFER CIEZAK-JENKINS, Army Research Laboratory, YASMIN KADRY, University of Maryland College Park, VITALY PRAKAPENKA, Advanced Photon Source, MOHAMMAD MAHMOOD, Howard University, ALEXANDER GONCHAROV, Carnegie Institution of Washington — Energetic materials are of great interest in energy and defense applications. In the search for new energetic materials with improved properties, such as reduced environmental impact, a crystalline solid Triaminoguanidinium 1-methyl-5-nitriminotetrazolate (TAG), $C_3H_{12}N_{12}O_2$, has recently been synthesized (Klapötke et. al. 2008). We have studied the properties of TAG under static compression, and under reaction initiation at high pressure, using Raman and IR spectroscopy and x-ray diffraction. TAG appears to remain a stable, crystalline solid up to at least 35 GPa at room temperature. Laser initiation at 10-15 GPa reveals a rapid self-propagating reaction (deflagration) that consumes the sample, similar to other energetic materials such as nitromethane. Post-initiation products include crystalline molecular nitrogen (delta-phase), and nitrogen crystallites with regular defects. The formation of bulk molecular nitrogen during deflagration - in both phase segregated and impurity-hosting forms - distinguishes TAG from other known energetic materials, and suggests a pathway for the generation of novel phases from element-enriched energetic substances.

[1]This research was conducted under U.S. Army Research Office grant # 56122-CH-H.

12:39PM Q31.00006 High pressure–high temperature studies of ammonia , JULIUS OJWANG, RYAN MCWILLIAMS, ALEXANDER GONCHAROV, Carnegie Institution of Washington — Raman scattering measurements and x-ray diffraction of ammonia have been made under simultaneous conditions of high temperature and high static pressure in the laser heated diamond anvil cell. The experimental results on phase transitions with pressure increase at room temperature are found to be in accord with previous studies [1]. Pressure was increased up to 52 GPa and temperature ramped up to 2000 K. On increasing temperature at high pressure, strong changes in the ammonia Raman spectra are observed, which could be associated with melting. On melting, ammonia undergoes partial decomposition into nitrogen and hydrogen. We also observed the appearance of new N-H stretch bands at high temperatures which may be related to the formation of new bonds. When quenched back to room temperature the starting phase of solid ammonia is recovered. The shift in frequencies of the vibron bands of nitrogen with pressure shows that it is phase segregated from ammonia.

12:51PM Q31.00007 Atomic structure and elastic properties at high pressure of aluminum oxynitride in cubic phase , I.G. BATYREV, J.W. MCCAULEY, B.M. RICE, G.A. GAZONAS, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD 21005, A.R. OGANOV, Department of Geosciences and Department of Physics and Astronomy, State University of New York, Stony Brook, NY 11794-2100 — The atomic structure and elastic properties of aluminum oxynitride spinel (AlON) at high pressure (up to 40 GPa) have been calculated from first principles. We have assumed an "ideal" stoichiometry of cubic AlON with 35.7 mole % AlN using the constant anion model. The elastic constants were calculated from independent strains that were applied to a unit cell, parameterizing the total energy as a function of the strain and from a stress-strain relationship. At ambient conditions a clustered distribution of N atoms has $\sim$ 1 eV per 55 atoms higher total energy than for a random distribution and slightly, but systematically lower elastic constants. The pressure dependence of C_{11}, C_{12} and C_{44} for random and cluster distributions of N atoms was calculated in the range of 0-40 GPa by performing six finite distortions of the lattice and deriving the elastic constants from the strain-stress relationship. The calculated values of dC_{11}/dP are in the range of 4.0-6.2 and for dC_{44}/dP $\sim$0.8-1.5. The estimates are in reasonable agreement with experimental measurements of polycrystalline AlON. The minimum energy structure of AlON was found using the evolutionary algorithm USPEX (Oganov & Glass, 2006)

1:03PM Q31.00008 In Situ Neutron and Synchrotron X-ray Diffraction Studies of Jarosite at High-Temperature High-Pressure Conditions , H. XU, Y. ZHAO, D. HICKMOTT, J. ZHANG, S. VOGEL, L. DAEMEN, M. HARTL, Los Alamos National Laboratory — Jarosite ($KFe_3(SO_4)_2(OH)_6$) occurs in acid mine drainage and epithermal environments and hot springs associated with volcanic activity. Jarosite is also of industrial interest as an iron-impurity extractor from zinc sulfide ores. In 2004, jarosite was detected by the Mars Exploration Rover Mössbauer spectrometer, which has been interpreted as a strong evidence for the existence of water (and possibly life) on ancient Mars. This discovery has spurred considerable interests in stability and structural behavior of jarosite and related phases at various temperature, pressure, and aqueous conditions. In this work, we have investigated the crystal structure and phase stability of jarosite at temperatures up to 900 K and/or pressures up to 9 GPa using *in situ* neutron and synchrotron X-ray diffraction. To avoid the large incoherent scattering of neutrons by hydrogen, a deuterated sample was synthesized and characterized. Rietveld analysis of the obtained diffraction data allowed determination of unit-cell parameters, atomic positions and atomic displacement parameters as a function of temperature and pressure. In addition, the coefficients of thermal expansion, bulk moduli and pressure-temperature stability regions of jarosite were determined.

1:15PM Q31.00009 Testing the minimum thermal conductivity model for amorphous polymers using high pressure , WEN-PIN HSIEH, Department of Physics, University of Illinois, Urbana, MARK LOSEGO, PAUL BRAUN, Department of Materials Science and Engineering, University of Illinois, Urbana, SERGEI SHENOGIN, PAWEL KEBLINSKI, Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, NY, DAVID CAHILL, Department of Materials Science and Engineering, University of Illinois, Urbana — Pressure dependence of thermal conductivity provides a critical test of the validity of the model of the minimum thermal conductivity for describing heat transport by molecular vibrations of an amorphous polymer. We measure the pressure dependence of the thermal conductivity of poly(methyl methacrylate) (PMMA) brushes grafted from SiC substrates using a combination of time-domain thermoreflectance and SiC anvil cell techniques. We also determine the pressure dependence of the thermal conductivity from a computational model of amorphous polystyrene. In both cases, thermal conductivity as a function of pressure is accurately predicted by the minimum thermal conductivity model via the pressure dependence of the elastic constants and density.

1:27PM Q31.00010 The Influence of Crystal Structure on the Thermal Expansion Behavior of $GeZn_2O_4$, MICHAEL CRAWFORD, R.L. HARLOW, W.E. GUISE, DuPont Company, R.A. FISHER, Los Alamos National Laboratory, W. WOERNER, J.B. PARISE, Stony Brook University, Q. HUANG, J.W. LYNN, NIST Center for Neutron Research, R. STEVENS, California Institute of Technology, B. WOODFIELD, J. BOERIO-GOATES, Brigham Young University, J. LASHLEY, Los Alamos National Laboratory, O. GOURDON, A. HUQ, Spallation Neutron Source, Oak Ridge National Laboratory, J. HORMADALY, Ben Gurion University, P.L. LEE, Y. ZHANG, Argonne National Laboratory — $GeZn_2O_4$ synthesized at ambient pressure adopts the rhombohedral phenacite crystal structure, whereas cubic or tetragonal inverse spinel phases are formed at high pressures. We have measured the thermal expansion for all three forms of $GeZn_2O_4$ at temperatures from 10 K to 400 K (or higher) using synchrotron x-ray powder diffraction. The phenacite form exhibits negative thermal expansion below 300 K, changing to positive thermal expansion above that temperature. In contrast to this behavior, the cubic and tetragonal inverse spinel phases exhibit positive thermal expansion below room temperature. Characterization of these materials using x-ray and neutron diffraction, as well as heat capacity and Raman spectroscopy, will be described. Possible structural reasons for the different thermal expansion behaviors of the phenacite and spinel forms of $GeZn_2O_4$ will be discussed.

1:39PM Q31.00011 First-principles calculation of Ca2RuO4 at high pressure , NOBUMI MIYAWAKI, TATSUYA SHISHIDOU, Hiroshima University, TAMIO OGUCHI, Osaka University — It has been observed that the layered perovskite antiferromagnetic insulator Ca_2RuO_4 reveals a phase transition into a ferromagnetic metal at 0.5GPa [1]. This insulator-metal transition is accompanied by a structural change with tilt and rotation of RuO_6 octahedron within the space group $Pbca$. Above about 9GPa, another transition from the ferromagnetic to superconducting phase has been recently reported [2]. The transition includes a structure change from $Pbca$ to $Bbcm$. In this study, a first-principles calculation is performed to study the electronic structure of Ca_2RuO_4, especially focusing on the changes of Ru $4d$ states, with pressure. As the pressure is increased, calculated ferromagnetic spin moment of Ru is gradually decreased in $Pbca$ owing to the widening of Ru $4d$ band. It is interesting that a ferromagnetic solution still exists in $Bbcm$. Similar structural changes (the tilt and rotation of RuO_6 octahedron) take place in $Ca_{2-x}Sr_xRuO_4$, where orbital hybridization with spin-orbit coupling (SOC) is crucial [3]. We also investigated effects of SOC, with the result that those appear even in the electronic structure of Ca_2RuO_4. Calculation results optimizing the structure will be also discussed. [1] F. Nakamura, et al., Phys. Rev. B **65**, 220402(R) (2002). [2] P. L. Alireza, *et al.*: J. Phys.: Condens. Matter **22**, 052202 (2010). [3] T. Oguchi, J. Phys. Soc. Jpn. **78**, 044702 (2009).

1:51PM Q31.00012 Effect of high pressure on transport and structural properties of topological insulator Bi_2Se_3[1] , J.J. HAMLIN, Department of Physics, University of California San Diego, J.R. JEFFRIES, Lawrence Livermore National Laboratory, N.P. BUTCH, P. SYERS, Department of Physics, University of Maryland, D. A. ZOCCO, Department of Physics, University of California San Diego, S.T. WEIR, Lawrence Livermore National Laboratory, Y.K. VOHRA, Department of Physics, University of Alabama at Birmingham, J. PAGLIONE, Department of Physics, University of Maryland, M.B. MAPLE, Department of Physics, University of California San Diego — We report a series of electrical resistivity, magnetotransport, and xray diffraction measurements on the topological insulator Bi_2Se_3 under pressures as high as 34 GPa. The results demonstrate that applied pressure can be used to controllably tune the transport properties without chemical substitution.

[1]Support from the DOE/NNSA and NSF-MRSEC is acknowledged.

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q32 DMP: Focus Session: Optical Properties of Semiconductor and Metal Nanostructures C144

11:15AM Q32.00001 Application of modified phonon confinement model in Raman characterization of Ge nanowires , K. ROODENKO, University of Texas at Dallas, I.A. GOLDTHORPE, P.C. MCINTYRE, Stanford University, Y.J. CHABAL, University of Texas at Dallas — Raman spectroscopy is an attractive tool for characterization of low-dimensional materials, such as carbon nanotubes, graphene sheets or semiconductor nanowires. Phonon confinement model [1,2] was proposed to interpret Raman signal obtained from low-dimensional materials. Due to the finite-size of the nanostructures, the fundamental q∼0 Raman selection rule is relaxed, allowing the contribution from phonons away from the Brillouin-zone center. In this contribution we address several unresolved issues, such as the factors within the confinement function, incorporation of crystallographic orientation, and the interplay between the temperature and the nanostructure size [3]. Application of the modified model to the interpretation of Raman signal from Ge nanowires will be discussed.

[1] H. Richter, et al., Solid State Commun. 39, 625 (1981).
[2] I. H. Campbell et al., Solid State Commun. 58, 739 (1986).
[3] K. Roodenko et al., Phys. Rev. B 82, 115210 (2010).

11:27AM Q32.00002 Laser-Induced, Local Oxidation of Copper Nanoparticle Films During Raman Measurements , ANGELA R. HIGHT WALKER, GUANGJUN CHENG, IRENE CALIZO, National Institute of Standards and Technology (NIST), Gaithersburg, MD 20899 — The optical properties of gold and silver nanoparticles and their films have been thoroughly investigated as surface enhanced Raman scattering (SERS) substrates and chemical reaction promoters. Similar to gold and silver nanoparticles, copper nanoparticles exhibit distinct plasmon absorptions in the visible region. The work on copper nanoparticles and their films is limited due to their oxidization in air. However, their high reactivity actually provides an opportunity to exploit the laser-induced thermal effect and chemical reactions of these nanoparticles. Here, we present our investigation of the local oxidation of a copper nanoparticle film induced by a visible laser source during Raman spectroscopic measurements. The copper nanoparticle film is prepared by drop-casting chemically synthesized copper colloid onto silicon oxide/silicon substrate. The local oxidation induced by visible lasers in Raman spectroscopy is monitored with the distinct scattering peaks for copper oxides. Optical microscopy and scanning electron microscopy have been used to characterize the laser-induced morphological changes in the film. The results of this oxidation process with different excitation wavelengths and different laser powers will be presented.

11:39AM Q32.00003 Observation of UV Surface-Enhanced Raman Spectra using Ga Nanoparticles , YANG YANG, Department of Physics, Duke University, JOHN CALLAHAN, Army Aviation and Missile RD&E Center, KEVIN LANTZ, Dept of ECE, Duke Univ, JOHN FOREMAN, Army Aviation and Missile RD&E Center, PAE WU, TONG-HO KING, APRIL BROWN, Dept of ECE. Duke Univ, HENRY EVERITT, Dept of Physics/ECE, Duke Univ; Army Aviation and Missile RD&E Center — Ultraviolet (UV) surface enhanced Raman spectra (SERS) are observed for the first time using gallium nanoparticles (Ga NPs). Ga NP ensembles were synthesized on sapphire substrates at room temperature by molecular beam epitaxy. In situ spectroscopic ellipsometry was used to tune the UV local surface plasmon resonance (LSPR) wavelengths of the Ga NP ensembles during deposition. Three samples were prepared with LSPR wavelengths of 325, 295, and 260nm. UV Raman spectra using a 325nm HeCd laser were collected from fixed thicknesses of cresyl violet, poly(3-hexylthiopene), or MEH-CN-PPV that were spin cast onto these three samples, each of which had a NP-free region. A sample¡¯s enhancement was measured by comparing selected Raman signal intensities from the NP-covered and bare surfaces. Enhancements were found to decrease with increasing detuning between the laser and LSPR wavelengths. Similar behavior was observed from Ga NPs after 3 months of exposure to air, demonstrating the resilience of Ga NPs to oxidation.

11:51AM Q32.00004 Electronic origin of photoluminescence from Si nanocrystal embedded in amorphous SiO2 matrix[1] , TIANSHU LI, Department of Civil and Environmental Engineering, George Washington University, FRANCOIS GYGI, Department of Applied Science & Department of Computer Science, University of California, Davis, GIULIA GALLI, Department of Chemistry & Department of Physics, Unversity of California, Davis — Through combining classical molecular dynamics and *ab initio* calculation, we have created composite models of Si nano crystal embedded in SiO_2 amorphous matrices, with the sizes of Si nanocrystals ranging from 1.3 nm $\sim$ 1.9 nm. Electronic structure calculations showed that the band gap of composite structure increases as the size of Si nanocrystal reduces, however the increase of gap is mainly attributed to the *lowering of valence band edge*, with conduction band edge virtually unchanged. It was also found that while the wavefucntions from conduction band edges are extended over the entire Si nanocrystal, those from the valence band edges are mainly distributed near the nanocrystal/matrix interface. Further analysis identified that the valence band edges are dominated by the local distortion of nanocrystal from diamond cubic structure, which increases as both approaching the surface of Si nanocrystal, and decreasing the size of Si nanocrystal. This finding suggests that the local strain induced by surrounding amorphous SiO_2 matrix may play a key role in the photoluminescence of Si nanocrystal/SiO_2 amorphous matrix composite structures.

[1]This work is supported by DOE/BES DE-FG02-06ER46262.

12:03PM Q32.00005 Enhanced luminescence in terbium-cerium co-doped tin oxide quantum dots , CHRISTIE LAROCHELLE, KELLY MCCUTCHEON, Franklin & Marshall College, REBECCA SOBEL, MIT — SnO_2 quantum dots doped with Tb^{3+} exhibit strong luminescence from the Tb^{3+} dopants due to efficient energy transfer from the SnO_2 donors to the Tb^{3+} acceptor ions. We report results from a study of the effect of co-doping the SnO_2 dots with both Tb^{3+} and Ce^{3+} on the photoluminescence properties of the samples. The dots were synthesized using a sol-gel technique and the Ce^{3+}/Tb^{3+} ratio was varied while keeping the total doping level at 1wt%. X-ray diffraction and TEM results confirm the presence of nanocrystals of less than 10 nm in diameter. Photoluminescence results indicate that the Tb^{3+} ions are incorporated in a crystalline environment and that co-doping with Ce^{3+} enhances the energy transfer efficiency and therefore the intensity of the Tb^{3+} luminescence.

12:15PM Q32.00006 Stabilization of fluorescent silver clusters by RNA homopolymers and their DNA analogs: C,G vs A,T(U) Dichotomy , DANIELLE SCHULTZ, ELISABETH GWINN, UCSB — We show that single-stranded RNA stabilizes fluorescent silver nanoclusters (Ag:RNAs) in aqueous solution, analogous to previously studied Ag:DNAs. To determine whether the different canonical nucleosides play similar roles in stabilizing fluorescent silver species in RNA and DNA hosts, we compare RNA homopolymers of rA,rC,rG and rU to their DNA counterparts, and observe the same base-dependent dichotomy: visible- to IR-emitting silver complexes are stabilized by C and G homopolymers, but not by A or T(U) homopolymers at neutral pH. Shifts in emission wavelengths between Ag:RNA and Ag:DNA analogs show that both base and sugar influence populations of fluorescent species. The data indicate a minimum binding-pocket size of roughly five C or G bases for fluorescent species. These findings open the scope of silver cluster fluorophores to the diversely structured and functional arena of RNA and have implications for rational designs of nucleic acid hosts. Supported by NSF CHE-0848375.

12:27PM Q32.00007 Electronic and Optical Excitations in Perylene Diimide Derived Dye Molecules from First Principles , KOPINJOL BAISHYA, SERDAR OGUT[1], University of Illinois at Chicago, ERSEN METE, Balikesir University, OGUZ GULSEREN, Bilkent University, SINASI ELLIALTIOGLU, Middle East Technical University, Turkey — Halogenated perylene diimide dyes, such as Br-PDI ($Br_2C_{24}H_8N_2O_4$) and their glycine (BrGly) and aspartine (BrAsp) derivatives are known to absorb and emit light in the visible range with high quantum yields, and have good heat and chemical stability. As such, they are promising alternatives to the expensive (Ru-based) metal-driven dye sensitizers for solar cell applications. In this talk, we present results for the electronic structures, quasiparicle gaps, and the absorption spectra of PDI-derived dye molecules BrPDI, BrGly, and BrAsp, computed within the time-dependent density functional theory as well as many body perturbation techniques such as the GW method and the solution of the Bethe-Salpeter equation. In addition to discussing our results for bare molecules, we also present our preliminary studies for the change in their electronic and optical properties when they are attached to stoichiometric and reduced rutile TiO_2 (110) surfaces.

[1]Supported by DOE Grant No. DE-FG02-03ER15488

12:39PM Q32.00008 Enhanced light emission via plasmonic and non-plasmonic effects in metal ion-implanted Silicon , AKHILESH SINGH, KAROL GRYCZYNSKI, ARKADII KROKHIN, FLOYD MCDANIEL, ARUP NEOGI, University of North Texas, Department of Physics, Denton, TX, USA — We have observed enhanced photoluminescence from metal implanted nanoscale Silicon light emitters. Low energy (30 keV) Au and Ag metal ions were implanted in crystalline silicon to achieve non-plasmonic and plasmonic enhancement of light emission over a broad spectral range. The emission in the UV region can be significantly enhanced by the surface plasmon (SP) induced radiative recombination process. The recombination of carriers in Si bound exciton is also influenced by transverse optical phonon due to the polarization of the surface of bound exciton complex. The recombination life time of the electron-hole pair as estimated from the time resolved PL measurement changes from $\sim$ 2 ns to 400 ps in the presence of Ag ion induced SP polaritons. The non-resonant emission can be enhanced by electrostatic-image charge effects. The emission in the visible (570 nm) and UV (370 nm) wavelength range can also be significantly enhanced by electrostatic image charge effects induced by Au nanoparticles

12:51PM Q32.00009 Exciton-plasmon and spin-plasmon interactions in hybrid semiconductor-metal nanostructures , ALEXANDER GOVOROV, Department of Physics and Astronomy, Ohio University, Athens, OH, 45701 — Coulomb and electromagnetic interactions between excitons and plasmons in nanocrystals cause several effects: energy transfer between nanoparticles, plasmon enhancement, Lamb shifts of exciton lines, Fano interference. In a complex composed of semiconductor quantum dot and metal nanoparticle, plasmons interact with spin-polarized excitons. This interaction leads to the formation of coupled spin-plasmon excitations and to spin-dependent Fano resonances. If an exciton-plasmon system includes chiral elements (chiral molecules or nanocrystals), the exciton-plasmon interaction is able to create new plasmonic lines in circular dichroism spectra.

1:03PM Q32.00010 Generalized Ellipsometry on Ferromagnetic Sculptured Thin Films. , DANIEL SCHMIDT, TINO HOFMANN, University of Nebraska-Lincoln, KAH MOK, HEIDEMARIE SCHMIDT, Forschungszentrum Dresden-Rossendorf, RALF SKOMSKI, EVA SCHUBERT, MATHIAS SCHUBERT, University of Nebraska-Lincoln — We present and discuss generalized ellipsometry and generalized vector-magneto-optic ellipsometry investigations on cobalt nanostructured thin films with slanted, highly-spatially coherent, columnar arrangement. The samples were prepared by glancing angle deposition. The thin films are highly transparent and reveal strong form-induced birefringence. We observe giant Kerr rotation in the visible spectral region, tunable by choice of the nanostructure geometry. Spatial magnetization orientation hysteresis and magnetization magnitude hysteresis properties are studied using a 3-dimensional Helmholtz coil arrangement allowing for arbitrary magnetic field direction at the sample position for field strengths up to 0.4 Tesla. Analysis of data obtained within this novel vector-magneto-optic setup reveals magnetization anisotropy of the Co slanted nanocolumns supported by mean-field theory modeling.

1:15PM Q32.00011 Coupled Quantum Dot-Metal Nanoparticle Systems: Hybrid Behavior and Excitation Transport , RYAN ARTUSO, University of Maryland-College Park, GARNETT BRYANT, National Institute of Standards and Technology — Transmission of information between qubits for quantum communication and quantum computing will require directed nanoscale transmission where the quality of the information can be maintained. One paradigm proposes to achieve directed nanoscale transmission by coupling qubits, for example in quantum dots, to plasmonic nanoantennas or nanoguides made from metallic nanowires and nanoparticles. We study theoretically the response of hybrid nanostructure molecules consisting of multiple semiconductor quantum dots (SQD), and metal nanoparticles (MNP) subject to an applied optical field. We consider the situation where the SQDs interact directly without an MNP and the case in which the interaction is mediated by a MNP. We find modifications to the previously predicted SQD-MNP hybrid response. We also find a new regime of behavior in which breaking the SQD-SQD identical particle symmetry causes the system to no longer reach a steady state and instead oscillate at a beating frequency. Lastly, we identify the effects that MNP size and shape, and the placement of the SQDs have on the SQD-SQD interaction.

1:27PM Q32.00012 Plasmon Behavior in Gold Nano-dot Media , N. LIMBEROPOULOS, J. DEROV, A. DREHMAN, E. CRISMAN, Air Force Research Laboratory, Hanscom AFB, MA — We present correlations between the plasmon resonance of a gold nano-dots medium suspended in Al_2O_3 and the plasmon resonance of a single layer film of solid gold. We also present the effective medium properties of multi-layered, dot-film media. The gold dots were fabricated on Al_2O_3 substrates by sputter-depositing the gold and then annealing the resultant films. The median dot size ranged from 70 to 250 nm depending on the processing. Successive Au-dot layers were made by depositing Al_2O_3 over the previous dot pattern followed by depositing another gold film, followed by re-annealing. We used attenuated-total-reflection to couple transverse-magnetic optical waves to the plasmon resonance and controlled the degree of coupling by varying the spacing between the dot medium and the coupling prism. The plasmon resonances for the dot media had asymmetric line shapes compared to that for the continuous gold film. We were able to show correlations between that asymmetry and the spatial parameters of the dot/Al_2O_3 media construction. Effective media parameters and the dispersion characteristics for nano-dot/Al_2O_3 bi-layer were determined.

1:39PM Q32.00013 Surface Plasmon Generation by Excitons in Carbon Nanotubes[1] , IGOR BONDAREV, TODOR ANTONIJEVIC, North Carolina Central University — Optical properties of semiconducting carbon nanotubes (CNs) originate from excitons and may be tuned by either electrostatic doping [1], or via the quantum confined Stark effect (QCSE) by means of an electrostatic field applied perpendicular to the CN axis[2]. In both cases exciton properties are mediated by surface plasmon excitations [2,3]. We have shown recently that the QCSE allows one to control the exciton-interband-plasmon coupling in individual CNs and their optical absorption, accordingly [2]. Here, we extend our studies to demonstrate the possibility of low-energy localized surface plasmon generation by optically excited excitons in small-diameter ($\sim$1nm) CNs. The stimulated character of such an energy transfer causes the buildup of the macroscopic population numbers of coherent localized surface plasmons and, as a consequence, high-intensity coherent optical-frequency fields localized at nanoscale, which can be used for various applications, such as near-field nonlinear-optical probing, sensing, or materials nanoscale modification. [1] M.Steiner, et al., NL9,3477. [2] I.V.Bondarev, et al., PRB80,085407. [3] C.D.Spataru and F.Leonard, PRL104,177402.

[1]NSF (ECCS-1045661, HRD-0833184), NASA (NNX09AV07A), and ARO (W911NF-10-1-0105) support acknowledged.

1:51PM Q32.00014 Nanocrystal optoelectronic devices by plasmon-based optical trapping , KENNETH EVANS, Rice University, Applied Physics Graduate Program, DANIEL WARD, Rice University, Department of Physics and Astronomy, GAUTAM KINI, MICHAEL WONG, Rice University, Department of Chemical and Biomolecular Engineering, DOUGLAS NATELSON, Rice University, Department of Physics and Astronomy — Optical trapping is an important tool for studying and manipulating nanoscale objects. In conventional laser trapping, the trapping volume is diffraction limited. Recent experiments have shown that subwavelength control of nanoparticles can be achieved by using plasmonic nanostructures, rather than using the laser directly, to generate the electric fields necessary for trapping. We present a numerical model describing the trapping forces on an individual semiconducting nanocrystal in a nanoscale metallic junction, and discuss initial experimental results. Calculations of the fields are performed in COMSOL, a commercial finite element solver package, and the trapping forces are computed using the full Maxwell stress tensor formalism. We propose the use of plasmonic optical trapping in this geometry as a method to fabricate electrically driven, single nanocrystal light-emitting devices.

2:03PM Q32.00015 The Morphology and Evolution of Bipyramidal Gold Nanoparticles for Plasmon-assisted Nanosheet Biosensor[1] , NICHOLAS GEITNER, Miami University, AMOS DEOPKE, MELODIE FICKENSCHER, University of Cincinnati, JAN YARRISON-RICE, Miami University, WILLIAM HEINEMAN, HOWARD JACKSON, LEIGH SMITH, University of Cincinnati — We examine the growth and evolution bipyramidal gold nanoparticles. These particles are then characterized based on their longitudinal LSPR peak and their physical dimensions. Bipyramidal particles are grown using a seed-mediated growth process, and variations in the particles are produced by varying silver nitrate concentration and growth time. While each growth's physical dimensions were well defined and consistent with previous results, two different distinct modes of temporal evolution are observed after the primary growth period. We also observe a distinct linear relationship between tip radius of curvature and wavelength of longitudinal LSPR peak, in agreement with numerical calculations. These particles are to be functionalized and dispersed onto CdS nanosheets for biosensor applications.

[1]Supported by NSF awards #070173, #0806700, and #0806572.

Wednesday, March 23, 2011 11:15AM - 2:03PM –

Session Q33 DMP DCOMP: Focus Session: Dielectric, Ferroelectric, and Piezoelectric Oxides: Interfaces and Optical Properties C143/149

11:15AM Q33.00001 Engineering exotic phenomena at oxide interfaces[1] , PHILIPPE GHOSEZ, Universite de Liege — Complex transition metal oxides form an important class of compounds, exhibiting a wide variety of functional properties exploited in many applications. Thanks to advances in deposition techniques, these oxides can also nowadays be combined in heterostructures, with a structural quality comparable to what is achieved for conventional semiconductors, and the appearance of new phenomena at the interfaces where oxides with different properties meet brought recently the field to an entirely new level. Such phenomena include, for instance, the appearance of a two- dimensional electron gas at the interface between insulator oxides, the possibility of unexpected coupling between structural instabilities at some interfaces yielding unusual functional properties or the tunneling through ferroelectric and multiferroic barriers. Concentrating on few selected examples, I will illustrate how first-principles calculations can efficiently help the experimentalists to characterize the interfaces between complex transition metal oxides and sometimes guide them toward the design of new interesting heterostructures with exotic properties.

[1]Work funded by the EC-FP7 OxIDes and IAP-Belgian QCN projects.

11:51AM Q33.00002 Harnessing competition in artificially layered ferroelectric superlattices to engineer enhanced piezoelectrics , MATTHEW DAWBER, BENEDIKT ZIEGLER, SARA CALLORI, JOHN SINSHEIMER, Dept of Physics and Astronomy, Stony Brook University, VALENTINO COOPER, Materials Science and Technology Division, Oak Ridge National Laboratory, TAHIR YUSUFALY, KARIN M. RABE, PREMALA CHANDRA, Department of Physics and Astronomy, Rutgers University — First principles calculations by Cooper and Rabe (V. R. Cooper and K.M. Rabe, Phys. Rev. B 79, 180101 (R) (2009)), predicted that in $PbTiO_3/BaTiO_3$ superlattices an enhancement of the d_{33} piezoelectric coefficient could be achieved at a particular ratio of the thickness of the constituent layers. We have fabricated high quality artificially layered $PbTiO_3/BaTiO_3$ superlattices on $SrTiO_3$ substrates (with $SrRuO_3$ bottom electrodes) using an off-axis RF magnetron sputtering technique, allowing us to perform x-ray diffraction, electrical measurements and atomic force microscopy on this system. The experimental results confirm the prediction from first principles calculations, and we apply a Landau theory model as a useful bridge between the first principles predictions and experimental results at elevated temperature. In this work we have demonstrated that by finely balancing competing material properties in artificial heterostructures, desirable properties that exceed those of the parent compounds can be achieved.

12:03PM Q33.00003 Ferroelectrical and Dielectric Properties of $BaTiO_3/Ba_{(1-x)}Sr_xTiO_3$ Superlattices , NORA ORTEGA, ASHOK KUMAR, RAM S. KATIYAR, University of Puerto Rico — Artificially designed superlattices (SL) composed of alternate layers of $BaTiO_3$ (BT) and $SrTiO_3$ (ST) have attracted interests due to the possibility of producing superior and new functional properties, which are attractive for device applications. We have fabricated SL of BT/$Ba_{(1-x)}Sr_xTiO_3$ (BST) with x = 0, 0.3, 0.4, 0.5, 0.6, 0.7, 1, utilizing multi-target by pulsed laser deposition technique. The modulation period (Λ) in all SL was Λ= 80 Å and the total thickness of each SL films were 600 nm. The x-ray diffraction revealed well oriented (00l) perovskite structure and the so-called satellite peaks. The polarized Raman spectra showed the substantial transformation of the ferroelectric E(1TO) soft mode, depending of the ratio of Ba/Sr in BST layer. The dielectric constant of SL showed linear frequency dispersion above of 20 kHz, and their values are in the range of 400 to 900 at 1 kHz, while the tangent loss values were below to 0.1 at 1 kHz. Well defined ferroelectric loop was observed in all the SL at different frequencies (1 kHz-10 kHz), with remanent polarization ($2P_r$) 10 $\mu C/cm^2$. Improvement in saturation in the ferroelectric loop was observed with increase of Ba composition in BST layer. All these superlattices show very low leakage current far above its coercive field.

12:15PM Q33.00004 Artificially layered $PbTiO_3/CaTiO_3$ superlattices , JOHN SINSHEIMER, YOUCEF BENKARA, JONATHAN DALEY, SARA CALLORI, MATTHEW DAWBER, Dept of Physics and Astronomy, Stony Brook University — It has been shown that in artificially layered $PbTiO_3/SrTiO_3$ superlattices, a form of improper ferroelectricity occurs where the rotations of the oxygen octahedra at the interfaces couple with the polar mode and increase the ferroelectric polarization of the material when the layers are very thin. $PbTiO_3/CaTiO_3$ superlattices grown on $SrTiO_3$ substrates are also highly likely to display this kind of behavior, as the $CaTiO_3$ ground state is dominated by rotational distortions. This system should also play host to a competition between in-plane ferroelectricity (as $CaTiO_3$ is subjected to a large tensile strain when grown on $SrTiO_3$) and out-of-plane ferroelectricity (the usual result when in $PbTiO_3$ is grown on $SrTiO_3$). Using off-axis RF magnetron sputtering, we have produced high quality superlattices of $PbTiO_3/CaTiO_3$ with various layer thicknesses on $SrTiO_3$ substrates with $SrRuO_3$ bottom electrodes. The samples were analyzed using x-ray diffraction, electrical measurements, and atomic force microscopy. Our experimental results reveal a fascinating transition region at certain ratios of the relative layer thicknesses.

12:27PM Q33.00005 Polarization switching and dielectric properties of ferroelectric bilayers , MANDANA MEISAMI AZAD, The University of Tulsa, DANIEL TINBERG, The Pennsylvania State University, DONALD WALKO, Argonne National Laboratory, SUSAN TROLIER-MCKINSTRY, The Pennsylvania State University, ALEXEI GRIGORIEV, The University of Tulsa — In this work, we analyze polarization switching and dielectric properties of ferroelectric multilayer thin films of lead zirconate titanate. The interlayer coupling and polarization dynamics of ferroelectric multilayers are largely unknown. The studies of multilayers present a significant interest due to both fundamental understanding of interlayer interactions and practical applications of ferroelectrics in nanoelectronics and nanoelectromechanical systems. It is predicted that unusual switching characteristics and domain configurations such as the antiparallel alignment of the spontaneous polarization in adjacent layers can be observed in these materials. Using electrical measurements and time-resolved x-ray microdiffraction we analyzed physical properties of $PbZr_{0.8}Ti_{0.2}O_3/PbZr_{0.6}Ti_{0.4}O_3$. Strong nonlinearities in piezoelectric and dielectric responses of the bilayer to applied electric fields, which were observed in our experiments, can be explained by unusual polarization domain dynamics and interface charging effects.

12:39PM Q33.00006 Metallic oxides as dielectrics in artificially layered ferroelectric superlattices , SARA CALLORI, Dept. of Physics and Astronomy, Stony Brook University, DONG SU, Center for Functional Nanomaterials, Brookhaven National Laboratory, JOHN SINSHEIMER, MATTHEW DAWBER, Dept. of Physics and Astronomy, Stony Brook University — Artificially structured oxides provide many opportunities to develop systems with novel and tunable properties. $SrRuO_3$ has a metal-insulator transition as a function of thickness, which suggested to us the idea that we could use extremely thin layers (less than 3 unit cells) of $SrRuO_3$ as a novel dielectric component within an artificially layered superlattice system. We have created high quality $PbTiO_3/SrRuO_3$ superlattices by using an off-axis RF magnetron sputtering technique. The samples were characterized by x-ray diffraction, atomic force microscopy, transmission electron microscopy, and electrical measurements. When the $PbTiO_3$ layers are above a certain critical thickness, significant out-of-plane ferroelectricity develops in the system and the overall material has a semiconducting character. In this talk we will present a detailed experimental investigation of the behavior of ferroelectric polarization and domain size as the relative thicknesses of the superlattice layers are varied. Our work serves as a demonstration that a new set of materials, metallic oxides, can be considered for inclusion as novel dielectric layers in ferroelectric superlattices.

12:51PM Q33.00007 Stabilizing ferroelectric polarization of ultrathin BaTiO3 films through interface engineering , XIAOHUI LIU, YONG WANG, PAVEL LUKASHEV, J.D. BURTON, EVGENY TSYMBAL, Department of Physics and Astronomy & Nebraska Center for Materials and Nanotechnology, University of Nebraska, Lincoln, NE 68588, UNIVERSITY OF NEBRASKA–LINCOLN TEAM — Ferroelectric tunnel junctions have recently attracted considerable interest due to their potential for device applications [1]. The main challenge for the implementation of these devices is to stabilize ferroelectricity in nanometer- thick films where depolarizing fields and interface effects play an important role. Here, we report results of first- principles calculations of ferroelectric polarization in epitaxial SrRuO3/BaTiO3/SrRuO3 junctions. We show that the ferroelectric polarization is very sensitive to the surface termination of the electrodes and film thickness. In particular, we find that the presence of RuO2/BaO interface is detrimental to ferroelectricity due to the pinning of polar displacements in BaTiO3 in the direction away from the interface making the polarization of ultra-thin films non- switchable. We find that ferroelectricity can be stabilized by adding a thin layer of SrTiO3 at this interface. A phenomenological model is developed to explain the correlation between ferroelectric properties and junction geometry.

[1] E.Y. Tsymbal and H. Kohlstedt, Science 313, 181 (2006).

1:03PM Q33.00008 Inverse layer capacitance in perovskite oxide superlattices , XIFAN WU, Temple University, MASSIMILIANO STENGEL, ICMAB(CSIC), Barcelona, DAVID VANDERBILT, Rutgers University — Ferroelectricity is one of the most important functionalities that can be tuned in perovskite oxide superlattices. At fixed displacement field D, the overall polar instability can be accessed by the inverse of the capacitance per basal area as $C^{-1} = \partial V/\partial D$, where V is the potential drop across the supercell.[1] Here we propose that C^{-1} can be further rigorously decomposed into contributions from individual AO or BO_2 layers, giving an *layer inverse capacitance* defined as $c_j^{-1} = \epsilon_0^{-1}(h_j + D\partial h_j/\partial D - \partial p_j/\partial D)$, where h_j and p_j are the layer height and Wannier-based layer polarization[2] of layer j, respectively. We compute the c_j^{-1} in several typical multicomponent perovskite superlattices such as $CaTiO_3/BaTiO_3$ and $PbTiO_3/SrTiO_3$, and demonstrate that they satisfy a *locality* principle: their behavior depends mainly on the local chemical environment (i.e., the identities of neighboring layers). Thus, we show that the c_j^{-1} can provide an insightful *local* analysis of the ferroelectric tendency at interfaces in functional oxide superlattices.

[1]M. Stengel, D. Vanderbilt, and N.A. Spaldin, Nature Mater. **8**, 392 (2009).
[2]X. Wu, O. Diéhuez, K.M. Rabe and D. Vanderbilt, Phys. Rev. Lett. **97**, 107602 (2006).

1:15PM Q33.00009 Light-Driven Ferroelectric Polarization Dynamics Probed with Time-Resolved X-ray Scattering , D. DARANCIANG, Stanford University, M. HIGHLAND, H. WEN, Argonne National Lab, N. BRANDT, H. HWANG, M.I.T., J. LARSSON, Lund University, K. SOKOLOWSKI-TINTEN, University of Duisberg-Essen, D. REIS, SLAC, K. NELSON, M.I.T., P. FUOSS, G.B. STEPHENSON, Argonne National Lab, A.M. LINDENBERG, SLAC — We report femtosecond resolution time-resolved x-ray scattering measurements of dynamical changes in the polarization of PbTiO3 (PTO) nanolayers on SrTiO3 (STO) and DyScO3 (DSO) substrates under 400 nm, 40 fs optical excitation. For PTO on STO, an optically-induced polarization enhancement occurs on picosecond timescales that can be associated with a carrier-induced screening of the depolarization field. For PTO on DSO, qualitatively different effects are observed, indicating that the light initially couples to c-domains. We also observe optically-driven ferroelectric to paraelectric phase transitions (and vice versa) near the Curie temperature. The optical response of PTO on STO in the monodomain phase is consistent with a bulk photovoltaic effect. Optical excitation in the stripe phase at 515 C drives strains of order 1 percent, with an associated non-thermal disordering of the stripe domains. For PTO on DSO, temperature-dependent in-plane and out-of-plane structural dynamics are simultaneously captured, allowing the complex coupling between a- and c-domain motions to be mapped out.

1:27PM Q33.00010 Optical Properties of Epitaxial Sr-Ti-O Compounds from First Principles[1] , ROBERT BERGER, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory — $SrTiO_3$ is a representative of the property-rich perovskite family, and a material whose ability to convert solar photons to H_2 fuel would be more efficient if its wide optical bandgap (3.25 eV) better matched the solar spectrum. The Sr- and Ti-based Ruddlesden-Popper (RP) phases, $Sr_{n+1}Ti_nO_{3n+1}$, are structural modifications of $SrTiO_3$ with potentially useful electronic properties. While bulk growth is limited to $n < 4$ and $n = \infty$ ($SrTiO_3$), thin films of larger finite n structures have been grown epitaxially. In optical experiments, bandgaps of these films decrease monotonically with increasing n.[2] In density functional theory (DFT), however, the $n = \infty$ gap is larger than those for finite $n > 3$. This disagreement could stem from limitations in both experiment and theory. We explore this issue in depth using DFT, many-body perturbation theory, and tight-binding techniques.

[1]This work was done at the Molecular Foundry (LBNL), and supported by the DOE through the Energy Materials Center (Cornell University).
[2]C.-H. Lee et al., to be published.

1:39PM Q33.00011 Spectroscopic investigation on the electronic structure of a $5d$ band insulator $SrHfO_3$, YUNSANG LEE, Y.K. SEO, D.J. LEE, Soongsil University, H.J. NOH, Chonnam National University — We investigated the high-energy electronic structure of a 5d perovskite $SrHfO_3$. By using optical spectroscopy and O $1s$ x-ray absorption spectroscopy, the values of electronic structure parameters are estimated properly. In particular, the crystal field splitting energy, which is closely associated with the $p-d$ hybridization strength, is as high as 5 eV, and the Sr $4d$ bands appear to be strongly mixed with the Hf $5d$ bands. Moreover, the emission spectra with a 325 nm light excitation exhibit a sizable strength near 500 nm at low temperatures due to oxygen defects. These findings in $SrHfO_3$ are compared with electronic properties of similar compounds, $3d$ $SrTiO_3$ and $4d$ $SrZrO_3$.

1:51PM Q33.00012 Precise measurements of index of refraction at Brewster angle , WEI-TAI HSU, Department of Physics, Lamar University, CHRISTIAN BAHRIM, Research Center for Adaptive Data Analysis, National Central University, Chungli, Taiwan — A simple and accurate method is proposed for finding the index of refraction of solid and liquid dielectrics using the polarization of light reflected by a dielectric surface near the Brewster angle. The method allows measuring the Brewster angle with a precision better than 0.01 degrees and the index of refraction with a precision of 0.0001 by running a parabolic fit of the parallel component of the reflectance normalized to the total reflectance in a narrow region of about 15 degrees around the Brewster angle [1]. Our measurement is about 100 times better than other existing methods. The best precision in our measurements is achieved when a computer-based filtering procedure of the experimental reflectance is used during the data acquisition [2]. Our apparatus allows measuring small variation of the index of refraction, such as due to the change in temperature or the interference with another E-field.

[1] Bahrim C and Hsu Wei-Tai, 2009 *Am. J. Phys.* **77** (4) 337-343; [2] Hsu Wei-Tai and Bahrim C, 2009 *Eur. J. Phys.* **30** 1325-1336.

Wednesday, March 23, 2011 11:15AM - 2:15PM –
Session Q34 DMP: Focus Session: Interfaces in Complex Oxides - Polar Interfaces C141

11:15AM Q34.00001 Effect of polar interfaces on thin-film ferroelectricity , YONG WANG, MANISH NIRANJAN, KAROLINA JANICKA, Department of Physics and Astronomy, University of Nebraska, Lincoln, NE, USA, JULIAN VELEV, Department of Physics, University of Puerto Rico, USA, MIKHAIL ZHURAVLEV, Kurnakov Institute for General and Inorganic Chemistry, Moscow, Russia, SITARAM JASWAL, EVGENY TSYMBAL, Department of Physics and Astronomy, University of Nebraska, Lincoln, NE, USA — Based on first-principles and model calculations we investigate the effect of polar interfaces on the ferroelectric stability of thin-film ferroelectrics [1]. We consider Vacuum/LaO/BaTiO3/LaO, LaO/BaTiO3, and SrRuO3/LaO/BaTiO3/LaO heterostructures as representative systems, where a LaO monolayer at the interface with a TiO2-terminated BaTiO3 produces a polar interface. The polar interfaces create an intrinsic electric field which produces electric polarization in BaTiO3 directed into the interior of the BaTiO3 layer. This creates a ferroelectric dead layer near the interfaces that is non-switchable and thus detrimental to ferroelectricity. The effect is stronger for a larger effective ionic charge at the interface and longer screening length due to a stronger intrinsic electric field that penetrates deeper into the ferroelectric. The predicted mechanism for a ferroelectric dead layer at the interface controls the critical thickness for ferroelectricity in systems with polar interfaces. [1] Y. Wang et al., Phys. Rev. B. 82, 094114 (2010).

11:27AM Q34.00002 Lattice screening of the polar catastrophe in $KNbO_3/BaTiO_3$ interfaces , PABLO GARCIA-FERNANDEZ, PABLO AGUADO-PUENTE, JAVIER JUNQUERA, CITIMAC, Universidad de Cantabria, Avda. de los Castros s/n, E-39005 Santander, Spain — The discovery of a bidimensional electron gas (2DEG) in the interface between two insulating lattices like $LaAlO_3$ and $SrTiO_3$ has triggered much interest around bidimensional conductivity in these heterostructures. In this work we study polar interfaces between $KNbO_3$ (KNO) and $BaTiO_3$ (BTO), equivalent from the layer by layer charge point of view to the LAO/STO. In particular we focus on: (a) the possibility of formation of a 2DEG, (b) its interaction with the ferroelectric distortions of these materials, and (c) the effect of external electric fields. For this, we have performed Density Functional Theory calculations for a KNO(m)/BTO($2m$)/KNO(m) slab (m= width in unit cells) with different kinds of interfaces (n or p). We find that a 2DEG is formed only in the unrelaxed configuration, where there is no rumpling between the atoms of a given layer. However, when geometry is relaxed, $KNbO_3$ polarizes and the 2DEG is effectively screened. This effect is robust even under application of electric fields of moderate size. Finally, we find that an easily-rotated [110] in-plane polarization, driven by electrostatic effects, appears in the vicinity of the KO/TiO_2-type interface even thought the system is under in-plane compressive strain.

11:39AM Q34.00003 Evolution of the Band Alignment at Polar Oxide Interfaces , J.D. BURTON, EVGENY TSYMBAL, University of Nebraska - Lincoln — The next generation of electronic devices and systems are envisioned to exploit the multifunctional properties of complex oxide interfaces. Fundamental to this endeavor is an understanding of the electronic band alignment across such interfaces. Engineering this band alignment in all-oxide systems by properly preparing the interfaces is highly desirable. Here we explore an all-oxide metal-insulator interface between, $SrTiO_3$ (STO), and $La_{1-x}A_xMnO_3$ (LAMO), where A is a divalent cation [1]. The doping level of the manganite, x, offers a parameter which can be varied to engineer the band alignment. We use first-principles density-functional calculations to determine the evolution of the band alignment at $La_{0.7}A_{0.3}MnO_3|La_{1-x}A_xO|TiO_2|SrTiO_3$(001) heterointerfaces as the interfacial composition, $La_{1-x}A_x$, is varied. The position of the valence band maximum (VBM) with respect to the Fermi level increases linearly with interfacial composition x due to the linear dependence of the screened electrostatic interface dipole on the interfacial ionic charge. The importance of the polar nature of LAMO and its background dielectric properties will be discussed. Our results are agreement with recent experimental data reported by Hikita *et al* [2].
[1] J. D. Burton and E. Y. Tsymbal, Phys. Rev. B 82, 161407 (2010).
[2] Y. Hikita *et al.*, Phys. Rev. B 79, 073101 (2009).

11:51AM Q34.00004 Polarization discontinuities and compensation mechanisms at oxide-oxide interfaces , MASSIMILIANO STENGEL, ICMAB (CSIC), DAVID VANDERBILT, Rutgers University — Polar interfaces between insulating perovskite materials have been the subject of special attention in the past few years, following the discovery of two-dimensional conductivity in $LaAlO_3/SrTiO_3$. In this talk I will introduce the problem by using general concepts of macroscopic electrostatics, in the framework of the modern theory of polarization [1]. Based on these ideas, I will show how we can understand the origin and the spatial distribution of the metallic electron gas in terms of few basic ingredients, which can be readily extracted from bulk calculations of $SrTiO_3$. These results provide an unified view over the factors determining the confinement and decay of the compensating free charge within arbitrary electrical boundary conditions.

[1] M. Stengel and D. Vanderbilt, Phys. Rev. B 80, 241103(R) (2009).

12:03PM Q34.00005 First-principles study of the band offset at the anatase $TiO_2/SrTiO_3$ (001) interface , ALEXANDER DEMKOV, HOSUNG SEO, CHANDRIMA MITRA, The University of Texas at Austin — Band offsets at the interface of two oxides have recently attracted considerable attention in the context of the high-k dielectric gate stack in field effect transistors. The problem is also important in oxide heteroepitaxy. Recently, Chambers et al. reported that using the x-ray photoelectron spectroscopy no valence band offset is found between anatase TiO_2 (001) and $SrTiO_3$ (001). In this talk we describe the electronic structure at the $TiO_2/SrTiO_3$ (001) interface. We calculate the valence band offset to be 0.94 eV in the Schottky limit and 0.76 eV when the oxides are brought in contact, in apparent contradiction with experiment. A careful analysis of the electronic structure evolution from the bulk region of $SrTiO_3$ to the interface and through anatase all the way to the surface allows us to clarify the experimental results. We compare local density approximation results to those obtained with the GW method.

12:15PM Q34.00006 Many-body effects on the capacitance of multilayers made from strongly correlated materials[1] , SIMON HALE, JIM FREERICKS, Georgetown University — Recent work by Kopp and Mannhart on novel electronic systems formed at oxide interfaces has shown interesting effects on the capacitances of these devices. In our work, we identify effects on the capacitance that stem from many-body physics and from other factors. In order to do so, we employ inhomogeneous dynamical mean- field theory to calculate the capacitance for multilayered nanostructures. These multilayered nanostructures are composed of semi-infinite metallic leads coupled via a strongly correlated dielectric barrier region. The barrier region can be adjusted from a metallic regime to a Mott insulator through adjusting the interaction strength. We are able to vary the barrier thickness allowing comparison to the expected geometric capacitance. We also examine the effects of varying the temperature, potential difference, screening length, chemical potential, and electron filling. We set up a system that depletes the charge from the barrier so that the capacitance approaches the geometric capacitance, allowing us to study nonlinear effects.

[1]NSF DMR-0705266 and DMR-1006605.

12:27PM Q34.00007 Electronic Reconstruction at oxide interfaces: from an electron-hole bilayer to a spin-polarized 2DEG , ROSSITZA PENTCHEVA, University of Munich — The origin of conductivity at the interface between the band insulators $LaAlO_3$ and $SrTiO_3$ has been subject of continued interest and debate. Density functional theory calculations can provide not only insight into the underlying mechanisms but also allow one to identify further parameters to tune the electronic reconstruction in this system in view of device applications. In particular, the potential build up induced by the polarity of the $LaAlO_3$ film is found to be counteracted by a strong lattice polarization in the $LaAlO_3$ film. The latter allows the system to remain insulating for the first several $LaAlO_3$ layers before a crossover to an electronic reconstruction takes place at around 4-5 monolayers (ML). We demonstrate that, owing to a dispersive surface state, an additional $SrTiO_3$ capping layer can trigger the insulator-to-metal transition already at two ML of $LaAlO_3$. As a result, two spatially separated sheets of carriers emerge: electrons at the interface and holes at the surface that are only 1 nm apart and can be used to study excitonic phenomena. Furthermore, we explore the effect of a metallic contact layer on top of the $LaAlO_3$ film which not only eliminates the potential build up but turns out to be a promising way to enhance the carrier concentration and possibly to realize a spin-polarized electron gas at the interface. Work in collaboration with W.E. Pickett, K. Otte, V. Ruiz López.

1:03PM Q34.00008 Electronic properties of the conducting interface in $LaAlO_3/SrTiO_3$ heterostructures - the view from x-ray spectroscopies , M. SING, G. BERNER, A. MULLER, J. WALDE, F. PFAFF, R. CLAESSEN, Wurzburg University, Germany, H. HOLLMARK, L.-C. DUDA, Uppsala University, Sweden, S. PAETEL, C. RICHTER, J. MANNHART, Augsburg University, Germany, S. THIESS, W. DRUBE, HASYLAB, Hamburg, Germany, S.A. PAULI, C.W. SCHNEIDER, P.R. WILLMOTT, Paul Scherrer Institut, Villigen, Switzerland — Novel phases with often unexpected electronic and magnetic properties may form at the interfaces of epitaxial heterostructures composed out of complex oxides. A case in point is $LaAlO_3$ (LAO) on TiO_2-terminated $SrTiO_3$ (STO), for which a conducting interface has been found if the LAO thickness exceeds 3 unit cells. Although there is growing evidence that the origin is intrinsic and involves a transfer of charge to the interface to compensate the electric potential due to the polar nature of LAO there are a number of open issues. These refer, e.g., to the LAO thickness dependence of the charge carrier concentration, the potential gradient and the role of defects in LAO, the band alignment and bending at the interface, the lateral mobility or confinement of the interface charge carriers etc. We address these questions from the viewpoint of high-energy spectroscopies, i.e. hard x-ray photoelectron spectroscopy and resonant inelastic soft x-ray scattering, both of which we applied for the first time to these materials.

1:15PM Q34.00009 Internal electric field in $SrTiO_3/LaAlO_3$ heterostructures probed with hard x-ray photoemission spectroscopy , ERIK SLOOTEN, University of Amsterdam, Z. ZHONG, H. MOLEGRAAF, University of Twente, S. DE JONG, F. MASSEE, E. VAN HEUMEN, University of Amsterdam, M. GORGOI, Helmholtz Zentrum Berlin, G. RIJNDERS, D. BLANK, M. HUIJBEN, P. KELLY, University of Twente, M. S. GOLDEN, University of Amsterdam — The origin of the conducting layer at the interface between insulating $SrTiO_3$ (STO) and $LaAlO_3$ (LAO) is still widely debated. The alternatingly charged layers within the LAO blocks give rise to an internal electric field, which at some point has to be screened. This built-in potential is predicted to close the LAO bandgap at a critical thickness of 4 layers of LAO. Using hard x-ray photoemission spectroscopy we study the core levels of these systems as a function of the LAO layer thickness. By measuring the La 4d and Al 2s core levels with respect to the Sr 3d core level we carefully determine the core level shifts for samples with 2 to 6 layers of LAO. Although the observed shifts are an order of magnitude smaller than predicted, we do find an interesting increase of the core level shifts for samples with more than 4 layers. We perform DFT slab calculations to show that oxygen vacancies can significantly reduce the potential build-up. Our results suggest that in real materials the electronic reconstruction is pre-empted by other effects of which oxygen vacancies are one possibility.

1:27PM Q34.00010 Interfacial Electronic Properties of $LaAlO_3/SrTiO_3$ superlattice Probed with Hard X-ray Photoemission , DI-JING HUANG, NSRRC, Taiwan, YING-YI CHU, Dept. NHTU, Taiwan, JAN-CHI YANG, Dept. of Materials Science and Engineering, Taiwan, KU-DING TSUEI, NSRRC, Taiwan, WEN-CHUNG LIU, Dept of Phys, NHTU, Taiwan, YEN-FA LIAO, NSRRC, Taiwan, YING-HAO CHU, Dept of Materials Science and Engineering, NCTU, Taiwan, JONAS WEINEN, STEFANO AGRESTINI, VALERIO OLIANA, HAO TJENG, MPI-CPfS, Dresden, Germany, C.T. HUANG, NSRRC, Taiwan — Unexpected electronic and magnetic properties at interfaces between distinct transition-metal oxides have received much attention recently. The electronic phase at the interface of a heterostructure often differs from those of the sandwiching bulks. For instance, the interface between two band insulators $LaAlO_3$ and $SrTiO_3$ exhibits rich interfacial phases, drastically different from their original bulks. Here we will present measurements of hard X-ray photoemission and x-ray absorption on a $LaAlO_3/SrTiO_3$ superlattice to address the issue of interfacial electron at interfaces.

1:39PM Q34.00011 ARPES studies in LaTiO3/SrTiO3 heterostructures[1] , YOUNG JUN CHANG, Advanced Light Source and Fritz-Haber-Institut, LUCA MORESCHINI, ALS, YONG SU KIM, ALS and Hanyang University, ANDREW L. WALTER, ALS and Fritz-Haber-Institut, DAVIDE INNOCENTI, ALS and University of Rome "Tor Vergata", AARON BOSTWICK, GEOFFREY A. GAINES, ALS, KARSTEN HORN, Fritz-Haber-Institut, ELI ROTENBERG, ALS — Electronic band structure of LaTiO3/SrTiO3 heterostructures was studied using angle resolved photoemission spectroscopy (ARPES). LaTiO3 films, grown by in situ pulsed laser deposition (PLD) on beamline 7.0.1 at Advanced Light Source, exhibit a thickness-dependent phase transition from the correlated metallic interface to Mott insulator. We observed the quasi-particle peak at the Fermi level explaining the metallic interface for ultrathin LaTiO3, and the band gap opened for thick LaTiO3 similar to the bulk. We compare the thickness dependent electronic structure with theoretically calculated phase diagram (S. Okamoto and A. J. Millis, Nature 428, 630 (2004)).

[1]Work supported by U.S. DOE (DE-AC02-05CH11231 for ALS), the Max Planck Society, and Swiss National Science Foundation (PBELP2-125484).

1:51PM Q34.00012 Direct Spectroscopic Evidence of Charge Reversal at PZT/LSMO Heterointerface , CHUNG-LIN WU, PEI-WEI LEE, YI-CHUN CHEN, Department of Physics, National Cheng Kung University, Taiwan, LO YUEH CHANG, CHIA-HAO CHEN, National Synchrotron Radiation Research Center, Taiwan, CHEN-WEI LIANG, Department of Materials Science and Engineering, National Chiao Tung University, Taiwan, PU YU, QING HE, RAMAMOORTHY RAMESH, Department of Physics, University of California, Berkeley, USA, YING-HAO CHU, Department of Materials Science and Engineering, National Chiao Tung University, Taiwan — At the heterointerface of a top ferroelectric $Pb(Zr_{0.2}Ti_{0.8})O_3$ (PZT) ultrathin film and a bottom $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) electrode, we used continuous synchrotron radiation photoelectron spectroscopy (SR-PES) to probe *in situ* and demonstrated that the interfacial charges are reversible and their affected valence-band barrier height becomes modulated on switching the polarization in the top layer. By monitoring the core-level shifting of the buried LSMO layer under continuous illumination of synchrotron radiation, we directly observed a temporal screening of polarization induced by the photon-generated carriers in the top PZT layer. This dynamic characterization of the core-level shifting of the buried layer demonstrates an effective method to probe the electric conduction and ferroelectric polarization of an ultra-thin ferroelectric oxide thin film.

2:03PM Q34.00013 Scanning tunneling microscopy investigation of the electronic structure across $LaAlO_3/SrTiO_3$ heterointerfaces , YA-PING CHIU, BO-CHAO HUANG, Department of Physics, National Sun Yat-sen University, JAN-CHI YANG, YING-HAO CHU, Department of Materials Science and Engineering, National Chiao Tung University — Atomically controlled polarity discontinuities induced unusual charge states have been found in the model interface between two insulating perovskite oxides, $LaAlO_3$ and $SrTiO_3$. In this work, by using cross-sectional scanning tunneling microscopy, local and direct evidence of nontrival local structural and electronic information across the heterointerfaces are investigated. A combination of scanning tunneling spectroscopy analysis with atomic resolution across the $LaAlO_3/SrTiO_3$ heterointerface reveals how the oppositely charged atomic planes undergo electronic reconstructions and introduce a built-in electric field across the polar $LaAlO_3$ thin films grown on $SrTiO_3$ substrates. Further analysis of the related electronic and geometrical properties not only realizes the properties both in bands of electron and hole characters across the $LaAlO_3/SrTiO_3$ heterointerfaces but also helps to elucidate the mechanism of the interface conductivity.

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q35 DCMP: Topological Insulators: Interactions C140

11:15AM Q35.00001 Fragile Mott Insulators[1] , STEVEN KIVELSON, Department of Physics, Stanford University, HONG YAO, Department of Physics, University of California Berkeley — We prove that there exists a class of crystalline insulators, which we call "fragile Mott insulators" which are not adiabatically connected to any sort of band insulator provided time-reversal and certain point-group symmetries are respected, but which are otherwise unspectacular in that they exhibit no topological order nor any form of fractionalized quasiparticles. Different fragile Mott insulators are characterized by different nontrivial one-dimensional representations of the crystal point group. We illustrate this new type of insulators with two examples: the d-Mott insulator discovered in the checkerboard Hubbard model at half-filling and the Affleck-Kennedy-Lieb-Tasaki insulator on the square lattice.

[1]This work was supported, in part, by DOE grants DE-FG02-06ER46287 and DE- AC02- 05CH11231

11:27AM Q35.00002 Correlation effects in quantum spin Hall states: a Quantum Monte Carlo study , THOMAS C. LANG, MARTIN HOHENADLER, FAKHER F. ASSAAD, Department of Theoretical Physics & Astrophysics, University of Wuerzburg — We consider a quantum spin hall insulator as realized by the Kane-Mele model with spin orbit coupling λ supplemented by a Hubbard U term. On the basis of projective auxiliary field quantum Monte Carlo simulations on lattice sizes up to 12×12, we map out the magnetic phase diagram. Beyond a critical value of $U > U_c$ the quantum spin Hall insulating state is unstable towards magnetic ordering. At $U < U_c$ we study the spin, charge and single particle dyanmics of the helical edge state by retaining the Hubbard interactions only on the edge of a ribbon. As U_c is approached we observe a substantial depletion of low-lying spectral weight in the dynamical charge structure factor, and a robust signature of the helical edge state in the single particle spectral function.

11:39AM Q35.00003 Quantum Monte Carlo simulations on interaction effects in the 2D Kane-Mele-Hubbard model , DONG ZHENG, The Department of Physics, Tsinghua University, CONGJUN WU, GUANG-MING ZHANG, The Department of Physics, University of California, San Diego — Interaction effects in topological insulators remain an open question. We have proved that the determinant quantum Monte-Carlo simulation on the two dimensional Kane-Mele model augmented by the Hubbard interaction is free of the sign-problem. Consequentially, the interplay between band topology and strong interaction can be studied at a high numeric precision. The process how the topological band insulator evolves into the antiferromagnetic Mott insulator as increasing interaction strength is studied by calculating both the bulk and edge electronic properties. The possibility of an exotic topological Mott-insulator is examined.

11:51AM Q35.00004 Interactions and doping effects in a topological insulator , STEPHAN RACHEL, KARYN LE HUR, Yale University, Department of Physics, New Haven, CT 06520 — We investigate the effect of repulsive and attractive onsite interactions on a Quantum Spin Hall Insulator (QSHI). For repulsive interactions, we show that the topological phase is stable up to quite large interactions $U \sim t$ before the system reaches a magnetically ordered phase [1]. For attractive interactions, we discuss superconductivity in a doped QSHI and compare it with a doped trivial band insulator. We also consider the effect of spin orbit coupling to zero–mode bound states at vortex cores.

[1] S.Rachel and K.Le Hur, Phys. Rev. B 82, 075106 (2010).

12:03PM Q35.00005 Mott Physics at the Boundaries of Topological Insulators[1] , AMAL MEDHI, PRAMOD KUMAR VERMA, VIJAY SHENOY, H. R. KRISHNAMURTHY, Indian Institute of Science, Bangalore — We address how the nature of linearly dispersing edge states of a topological insulating solid evolves with increasing electron-electron correlation engendered by a Hubbard like on-site repulsion. We report studies on strips (2D) and slabs (3D) of varying widths and thicknesses of topological insulators described by model Hamiltonians using an inhomogeneous slave rotor mean-field theory. Motivated by these studies, we construct variational wavefunctions with approriate Gutzwiller-Jastrow correlations and study them using the Monte-Carlo method. These studies reveal the width/thickness dependence of the critical on-site repulsion that obtains an edge Mott insulating state, and uncover the mechanism of the Mott transition in such systems.

[1]Work supported by DAE, SRC and DST, India

12:15PM Q35.00006 Interaction and distortion driven topological phases in multi-band lattices[1] , JUN WEN, MEHDI KARGARIAN, GREGORY FIETE, University of Texas at Austin — In this work we investigate the phase diagram of $5d$ transition metal oxides on the pyrochlore lattice. In particular, the competition between Coulomb interaction, spin-orbit coupling and distortion are discussed. Spin-orbit coupling entangles the spin and t_{2g} orbitals giving rise to doublet $j = 1/2$ and quadruplet $j = 3/2$ states. While most pervious works discussed the doublet manifold, we focus on the quadruplet manifold which is relevant for several perovskites. Coulomb interaction is taken into account using the slave-rotor mean field theory and we obtain a phase diagram for this model, which includes exotic phases. We extend the model by including lattice distortion which further splits the quadruplet $j = 3/2$ manifold. Under a variety of distortions a topological phase is stabilized, and we discuss how the overall phase diagram is altered with lattice distortions.

[1]We gratefully acknowledge funding from ARO grant W911NF-09-1-0527.

12:27PM Q35.00007 Magnetic responce in the quantized spin Hall system with electron correlation , JUN GORYO, Institute of Industrial Science, the University of Tokyo, NOBUKI MAEDA — We investigate the magnetic response in the quantized spin Hall (SH) phase of layered-honeycomb lattice system with intrinsic spin-orbit coupling $\lambda_{\rm SO}$ and on-site Hubbard U. The response is characterized by a parameter $g = 4Ua^2d/3$, where a and d are the lattice constant and interlayer distance, respectively. When $g < (\sigma_{xy}^{s2}\mu)^{-1}$, where σ_{xy}^{s} is the quantized spin Hall conductivity and μ is the magnetic permeability, the magnetic field inside the sample oscillates spatially. The oscillation vanishes in the non-interacting limit $U \to 0$. When $g > (\sigma_{xy}^{s2}\mu)^{-1}$, the system shows perfect diamagnetism, i.e., the Meissner effect occurs. We find that superlattice structure with large a is favorable to see these phenomena. We also point out that, as a result of Zeeman coupling, the topologically-protected helical edge states shows weak diamagnetism which is independent of g.

12:39PM Q35.00008 Electrostatic Effects in Topological Insulators , DIMITRIS GALANAKIS, Nanyang Technological University, Singapore, TUDOR STANESCU, West Virginia University — We study electrostatic effects in topological insulators generated by non-uniform charge distributions and by external electric fields. The system is modeled using a tight-binding model and the Coulomb interaction is included at a mean-field level within a self-consistent calculation. The self-consistent charge profiles are calculated numerically for both insulating and low density metallic systems. Using this approach, we investigate the bending of the bulk bands due to the presence of surface states and of charged surface impurities and the effect of applying gate voltages to topological insulator films of variable thickness. Our results shed new light on the potential differences between surface- and bulk-sensitive measurements of topological insulators.

12:51PM Q35.00009 Coulomb drag between helical edge states , VLADIMIR ZYUZIN, GREGORY FIETE, University of Texas at Austin — We theoretically investigate the Coulomb drag between the edge states of two quantum spin Hall systems. Using an interacting theory of the one-dimensional helical edge modes, we show that the drag vanishes at second order in the inter-edge interaction, where it is typically finite in other systems, due to the absence of backscattering within the edges. However, in the presence of a small external magnetic field, the drag is finite and scales as the fourth power of the magnetic field, a behavior that sharply distinguishes it from other systems. We obtain the temperature dependence of the drag for regimes of both linear and quadratic edge dispersion in the presence of a finite field. This work was financially supported by ARO under Grant No. W911NF-09-1-0527. V. A. Zyuzin and G. A. Fiete, Phys. Rev. B 82, 113305 (2010).

1:03PM Q35.00010 Effect of electron-electron interaction on surface transport in three-dimensional topological insulators , HRIDIS PAL, DMITRII MASLOV, University of Florida — We study the effect of electron-electron interaction on the temperature dependence of surface charge transport in three dimensional topological insulators. In conventional two dimensional materials at small temperatures, the presence or absence of T^2 dependence in the resistivity is found to depend on the Fermi surface geometry- whether it is concave or convex and whether it is simply connected or multiply connected. In the recently discovered three-dimensional topological insulators such as Bi_2Te_3, Bi_2Se_3, and Sb_2Te_3 the Fermi surface of the two dimensional surface states, owing to the underlying lattice symmetry, changes curvature from convex to concave as a function of energy. The contribution from electron-electron interaction is therefore expected to affect the resistivity in these materials which we investigate in this study.

1:15PM Q35.00011 Cooper Pair Injection into Topological Insulators , KOJI SATO, University of California, Los Angeles — We theoretically study tunneling of Cooper pairs (CP's) from a superconductor spanning a two-dimensional topological insulator strip into its helical edge states. The coherent low-energy electron-pair tunneling sets off positive nonlocal current cross-correlations along the edges, which reflect an interplay of two quantum-entanglement mechanisms. First of all, superconducting spin pairing dictates a CP partitioning into the helical edge liquids, which transport electrons in the opposite directions for opposite spin orientations. Luttinger-liquid (LL) correlations for the electron-density fluctuations are, furthermore, forcing paired electrons to enter into opposite insulator-strip edges, revealing CP spin entanglement in the inter-edge current correlations. At the same time, the LL behavior, in the absence of Fermi-liquid leads, fractionalizes electrons injected at a given edge into counter-propagating charge pulses carrying definite fractions of the elementary electron charge. The superconductivity as well as LL correlations thus introduce positive current cross-correlations, which reveal a wealth of information about both subsystems. Sato, Loss, Tserkovnyak, arXiv:1003.4316v1. To be published in Physical Review Letters

1:27PM Q35.00012 Instabilities of quadratic band crossing points , STEFAN UEBELACKER, CARSTEN HONERKAMP, RWTH Aachen University — The variation of the orbital composition of bands around band crossing points near the Fermi level can generate interesting effects. In particular, rather simple interactions can give rise to the spontaneous formation of topological insulating phases (S. Raghu et al., Phys. Rev. Lett. 100, 156401 (2008)). In contrast with Dirac points, quadratic band crossing points offer the advantage of a nonzero density of states at the crossing point, and instabilities occur already at small interaction strengths. Here, we present results of functional renormalization group calculations for models with a quadratic band crossing point and discuss the possibilities for nontrivial insulating phases induced by local interactions.

1:39PM Q35.00013 Fractionalization and topological point defects in the charge-ordered kagome lattice[1] , ANDREAS RUEGG, GREGORY A. FIETE, The University of Texas at Austin — The charge-ordered state on the kagome lattice shows some features which are closely related to two-dimensional topological insulators. This motivated us to study a two-dimensional system of spin-polarized fermions on the kagome lattice at filling fraction $f = 1/3$ interacting through a nearest-neighbor interaction V using the unrestricted mean-field approach. Above a critical interaction strength V_c, a charge-density wave is stabilized. We find that topological point defects in the charge order bind a fractional charge. The value of the bound charge is $1/2$ as long as an effective sublattice symmetry is preserved but changes continuously with the strength of the symmetry-breaking field. Moreover, we compute the confinement potential between two fractionally charged defects and argue that the polaron state, formed upon doping the charge-density wave, can be viewed as a bound state of two defects.

[1]Funding: ARO W911NF-09-1-0527

1:51PM Q35.00014 Stability of spontaneous quantum Hall state in the Triangular Kondo-lattice model , YASUYUKI KATO, IVAR MARTIN, CRISTIAN BATISTA, Theoretical Division, Los Alamos National Laboratory — We study the behavior of the quarter-filled Kondo lattice model on a triangular lattice by combining a zero-temperature variational approach and finite-temperature Monte-Carlo simulations. For intermediate coupling between itinerant electrons and classical moments $\mathbf{S}_j$, we find a thermodynamic phase transition into an exotic spin ordering with uniform scalar spin chirality and $\langle \mathbf{S}_j \rangle = 0$. The state exhibits spontaneous quantum Hall effect. We also study how its properties are affected by the application of an external magnetic field.

2:03PM Q35.00015 Quantum corrections to conductivity in topological insulator thin films: Weak localization and electron-electron interaction , ASHLEY DASILVA, JIAN WANG, Penn State University, CUI-ZU CHANG, Chinese Academy of Sciences and Tsinghua University, KE HE, XU-CUN MA, Chinese Academy of Sciences, QI-KUN XUE, Tsinghua University, JAINENDRA JAIN, NITIN SAMARTH, MOSES CHAN, Penn State University — We study quantum corrections to transport in topological insulator candidate Bi_2Se_3, with and without doping with Pb. We study thin films with the expectation that the topological surface states will have substantial contribution to transport. Our observations are not consistent with the theory of diffusive transport of noninteracting electrons, because while the temperature dependence is consistent with weak localization, the magnetoresistance is positive, suggestive of weak anti-localization. We show that the theory including quantum corrections from both electron-electron interaction and disorder is qualitatively correct in all magnetic field directions that we have studied. We mention the implications of our results to the possibility of conducting surface states.

Wednesday, March 23, 2011 11:15AM - 1:39PM –

Session Q36 DMP: Focus Session: Graphene Structure, Dopants, and Defects: Nanoparticles

11:15AM Q36.00001 Manipulating graphene mobility and charge neutral point with ligand-bound nanoparticles as charge reservoir[1] , DEQI WANG, Department of Physics & Astronomy, University of California, Riverside, XINFEI LIU, LE HE, YADONG YIN, DI WU, JING SHI — In this work, we first demonstrate a significant enhancement in carrier mobility in SiO2-supported graphene decorated with a layer of ligand-bound nano-particles (NPs) such as iron oxide, titanium dioxide, or cadmium selenide acting as a charge reservoir. By transferring charges between graphene and the NP reservoir through the molecules, we show a remarkable reversible tunability in mobility (4,000 – 19,000 cm2/Vs) in the same device, which unambiguously proves that the charged impurity scattering is the prevailing mechanism for graphene mobility. In addition, the charge neutral point can also be independently tuned over a wide gate voltage range. Finally, we study the thermopower of graphene sample with different mobility. By properly taking account of the high temperature effects, we obtain good agreement between the Boltzmann transport theory and our experimental data.

[1]This work was supported in part by a DOE grant.

11:27AM Q36.00002 Imaging grain boundaries in monolayer graphene by transmission electron microscopy , KWANPYO KIM, Department of Physics, UC Berkeley, ZONGHOON LEE, National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, WILLIAM REGAN, Department of Physics, UC Berkeley, C. KISIELOWSKI, National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, M. CROMMIE, A. ZETTL, Department of Physics, UC Berkeley — Using transmission electron microscopy (TEM), we investigate the structure of grain boundaries in large-area monolayer polycrystalline graphene sheets at micron and atomic length scales. At micron scale, grain boundary mapping is performed by electron diffraction and dark field imaging techniques. The atomic scale imaging by an aberration-corrected ultra-high resolution TEM reveals an alternating pentagon-heptagon structure along the high-angle tilt grain boundary.

11:39AM Q36.00003 Electromagnetic interaction of graphene with nanoparticles: applications to nanoscale imaging spectroscopy and plasmonics , L.M. ZHANG, A.H. CASTRO NETO, Boston U, MICHAEL FOGLER, UCSD — Interaction of graphene-covered substrate with a nearby nanoscale particle is studied theoretically. Graphene is shown to induce broadening and frequiency shifts of electromagnetic resonaces (cavity modes) localized near the particle. The effect is strongly enhanced for substrates that possess narrow surface polariton excitations. In turn, the coupling to polaritons modifies the spectrum of graphene plasmons. The theory is applied to model scanning near-field optical microscopy (SNOM) experiments where the role of nanoparticle is played by the sharp tip of the scanned probe. The origin of the extraordinary fine spatial resolution of SNOM is explained and proposals for detecting the novel modes by SNOM in the infrared and THz domains are outlined. Also discussed are other applications, including infrared and Raman scattering from graphene covered by a layer of colloidal nanoparticles.

11:51AM Q36.00004 Interlayer Physics in Few Layer Graphenes[1] , E.J. MELE, University of Pennsylvania — Few layer graphenes (FLG's) represent a family of materials with physical properties distinct from those of single layer graphene and bulk graphite. Their electronic behavior is determined by the nature of electronic motion between layers and by the interactions of electrons in different layers. This talk reviews our experimental and theoretical work studying aspects of nanoparticle growth on FLG's that are determined by this interlayer physics. We observe and analyze: (1) a systematic film thickness dependence of the surface potential for FLG's deposited on SiO_2 substrates, (2) a related thickness dependence of the sizes of gold nanoparticles that nucleate on the exposed surface of FLG's and (3) a shape instability for growing nanoparticles formed from low workfunction metals adsorbed on FLG's. Finally we discuss some novel aspects of the interlayer electronic motion that are controlled by the rotational registry of neighboring layers.

[1]Work done in collaboration with: Y. Dan, S.S. Datta, A.T. Johnson, N.J. Kybert, Z. Luo, T. Ly, L.A. Somers, D.R. Strachan and N. Zimbovskaya.

12:27PM Q36.00005 Energetics and Electronic Structure of Transition Metal Adatoms and Clusters on Graphene[1] , CHRISTOPHER PORTER, DAVID STROUD, Ohio State University — Using density functional theory (DFT), we calculate both the atomic arrangement and electronic structure of transition metal (TM) adatoms, and clusters of adatoms, on graphene. We use a periodic arrangement of unit cells which typically include about 64 C atoms. For Fe on graphene, we have found that the stable position of the adatom is above the center of a hexagon of C and that most of the relaxation in the graphene occurs in the six C atoms closest to the adatom. We use DFT to map out a potential energy surface for Fe adatoms on graphene at any point in the unit cell, allowing an estimate of the energy barrier for an adatom to hop from one energy minimum to another. We also calculate the lowest energy configurations of pairs and larger clusters of TM adatoms on graphene. Finally, we have calculated the electronic structure and density of states associated with the adatoms and clusters on graphene, and have extended these calculations to spin- dependent properties, using a spin density functional approach. These results should be relevant to electronic and spin transport properties of graphene, both of which are expected to be strongly influenced by TM adatom impurities.

[1]Work supported by the NSF through MRSEC grant DMR - 0820414.

12:39PM Q36.00006 Doping efficiencies and physisorption of small molecules on graphene , ALEXANDER SAMUELS, DAVID CAREY, University of Surrey — Ab initio calculations have been employed to study the doping efficiencies of NO_2, NO and NH_3 on graphene. We have used both the local density approximation (LDA) and the generalised gradient approximation (GGA) to obtain the molecular binding energies and have employed the Hirshfield charge transfer method to calculate the charge transfer. Spin polarised calculations were employed for the open shell molecules (NO and NO_2) and we explored the effects of different adsorption sites and orientations. It was found that for all orientations of the molecule and using both LDA and GGA functionals that the adsorption of NO_2 results in p type doping of graphene with 0.06 e transferred to the molecule. For NO, LDA calculations show a p type behaviour with 0.03 e transferred per molecule but both n and p type doping of 0.003 – 0.004 e/molecules is calculated using a GGA functional. Finally for NH_3 both donor and acceptor behaviour (0.03 – 0.05 e/molecule) is calculated. In all cases the origin of the doping is related to the relative position of the HOMO and LUMO molecular orbitals with respect to the graphene Dirac point and low energy density of states. The effect of molecular adsorption on electron scattering is also discussed.

12:51PM Q36.00007 Surface Functionalization of Graphene Field Effect Transistors with Polyhistidine-Tagged Proteins[1] , YE LU, JOSEPH MITALA, JONG-HSIEN LIM, MITCHELL LERNER, ZHENGTANG LUO, NICHOLAS KYBERT, BRETT GOLDSMITH, BOHDANA DISCHER, A.T. CHARLIE JOHNSON, University of Pennsylvania, PHYSICS AND ASTRONOMY TEAM, BIOCHEMISTRY AND BIOPHYSICS TEAM — We have developed a facile and reliable method to covalently functionalize the surface of graphene field effect transistors (FETs) with polyhistidine-tagged proteins We demonstrated success of chemical functionalization by both atomic force microscopy (AFM) and Raman spectroscopy. Additionally, we characterized the electronic properties of graphene FETs at successive functionalization stages. The specificity enabled by such functionalization, along with the two dimensional nature and intrinsic high sensitivity of graphene, facilitates the emergence of graphene as a promising candidate in surface biochemistry research as well as graphene-based biosensor applications.

[1]Funding: NSF-NSEC/NBIC DMR-0425780

1:03PM Q36.00008 First principles simulations of molecules and nanostructures subjected to ion irradiation[1] , KALMAN VARGA, SERGIY BUBIN, BIN WANG, SOKRATES PANTELIDES, Vanderbilt University — In the framework of real-time real-space time-dependent density functional theory complemented with classical molecular dynamics for ions, we have studied the behavior of small molecules and nanostructure fragments, such as graphene sheets, irradiated by charged energetic particles. In particular, we have investigated the importance of electronic excitations and examined the regime when bond breaking (or defect formation) occurs. Based on the microscopic description of these processes, several quantities that are of interest for ion beam physics have been determined, such as the amount of energy transferred to the target system and the distribution of this energy between electronic excitations and vibrational motion.

[1]This work has been supported by NSF grants ECCS-0925422 and CMMI-0927345 and DTRA grant HDTRA1-10-1-0016

1:15PM Q36.00009 Point and Line Defect-mediated Binding of Metal Nanoparticles to Graphene , IOANNA FAMPIOU, ASHWIN RAMASUBRAMANIAM, University of Massachusetts Amherst — The synthesis of well dispersed, size-controlled metal nanoclusters on carbon supports is highly desirable since such clusters have been shown to possess enhanced catalytic activity and selectivity in a variety of chemical reactions. However, metal clusters interact rather weakly with defect-free carbon supports and can coarsen over time leading to loss of surface area and thence catalytic activity. Defects in carbon supports play an important role in enhancing metal-carbon bonding, thereby reducing the propensity for cluster coalescence. Using a combination of density functional theory and empirical potential simulations, we examine the interaction of metal Pt clusters with point (vacancies, holes) and line defects (dislocations, grain boundaries) in graphene. We compare and contrast the binding energies and diffusivities of clusters bound at defects and on pristine graphene. Our results suggest possible avenues for controlling the dispersion of Pt catalyst clusters on carbon supports via defect engineering.

1:27PM Q36.00010 Molecular Mechanics on Graphene Surface and its Detection[1] , KABEER JASUJA, NIHAR MOHANTY, VIKAS BERRY, Kansas State University — In this talk, we demonstrate that the light-induced reversible mechanical motion of an azo-molecule-tethered on graphene can be sensitively detected electronically by motion-induced molecular-gating of graphene (without external gate). The *in-situ* mechanical actuation of the azo-molecule is shown to redistribute the fermionic density *via* due to the change in the proximity of electron-rich benzene moiety of the azo molecule. The results demonstrate that the ultra-sensitive platform offered by graphene makes it possible to electrically detect molecular-scale mechanics. We envision that this research will enable development of next-generation graphene based actuating systems with applications including FETs, optoelectronic-switches and nano-pistons.

[1]Start-Up Kansas State University

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q37 DMP: Focus Session: Graphene Structure, Dopants, and Defects: Transport II

C146

11:15AM Q37.00001 Quantum motion of electrons and holes in the random puddle landscape of graphene[1] , ENRICO ROSSI, Department of Physics, College of William and Mary — The transport properties of graphene, especially close to the Dirac point, have puzzled physicists since its discovery in 2004. Only recently a fairly complete understanding of transport in graphene has emerged [1]. The interplay of disorder, gapless nature of the dispersion, and chirality of the quasiparticles induces the anomalous transport properties of graphene close to the Dirac point. In particular, in presence of long-range disorder the carrier density landscape close to the Dirac point breaks up in electron-hole puddles. In this highly inhomogeneous density landscape the standard theoretical approaches to transport are not valid. I will present a transport theory for graphene, and bilayer graphene, that is able to properly take into account the strong disorder-induced density inhomogeneities. The theory has three main features: *1)* it treats disorder microscopically and can therefore take into account its long-range nature, *2)* it provides a fully quantum mechanical analysis of transport, *3)* it is able to model experimentally relevant sizes. In particular the theory presented can be used to calculate the transport properties in the crossover regime, particularly relevant for graphene, between the ballistic and the diffusive regime. I will present results for single layer graphene and bilayer graphene. In addition I will discuss the transport properties of disordered graphene p-n-p junctions for which the semiclassical approaches are inadequate and the full quantum transport analysis is necessary.

[1] S. Das Sarma, S. Adam, E. H. Hwang, E. Rossi, *Electronic transport in two dimensional graphene*, arXiv:1003.4731 (2010), to be published in Rev. Mod. Phys.

[1]Work done in collaboration with S. Adam, J.H. Bardarson, P.W. Brouwer, S. Das Sarma, M.S. Fuhrer, E.H. Hwang and supported by NSF-NRI-SWAN and U.S.-ONR.

11:51AM Q37.00002 Interplay between density inhomogeneity and temperature in graphene transport[1] , QIUZI LI, EUYHEON HWANG, SANKAR DAS SARMA, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, MD 20742 — Motivated by recent experimental measurements of the temperature-dependent resistivity in graphene, we study the transport properties in monolayer graphene in the presence of electron-hole puddles induced by charged impurities in the environment. We explain the apparent insulating behavior of temperature-dependent conductivity observed in low mobility samples using an analytic statistical theory, which takes into account the non-mean-field nature of transport in the highly inhomogeneous density and potential landscape. In particular, the existence of puddles allows local activation of carriers in low density samples, mimicking an insulating temperature dependence in graphene conductivity.

[1]Work supported by ONR-MURI, NRI-NSF-SWAN and CNAM.

12:03PM Q37.00003 Electron scattering in graphene by a correlated charged impurities[1] , MICHAEL FUHRER, JUN YAN, JIANHAO CHEN, SHUDONG XIAO, Center for Nanophysics and Advanced Materials, Univesity of Maryland — We study charge transport in graphene with correlated charged impurities. Potassium is deposited on graphene in ultra-high vacuum at temperatures below 20 K, and the conductivity of graphene is measured as a function of carrier density in situ. Upon heating, the potassium ions order due to repulsive interactions, resulting in significant improvement of device mobility due to decrease of long range scattering. The charge density dependence of the conductivity becomes increasingly non-linear with increase of annealing temperature of the potassium/graphene. We find the experimental carrier-density-dependent conductivity in good agreement with a model of correlated charged impurities including a Gaussian-broadened structure factor at a finite wavevector corresponding to the potassium lattice.

[1]This work is supported by ONR-MURI and the UMD NSF MRSEC grant no. DMR 05-20471

12:15PM Q37.00004 Tunneling between two independently contacted graphene layers , CHRISTOPHER CORBET, SEYOUNG KIM, DAVID C. DILLEN, BABAK FALLAH, MICHAEL RAMON, EMANUEL TUTUC, SANJAY BANERJEE, The University of Texas at Austin — We study the tunneling between two overlapped, independently contacted graphene monolayers. We use micromechanical exfoliation to deposit graphene monolayers on separate substrates. Using electron beam lithography (EBL) patterning and etching we isolate the two monolayers and remove the multilayer graphene in their close proximity. Once patterned, one monolayer was removed from the substrate and manually aligned to the other monolayer with an overlap region of a few square micrometers. EBL and metal deposition were used to define hall bars on the two separate monolayers. This design allows the extraction of each sheet's mobility and density using standard four-point resistance measurements. Using a finite element model, we calculate the current flow in each layer, as well as in between the two layers. The tunneling resistance is modeled as a contact resistance between the two graphene layers in this overlap region. We extract an upper limit for the specific tunneling resistance between the two graphene layers of 1.4E-4 Ohms*cm^2. We discuss the current density and potential dependence on the shape of the overlap region.

12:27PM Q37.00005 Electron Hole Asymmetry in Graphene Coupled to an SiO2 Substrate , ROBERT HIGGINBOTHAM, University of Notre Dame, NAN SUN, GERALD ARNOLD, STEVEN RUGGIERO — The conductance of graphene generally exhibits an asymmetry in the electron and hole branches. We propose a contribution to this asymmetry that is based upon the coupling between the graphene and an SiO2 substrate. Treating the coupling in the tight-binding approximation, we calculate an exact Green's function for the coupled graphene/SiO2 system.

12:39PM Q37.00006 Electron-hole interference in graphene[1] , ATIKUR RAHMAN, JANICE WYNN GUIKEMA, SOO HYUNG LEE, NINA MARKOVIC, Johns Hopkins University — The crystal symmetry of graphene gives rise to massless Dirac low-energy quasiparticles which are described by a two-component spinor that has contributions from two interpenetrating sublattices. As a result, the electron and hole states are interconnected, in sharp contrast to conventional semiconductors. Through the Aharonov-Bohm effect, we demonstrate that the electrons and holes in graphene exhibit quantum interference with each other. Our device is made of a graphene ring in contact with gold leads. A top gate on one arm of the ring independently controls the carrier type and concentration in that arm, while the back gate acts on both arms. We observe clear Aharonov-Bohm oscillations (overall visibility $\sim$10%) in the magnetoresistance when the charge carriers are holes in one arm and electrons in the other arm. This indicates phase coherence between the electrons and holes in the two arms of the interferometer. Phase coherence is further substantiated by our observations of $T^{-1/2}$ temperature dependence of the oscillation amplitude.

[1]This work is supported in part by NSF DMR 0547834 (CAREER) and DMR 0520491 (MRSEC).

12:51PM Q37.00007 Measurements of the energy gap in biased bilayer graphene[1] , CONOR PULS, YING LIU, Physics Department, The Pennsylvania State University — The application of bilayer graphene in logic-based electronics necessitates the demonstration of reliable bandgap opening, a matter complicated by charge inhomogeneity and midgap states due to local impurities and other disorder. We use dual-gated field effect transistor (FET) and planar tunnel junction devices prepared on mechanically exfoliated bilayer graphene flakes to probe the temperature dependent resistivity and density of states near the charge neutrality point. In both devices, the Fermi level and theoretical bandgap width are simultaneously controlled with a perpendicular displacement field. We report that at high displacement fields and with the Fermi level at the charge neutrality point, the temperature dependence of the resistivity follows a simple thermal activation across a gap width of up to 110 meV at high temperatures. Low temperature transport is dominated by hopping channels whose presence also increase conductivity at high temperatures, reducing the achievable σ_{ON}/σ_{OFF} ratio, a value of great interest for FET devices. We explore the role of charged impurities found in the deposited dielectric in limiting FET performance in this respect.

[1]Work supported by DARPA under the CERA program.

1:03PM Q37.00008 A Unified Description of the DC Conductivity of Monolayer and Bilayer Graphene Based on Resonant Scatterers , AIRES FERREIRA, J. VIANA-GOMES, University of Minho, Portugal, JOHAN NILSSON, University of Gothenburg, Sweden, EDUARDO R. MUCCIOLO, University of Central Florida, USA, NUNO M.R. PERES, University of Minho, Portugal, ANTONIO H. CASTRO NETO, Boston University, USA, and National University of Singapore — We show that a coherent picture for the dc conductivity of monolayer and bilayer graphene emerges from considering that strong short-range potentials are the main source of scattering in these two systems. The origin of the strong short range potentials may lie in adsorbed hydrocarbons at the surface of graphene. The equivalence between results based on the partial wave description of scattering, the Lippmann-Schwinger equation, and the T-matrix approach is established. Scattering due to resonant impurities close to the neutrality point is investigated via a numerical computation of the Kubo formula using a kernel polynomial method. We find that realistic adsorbates originate impurity bands in monolayer and bilayer graphene close to the Dirac point. In the midgap region, a plateau of minimum conductivity of about e^2/h (per layer) is induced by the resonant disorder. In bilayer graphene, a large adsorbate concentration can develop an energy gap between midgap states and high energy states. As a consequence, the conductivity plateau is supressed near the edges and a "conductivity gap" takes place.

1:15PM Q37.00009 Dynamic Screening and Spectral Functions in Bilayer Graphene[1] , RAJDEEP SENSARMA, EUYHEON HWANG, SANKAR DAS SARMA, Condensed Matter Theory Center, University of Maryland, College Park — We study the dynamic screening of Coulomb interactions in a bilayer graphene system within Random phase approximation. We derive an analytic expression for the dielectric function of the system and study the dispersion and damping of low energy plasmon modes. The quadratic dispersion and chirality of bilayer graphene systems lead to a plasmon dispersion which is distinct both from 2D electron gas and monolayer graphene plasmons. We also look at the effects of dynamic screening on the single particle spectral function of the system. We determine the quasiparticle weight, the effective mass and the damping of quasiparticles, which give a complete description of the low energy spectral function of the system.The compressibility of the system is also obtained from the self-energy renormalization of the chemical potential. We find that the presence of the second band leads to a well screened effective interaction, leading to much smaller renormalization of the Fermi liquid parameters in comparison to a 2D electron gas. However, the dynamic nature of the screening is very important in obtaining the single particle properties of this system.

[1]The authors acknowledge support from CNAM, Univ. of Maryland, and US-ONR MURI

1:27PM Q37.00010 Electron transport properties of bilayer graphene , KOSTYANTYN BORYSENKO[1], [1] Department of Electrical and Computer Engineering, North Carolina State University, Raleigh, NC 27695-7911, JEFFREY MULLEN[2], [2] Department of Physics, North Carolina State University, Raleigh, NC 27695-8202, XIAODONG LI[1], YURIY SEMENOV[1], JOHN ZAVADA[1], MARCO BUONGIORNO NARDELLI[2,3], [3] CSMD, Oak Ridge National Laboratory, Oak Ridge, TN 37831, KI WOOK KIM[1] — We investigate the role of different phonon scattering mechanisms in determining the electron transport properties of bilayer graphene (BLG). The ever-present electron-phonon interaction imposes the limitations on transport characteristics of any device and thus, must be always taken into account. However, in a realistic device setup, when BLG is laid (or epitaxially grown) on the top of a substrate, extrinsic scattering mechanisms (due to charged impurities, surface polar phonons, etc.) will dominate. The electron coupling with surface polar phonons of the substrate is always present and this scattering mechanism can be dominant. Using first principles approach (density functional perturbation theory) we calculate the electron-phonon matrix elements of BLG and estimate the intrinsic electron scattering rates. We show that the transport properties of the free-standing BLG resemble those of the bulk graphite. Using the Monte Carlo simulation we estimate the low-field mobility and saturation velocity of the free-standing BLG, as well as BLG on various substrates (SiC, SiO_2, HfO_2).

1:39PM Q37.00011 Dual Gating of Suspended Graphene Devices via Contactless Gates , JAIRO VELASCO JR., LEI JING, GANG LIU, PHILIP KRATZ, YONGJIN LEE, WENZHONG BAO, JEANIE LAU — Monolayer and Bilayer graphene devices with local electrostatic gates present a rich platform for both academic and application driven inquiry. Realization of the veselago lensing effect and band gap engineering are a few of the most dazzling and promising physical phenomena that these systems are predicted to host. However, a major roadblock in this quest is the strict requirement of exceedingly clean samples. We have developed a method to fabricate suspended top gates above a freestanding graphene flake to address this challenge. Using this technique we demonstrate dual gating of a suspended graphene flake. We will discuss the latest experimental progress towards the electrical transport of such a device in the zero-magnetic field regime, as well as in the quantum Hall regime.

1:51PM Q37.00012 Current Annealing of Suspended Graphene Atomic Membranes , FENGLIN WANG, UCR Department of Physics and Astronomy, JAIRO VELASCO JR., ZENG ZHAO, HANG ZHANG, PHILIP KRATZ, LEI JING, WENZHONG BAO, CHUNNING LAU — Using a multi-level lithographical technique, we are able to suspend graphene membranes coupled to vast majority of electrode materials. The device's mobility is significantly improved upon current annealing. By combining transport measurement with in-situ SEM imaging, we are able to monitor morphological changes in graphene and correlate with its current-voltage characteristics, thus optimizing the current annealing process.

2:03PM Q37.00013 Pulsed current-voltage measurements of GFETs[1] , INANC MERIC, CORY DEAN, ANDREA YOUNG, PHILIP KIM, KENNETH SHEPARD, Columbia University — Pulsed current-voltage measurements are used to measure high-bias characteristics of graphene field-effect transistors (GFET). In contrast to standard DC measurements, current saturation for channel lengths as small as 100 nm is observed when measured by this method. Our results indicate that hot carrier injection into traps in the gate oxide masks saturating characteristics in standard DC measurements. Devices exhibit constant transconductance and output conductance with scaling channel length, despite a variation in low field mobility, supporting a velocity saturation model due to optical phonon scattering.

[1]This work is supported in part by the SRC Focus Center Research Program and by DARPA CERA program.

Wednesday, March 23, 2011 11:15AM - 2:03PM –

Session Q38 DMP DPOLY GERA: Focus Session: Organic Electronics and Photonics – Morphology in polymer-based solar cells A130/131

11:15AM Q38.00001 Structural measurements of polymer-fullerene blend films for organic photovoltaics , DEAN DELONGCHAMP, NIST — Organic photovoltaic (OPV) technology has the potential to greatly lower the cost of solar cell fabrication by enabling ink-based deposition of active layers. In bulk heterojunction (BHJ) OPV devices, the power conversion efficiency critically depends on the distribution of the polymer absorber and the fullerene electron acceptor (e.g., the blend morphology). I will describe measurement methods to probe the structure of OPV devices, with a focus on the morphology of the BHJ layer. For example, the vertical distribution of absorber and electron acceptor in BHJ films follows segregation behavior similar to that of miscible polymer blends. The top (air) interface becomes rich in the polymer absorber, whereas the bottom interface composition depends on the substrate surface energy. Thin film transistors fabricated from BHJs can therefore exhibit ambipolar or hole-only transport depending on the dielectric, because of different interfacial segregation. We extend these results to practical photovoltaic devices by comparing BHJs cast upon hole transport layers that have similar work functions but different surface energies. This study includes the application of variable angle spectroscopic ellipsometry (VASE) to BHJ films, and emphasizes the importance of absorber anisotropy and vertical heterogeneity in the optical model. Additional results will describe the nanometer-scale structure in the BHJ interior. The application of solid-state nuclear magnetic resonance (SS-NMR) can reveal details about the segregation of absorber and acceptor in a BHJ film. Nanoscale BHJ morphology information can also be collected using tomographic transmission electron microscopy (TEM). Together these measurements allow us to reveal a detailed picture of BHJ morphology, explain how the morphology originates from materials and processing choices, and relate the morphology to device performance and stability.

11:51AM Q38.00002 Tuning Rod-Rod Interactions in Poly(3-alkylthiophene) Derivatives , BRYAN BOUDOURIS, VICTOR HO, RACHEL SEGALMAN, University of California, Berkeley — Poly(3-alkylthiophene) (P3AT) derivatives are used commonly in polymer semiconducting applications. However, during the coating of P3AT thin films strong intermolecular interactions generally lead to the formation of semiconducting fibers. This prevents the formation of long-range ordered domains and complicates analysis of structure-property relationships in P3AT-containing devices (e.g., organic photovoltaic cells). Here, we show rod-rod interactions can be controlled by rational polythiophene side chain design. The effects of side chain passivation are evidenced by a depressed melting temperature and the presence of a liquid crystalline region. We show also that while the rod-rod interactions are lowered significantly in a polythiophene derivative with a branched side chain relative to straight chain P3ATs, the optoelectronic properties remain approximately constant. Importantly, this reduced melting temperature allows for the real-time evolution of a P3AT crystal structure at room temperature to be monitored on an experimentally convenient time scale. These structural data correlate well with field-effect charge carrier mobility measurements and provide a path for studying the mechanism of ordering in plastic electronics.

12:03PM Q38.00003 Polymer/Polymer Heterojunctions for Ambipolar Charge Transport in Organic Electronics , FELIX KIM, SELVAM SUBRAMANIYAN, SAMSON JENEKHE, University of Washington — Understanding of charge transport in polymer semiconductor heterojunctions is of basic interest in developing high-performance organic optoelectronic devices based on multicomponent polymer semiconductors. We report ambipolar charge transport in thin films of layered heterojunctions and bulk heterojunctions of solution-processable unipolar polymer semiconductors. Selective solubility of the polymer semiconductors, poly(thiazolothiazole)s and ladder-type poly(benzobisimidazo-benzophenanthroline), in organic and acidic solvents enabled the sequential deposition or blending of the polymer semiconductors. Charge carrier mobilities of 0.001-0.01 cm2/Vs were observed for both electrons and holes in the polymer/polymer heterojunction field-effect transistors. Thin film deposition and processing with various solvents are effective to improve charge-carrier mobilities by a factor of 100-1000. We have investigated the effects of the processing methods on morphology, and photophysical and charge transport properties of the polymer semiconductor heterojunctions. Integrated circuits and solar cells based on the polymer semiconductor heterojunctions are also demonstrated.

12:15PM Q38.00004 The role of donor-acceptor intermixing in the performance of polymer-polymer OPVs , ELENI PAVLOPOULOU, STEPHANIE LEE, CHANG SU KIM, YUEH-LIN LOO, Department of Chemical and Biological Engineering, Princeton University, ZHIHUA CHEN, ANTONIO FACCHETTI, Polyera Corporation, MICHAEL F. TONEY, Stanford Synchrotron Radiation Lightsource — We investigated the effect of donor-acceptor intermixing in bulk-heterojunction active layers on device performance of polymer-polymer organic photovoltaics (OPVs). Poly(3-hexylthiophene) (P3HT) was blended with poly{[N,N'-bis(2-octyldodecyl) -naphthalene-1,4,5,8-bis(dicarboximide)-2,6-diyl]-alt-5,59-(2,29-bithiophene)} (PNDI) and P3HT/PNDI films were spin-cast from dichrolobenzene, a good solvent for PNDI; chlorobenzene, a good solvent for P3HT; and xylene, a bad solvent for both. The short-circuit current densities and device efficiencies vary with casting solvent quality; devices with active layers cast from xylene exhibit the highest efficiencies while those cast from dichlorobenzene the lowest. Grazing Incidence X-ray Diffraction show that intermixing on a molecular scale increases with decreasing dissolution of the polymers in the parent solutions. Accordingly, increasing intermixing enhances device efficiencies.

12:27PM Q38.00005 Phase purity in organic solar cells , BRIAN COLLINS, ELIOT GANN, LEWIS GUIGNARD, North Carolina State University, XIAOXI HE, CHRISTOPHER MCNEILL, University of Cambridge, HARALD ADE — To date, the device function of organic bulk heterojunction solar cells has been commonly interpreted to arise from two interpenetrating, phase-separated donor and acceptor materials with charge separation of excitons occurring at discrete interfaces. However, little attention has been paid to phase purity and the consequences of a mixed phase on the operation of devices. To probe this possibility and its implications, the miscibility of common fullerenes in (3-hexylthiophene) (P3HT) and a number of new low bandgap polymers including PCDTBT have been measured directly via x-ray absorption spectroscopy in a scanning transmission x-ray microscope on films brought to thermodynamic equilibrium. A mixed amorphous phase is always observed, along with a fullerene-rich phase and possibly a pure crystalline polymer phase if the polymer is able to crystallize. For example, grazing incidence x-ray scattering shows no intercalation of fullerenes into P3HT crystallites, while amorphous portions of the polymer contain ∼20 wt.% of the fullerene. In fact, all systems tested to date have failed to exhibt a pure amorphous polymer phase, suggesting that the device paradigm of pure phases and discrete interfaces requires modification.

12:39PM Q38.00006 Diffusion rates and crystallization of phenyl-C61-butyric acid methyl ester in poly(3-hexylthiophene)[1] , L. GUIGNARD, B. COLLINS, J. SEOK, H. ADE, North Carolina State University — Bulk heterojunction (BHJ) solar cells based on poly(3-hexylthiophene) (P3HT) and phenyl-C61-butyric acid methyl ester (PCBM) are an important model system for studying organic solar cell operation. Recent experiments reveal that PCBM is partially miscible in the amorphous regions of P3HT [1-3], implying that P3HT:PCBM devices have three phases. The miscibility depends on temperature and regioregularity of the P3HT. To better understand the influence of P3HT regioregularity and molecular weight on the the P3HT:PCBM system, diffusion rates of PCBM are determined as a function of regioregularity of P3HT and temperature with visible light microscopy by analyzing the growth of the PCBM depletion region near PCBM crystals or agglomerates. Lower diffusion constants are found for less crystalline regiorandom P3HT than highly regioregular P3HT. The shape and growth behavior of PCBM crystal or agglomerate is also found to vary greatly.

[1] B. Watts *et al.*, Macromolecules **42**, 8392 (2009)
[2] B. A. Collins *et al.*, J. Phys. Chem. Lett **1**, 3160 (2010)
[3] J. W. Kiel *et al.*, Phys. Rev. Lett. **105**, 168701 (2010) and N. D. Treat *et al.*, Adv Funct Mater

[1]DOE DE-FG02-98ER45737

12:51PM Q38.00007 Structural evolution in polythiophene-fullerene mixtures , ENRIQUE GOMEZ, DEREK KOZUB, KIARASH VAKHSHOURI, The Pennsylvania State University — The morphology of organic semiconductor mixtures employed as the active layer of organic solar cells is a result of the complex interplay between the crystallinity of the constituents and the chemical incompatibility. Given that device performance can depend critically on the morphology of the active layer, efforts aimed identifying at the critical parameters for the structure formation process are important for the development of high-performance devices. We demonstrate that polythiophene-fullerene mixtures are partially miscible and that the crystallization of the electron donor drives the characteristic length scales of the structure. By modeling fullerene as a solvent for polythiophene, we have estimated the Flory-Huggins interaction parameter from measurements of the melting point depression of polythiophene. The miscibility between poly(3-hexylthiophene) (P3HT) and fullerene at P3HT volume fractions greater than 0.4 leads to a severe suppression of the crystallization of fullerene. Our efforts have enabled us to develop a hypothesis for the structure formation process in polythiophene/fullerene mixtures.

1:03PM Q38.00008 Miscibility Study of PCBM/P3EHT Organic Photovoltaics via Small Angle Neutron Scattering , WEN YIN, Department of Chemistry, University of Tennessee, BRYAN MCCULLOCH, RACHEL SEGALMAN, Department of Chemical Engineering, University of California , Berkeley, MARK DADMUN, Department of Chemistry, University of Tennessee — Organic photovoltaics (OPV) attracted considerable interest as lightweight, inexpensive, and easily processable replacement of inorganic photovoltaics. Current results indicate that the morphology of these photovoltaic materials is essential to their solar energy conversion efficiency but a detailed and fundamental understanding is absent. In this paper, the miscibility and structure of P3EHT/PCBM composites with varying PCBM loading level are investigated via small angle neutron scattering (SANS). With P3EHT having a melting temperature below 100°C, SANS experiments of the blends are conducted above the melting point to unequivocally determine the miscibility of PCBM and P3EHT without the added complexity of polymer crystals. Our SANS results show that blends with 20 and 50 wt% PCBM exhibit dramatically larger scattering at low-Q regime relative to 10 and 15wt% PCBM samples. This result implies that the miscibility limit of PCBM and P3EHT lies between 15:85 and 20:80. Further analysis is underway to correlate these results to OPV efficiency.

1:15PM Q38.00009 Characterization and Improvement on the Morphology in Polymer-Based Solar Cells , HAO SHEN, WENLUAN ZHANG, BRETT GURALNICK, MICHAEL MACKAY, University of Delaware, BRIAN KIRBY, CHARLES MAJKRZAK, National Institute of Standards and Technology — Polymer-based solar cells are promising for their cost-effective solar energy, yet this technology is still far from practical application owing to its low energy conversion efficiency. It has been known that the morphology in the active layer, or the nano-scaled intermixing between the polymer and fullerene derivative, is critical to the device performance. We have quantitatively measured the morphology in one of the most-studied polymer-based solar cells consisting of poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl-C61-butyric acid methyl ester (PCBM), by means of neutron and x-ray scattering techniques. In particular, the effects of thermal and co-solvent-assisted annealing on the PCBM cluster formation and vertical distribution are characterized. Basing on the observations, we are proposing a new design of solar cell architecture to approach a more controlled morphology in the active layer, by utilizing a thermodynamically-driven assembly of fullerenes onto the surface of silica microspheres. This presentation will focus on its application in the P3HT:PCBM system.

1:27PM Q38.00010 Investigation of fullerene concentration profile in polymer based solar cell by using magnetic contrast neutron reflectivity , WENLUAN ZHANG, Department of Materials Science and Engineering, University of Delaware, BRIAN KIRBY, National Institute of Standards and Technology Center for Neutron Scattering, MICHAEL MACKAY, Department of Materials Science and Engineering, University of Delaware, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING, UNIVERSITY OF DELAWARE COLLABORATION, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY CENTER FOR NEUTRON SCATTERING COLLABORATION — Poly(2,5-bis(3-tetradecyllthiophen-2-yl)thieno[3,2-b] thiophene) (pBTTT) has recently caused great interest as the electron donor in organic photovoltaics. It was demonstrated that fullerene molecules intercalate between side-chains of this semiconducting polymer creating a stable crystalline structure, so, a large concentration of fullerene must be used relative to the polymer to promote phase separated electron conductive pathways. We used state-of-the-art neutron reflectivity methods, with the application of magnetic contrast variation, to investigate the concentration profile of [6,6]-phenyl-C_{71}- butyric acid methyl ester($PC_{71}BM$) in order to understand the internal structure within the active layer. The $PC_{71}BM$ concentration profile greatly depends on the weight ratio of polymer to fullerene. XRD and other data are also used to show the morphology change of active layer.

1:39PM Q38.00011 Correlation of Structure and Roughness with Fabrication Conditions of P3HT-PCBM Bilayer Interfaces with X-Ray Reflectometry[1] , STUART KIRSCHNER, MING-LING YEH, NATHANIEL SMITH, HOWARD KATZ, DANIEL REICH, Johns Hopkins University — Organic semiconductors, including poly(3-hexylthiophene) (P3HT) and polymer-phenyl-C61-butyric acid methyl ester (PCBM), are considered as promising materials for applications such as photovoltaics, transistors, sensors, thermoelectrics, optoelectronics, and magnetoelectronics. In many cases, the interface plays a crucial role in device performance and in determining the origins of many effects. In this research, neat bilayers of P3HT-PCBM, and PCBM blended with polystyrenes, were studied with X-ray reflectometry (XRR), atomic force microscopy, and ultraviolet-visible spectroscopy. A polymer with a high atomic number element was included to improve the scattering length density contrast, and provided improved XRR resolution. A mobility of order 10^{-4} cm^2/V*s was maintained. The effect of different annealing, solvent, spin coating, and other fabrication conditions, was explored. Applicability of XRR to study interface characteristics, in these systems, will be discussed.

[1]Supported by NSF ECCS-0823947

1:51PM Q38.00012 Polymer Solar Cells, Deconstructed , YUEH-LIN LOO, JONGBOK KIM, HE WANG, STEPHANIE LEE, Chemical and Biological Engineering Department, Princeton University, ZELEI GUAN, ANTOINE KAHN, Electrical Engineering Department, Princeton University — Soft-contact lamination and delamination has enabled us to construct polymer solar cells for testing, and deconstruct them subsequently for structural characterization of the active layers and electronic characterization of relevant charge transfer interfaces. We have thus been able characterize buried active layers and interfaces that are otherwise inaccessible. Structural characterization post-device fabrication and testing reveals simultaneous crystallization of the polymer donor and the electron acceptor in the once-buried bulk-heterojunction active layers to be responsible for photocurrent enhancement in these devices. Electronic characterization of the active layer-bottom electrode interface reveals an electronic band gap of 1.5 eV, attributable to the difference between the ionization potential of the polymer donor and the electron affinity of the electron acceptor. This value is significantly larger than the band gap predicted by examining the energy levels of the individual constituents, likely due to the presence of interfacial dipoles when the polymer donor and the electron acceptor are intimately mixed.

Wednesday, March 23, 2011 11:15AM - 2:03PM –
Session Q39 GSNP DBP: Information Processing in Biological Systems A124/127

11:15AM Q39.00001 TBD , YUHAI TU, IBM T J Watson Res Ctr — This abstract not available.

11:51AM Q39.00002 Adaptive processing of natural signals in the fly peripheral visual system , LIMING ZHOU, Indiana University Dept. of Physics, ROB DE RUYTER VAN STEVENINCK, Indiana University Bloomington Dept. of Physics — For modest light intensity variations, fly photoreceptors and their postsynaptic targets, the Large Monopolar Cells (LMCs) behave approximately linearly. In this linear and stationary regime, signal transmission is described by a combination of impulse response and noise autocorrelation function. But natural visual signals often show fast and large intensity variations, and cells adapt to cope with such strong variations. As a result, responses to small contrast perturbations are still linear, but the system is no longer stationary. We study signal transfer under these conditions by measuring responses to small pseudorandom contrast perturbations that ride on large cyclically repeated intensity fluctuations. Those measurements allow us to describe signal transmission by matrices representing nonstationary analogs of the impulse response and the noise autocorrelation function. This description makes it possible to quantify information transmission as the system is continuously adapting to large intensity fluctuations, and to study trade off in adaptation and reliable information transmission in a natural context.

12:03PM Q39.00003 Optogenetic dissection of neural circuit underlying locomotory decision-making in Caenorhabditis Elegans[1] , ASKIN KOCABAS, Harvard University, ZENGCAI GUO, SHARAD RAMANATHAN — Despite the knowledge of the physical connectivity of the entire nervous system of C.elegans, we know little about how neuronal dynamics results in decision-making. Detailed understanding of functional and dynamic relations of the neural circuitry requires spatiotemporal control of the neuronal activity. Recent discoveries of light gated ion channels have allowed temporal optical control of neural activity. However, excitation of a specific neuron from among many expressing the channel has been a challenge. By combining optogenetic tools, micro mirror array technology and fast real time image processing, we have developed a technique to activate specific single or multiple neurons in an intact crawling animal while tracking its behavior. Using this setup we traced the neural pathway controlling the gradual turning of the animal during the locomotion. We found that the activity of a specific neuronal circuit that receives inputs from sensory neurons is coordinated with head movement. This coordination allows the animal to turn left or right based on the variation of sensory stimulus during head movement. By directly modulating the activity of the neural circuit, we can force the animal to turn in a specific direction independent of sensory stimuli.

[1]Human Frontier Science Program

12:15PM Q39.00004 Physical limits to concentration sensing in biochemical signaling[1] , NICHOLAS LICATA, SIMA SETAYESHGAR, Indiana University — In many biological systems, signals are carried by changes in the concentration of diffusable molecules which are transduced by receptors. It has been demonstrated experimentally that many signaling systems, from regulation of gene expression during development to bacterial chemotaxis, operate with remarkable sensitivity as indicated by a reliable response to small fractional changes in concentration. This sensitivity has contributions from an irreducible noise arising from the inherent random nature of the diffusing input signal, as well as from the chemical measurement process. By explicitly evaluating these theoretically derived contributions for the experimentally well- characterized bacterial chemotaxis network and motor response, we show that they are comparable to within factors of order unity, consistent with the observation that the measurement error approaches the physical lower limit set by diffusion. We extend our analysis to a class of ligand-gated ion channels, demonstrating the generality of this result where accuracy is especially important for the signaling system.

[1]This work was supported by the National Science Foundation.

12:27PM Q39.00005 Spatial phase patterns in locally coupled Kuramoto oscillators with repulsive interactions , ZAHERA JABEEN, MICHAEL GIVER, DAPENG BI, BULBUL CHAKRABORTY, Martin A. Fisher School of Physics, Brandeis University — Recent experiments in microfluidic arrays of interacting Belousov-Zhabotinsky droplets, which belong to the class of active emulsions, show a rich variety of spatial patterns [J. Phys. Chem. Lett. 1, 1241-1246 (2010)]. The predominant coupling between these droplets is inhibitory. Motivated by this experimental system, we study repulsively coupled Kuramoto oscillators with nearest neighbor interactions on a triangular lattice in two dimensions. We show that the geometry of the lattice constrains the phase difference between two neighboring oscillators to $2\pi/3$. We report the existence of domains with either clockwise or anticlockwise helicity, leading to defects in the lattice. We study the time dependence of these domains and show that at large coupling strengths the domains freeze due to frequency synchronization. A variant of this model, in which amplitude variations are introduced by an additional Ising-like coupling between the oscillators, explores the strong coupling limit phenomenon in the experimental system. We discuss these results in the context of the experiments.

12:39PM Q39.00006 Monte-Carlo Study of Axonal Transport in a Neuron[1] , UTTAM SHRESTHA, CLARE YU, ZHIYUAN JIA, ROBERT ERICKSON, STEVEN GROSS, University of California, Irvine — A living cell has an infrastructure much like that of a city. A key component is the transportation system that consists of roads (filaments) and molecular motors (proteins) that haul cargo along these roads. We will present a Monte Carlo simulation of intracellular transport inside an axon in which motor proteins carry cargos along microtubules and are able to switch from one microtubule to another. The breakdown of intracellular transport in neurons has been associated with neurodegenerative diseases such as Alzheimer's, Lou Gehig's disease (ALS), and Huntingdon's disease.

[1]This work was supported by NIGMS grant number 5R01GM79156.

12:51PM Q39.00007 Phase and frequency entrainment in locally coupled phase oscillators with repulsive interactions , MICHAEL GIVER, ZAHERA JABEEN, BULBUL CHAKRABORTY, Martin A. Fisher School of Physics, Brandeis University — Recent experiments in one and two-dimensional microfluidic arrays of droplets containing Belousov - Zhabotinsky reactants show a rich variety of spatial patterns [J. Phys. Chem. Lett. 1, 1241-1246 (2010)]. These experiments provide the first steps towards creating easily reproducible model active emulsion systems. Motivated by this experimental system, we study repulsively coupled Kuramoto oscillators with nearest neighbor interactions on a linear chain as well as a ring in one dimension. We show using linear stability analysis as well as numerical study, that the stable phase patterns depend on the geometry of the lattice and that a transition to the ordered state does not exist in the thermodynamic limit. We will also present results comparing our Kuramoto model with finite element simulations of the Brusselator model in geometries similar to those of the experiment.

1:03PM Q39.00008 Simulation studies of creeping flexible nematogens: flocking and rectifying barriers[1] , ADAM NICHOLAS, Beloit College, ROBIN SELINGER, Kent State Univ. — Recent simulation studies of active nematics have focused on rigid rods or swimming bacteria undergoing collisions via simple rules. Here we present a more physically detailed model of self-propelled creeping flexible nematogens. Each segmented "worm" is represented as nine interaction sites connected by springs. The springs' equilibrium length is modulated, causing each worm to elongate and contract periodically. Each worm alternately grips the substrate at its leading or trailing end, producing creeping locomotion. Inter-worm interactions are described via the Weeks-Chandler-Anderson potential between nearby interaction sites. Random forces and damping are also added. For worms that reverse crawling direction at random intervals, we observe a homogeneous nematic phase, and study its behavior in the presence of a rectifying barrier. For worms that move only in a single direction, we observe flocking behavior characterized by evolving stripes of densely crowded particles interspersed with low-density regions. We compare these results with relevant experiments and related theory/simulation approaches.

[1]Supported by NSF-CHE-1004987 (Kent State REU)

1:15PM Q39.00009 ABSTRACT WITHDRAWN –

1:27PM Q39.00010 Glass-like dynamics in collective cell migration , THOMAS ANGELINI, University of Florida, DAVID WEITZ, Harvard University — The collective movement of tissue cells is essential to fundamental biological processes in both health and disease, and occurs throughout embryonic development, during wound healing, and in cancerous tumor invasion. Most knowledge of cell migration, however, comes from single cell studies. Single cells migrate by executing cyclic processes of extension, adhesion, and retraction, during which the cell body fluctuates dramatically and the cell changes direction erratically. These sub-cellular motions must be coupled between neighbors in confluent layers, yet the influence of this coupling on collective migration is not known. In this talk we present a study of motion in confluent epithelial cell sheets. We measure collective migration and sub-cellular motions, covering a broad range of length-scales, time-scales, and cell densities. We find that that collective cell migration exhibits many behaviors characteristic of classical supercooled particulate fluids, including growing dynamic heterogeneities in the migration velocity field, non-Arrhenius relaxation behavior, and peaks in the density of states analogous to the Boson peak. These results provide a suggestive analogy between collective cell motion and the dynamics of supercooled fluids approaching a glass transition.

1:39PM Q39.00011 Active Chemical Thermodynamics promoted by activity of cortical actin , BHASWATI BHATTACHARYA, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore-560064, India, ABHISHEK CHAUDHURI, KRIPA GOWRISHANKAR, Raman Research Institute, C.V. Raman Avenue, Bangalore 560080,India, MADAN RAO, Raman Research Institute, C.V. Raman Avenue, Bangalore 560080/National Centre for Biological Sciences (TIFR), Bellary Road, Bangalore 560065, India — The spatial distribution and dynamics of formation and breakup of the nanoclusters of cell surface proteins is controlled by the active remodeling dynamics of the underlying cortical actin. To explain these observations, we have proposed a novel mechanism of nanoclustering, involving the transient binding to and advection along constitutively occuring "asters" of cortical actin. We study the consequences of such active actin-based clustering, in the context of chemical reactions involving conformational changes of cell surface proteins. We find that the active remodeling of cortical actin, can give rise to a dramatic increase in efficiency and extent of conformational spread, even at low levels of expression at the cell surface. We define a activity temperature (τ_a) arising due to actin activities which can be used to describe chemical thermodynamics of the system. We plot TTT (time-temparature-transformation) curves and compute the Arrhenius factors which depend on τ_a. With this, the active asters can be treated as enzymes whose enzymatic reaction rate can be related to the activity.

1:51PM Q39.00012 Brown movement in complex asymmetric periodic potential under the influence of colored noise , MIKHAIL SVIRIDOV, SERGEY GUZ, Moscow Institute of Physics and Technology — The idea of the molecular motor in an asymmetric periodic potential is a well-known problem. The motion of a Brownian particle is often studied when the system is subjected to the action of white noise. In practical situations noise is colored ("red") random process. The red noise is the Ornstein-Uhlenbeck process. In this work we consider noise when the spectral density of the external noise is equal to zero on the zeroth frequency. In our previous works such a noise is been called as "green" noise. For the analytical study of green noise action, we use an approach based on a Krylov-Bogoliubov averaging method which is modified to study the action of noise with arbitrary intensity. A certain effective potential can be built which determines the basic features of the system dynamics. Further, we compare two numerical cases. The first one is the time-derivative of the Ornstain-Uhlenbeck process (green noise). The complex potentials when the system does not work as a molecular motor in the case of red noise, i.e. the average motion of the particle does not exhibit a drift in a given direction. If green noise operates on the same system, it turn out the effective molecular motor. We demonstrate this fact by a histograms for realizations of these processes.

Wednesday, March 23, 2011 11:15AM - 2:03PM –

Session Q40 DCP: Theoretical Methods and Algorithms for Chemical Physics A122/123

11:15AM Q40.00001 Primordial Particles; Collisions of Inelastic Particles , GEORGE SAGI, George S. Sagi Research — Three-dimensional matter is not defined by Euclidian or Cartesian geometries. Newton's and Einstein's laws are related to the motions of elastic masses. The study of collisions of inelastic particles opens up new vistas in physics. The present article reveals how such particles create clusters composed of various numbers of particles. The Probability of each formation, duplets, triplets, etc. can be calculated. The particles are held together by a binding force, and depending upon the angles of collisions they may also rotate around their center of geometry. Because of these unique properties such inelastic particles are referred to as primordial particles, Pp. When a given density of Pp per cubic space is given, then random collisions create a field. The calculation of the properties of such primordial field is very complex and beyond the present study. However, the angles of collisions are infinite in principle, but the probabilities of various cluster sizes are quantum dependent. Consequently, field calculations will require new complex mathematical methods to be discovered yet.

11:27AM Q40.00002 Aggregation of Thermal Particles in Simulation[1] , IAT NENG CHAN, University of Macau — Based on the Schrodinger Equation, energy levels are evaluated for charged particle or atom surrounded by few atoms imitated to atomic cavity situations under multipole or Lennard-Jones interactions. To examine the states of corresponding eigenvalues, the associated wave functions from simulation are plotted in three-dimension to elucidate the space distribution of particles. In cases for testing on effect of different adjacent atomic structures, concentration region of distribution is revealed from a series of results. The range of localization shown also is affected by the type and strength of interactions between particles and atoms, besides the number and position of surrounding atoms. The thermal effect considered in the computation is modeled by average over results from random fluctuation of atom positions for a given heating grade. Moreover, analysis with fuzzy conditions is applied to reduce the complicated and time-consumption approach, also for the training in science education. Even the investigation is limited and tentative, qualitative studies on different parameters and structures can provide the influence of factors and approximate information to compare with the experience evidences.

[1]Supported by UM grant No. RG062/09-10S/CIN/FST.

11:39AM Q40.00003 Many Body Density Matrix Theory[1] , C.J. TYMCZAK, Texas Southern University — One fundamental limitation of quantum chemical methods is the accuracy of the approximate many-body theoretical framework. Accurate many-body formalisms for quantum chemical methods do exist, but these methods are computationally very expensive. Methods also exist that are much less computationally expensive such as Hatree-Fock, Density Functional and the Hybrid Functional theories, but at a reduced representation of the exact many-body ground state. This severely limits either the system size that can be addressed accurately, or the accuracy of the representation. What is needed is a method that represents the many-body ground states accurately, but with a low computational cost. Recently, a method for determining the response, to any order of the perturbation, within the density matrix formalism has been discovered. This method opens up the possibility of computing the variational many-body ground states to unprecedented accuracy within a simplified computational approach. We report on the theoretical development of this methodology, which we refer to as Many Body Density Matrix Theory. This theory has many significant advantages over existing methods. One, its computational cost is equivalent to Hartree-Fock or Density Functional theory. Two it is a variational upper bound to the exact many-body ground state energy. Three, like Hartree-Fock, it has no self-interaction. And four, it is size extensive.

[1]Funded by Welch Foundation Grant J-1675

11:51AM Q40.00004 Probing the Surface-to-Bulk Transition: A Closed-Form, Constant-Scaling Algorithm for Computing Subsurface Green Functions , MATTHEW REUTER, Department of Chemistry, Northwestern University, TAMAR SEIDEMAN, MARK RATNER — A closed-form algorithm for computing subsurface Green functions—the blocks of a material's Green function between the surface and the bulk—is presented, where we assume the system satisfies a common principal layer approximation. By exploiting the block tridiagonal and nearly block Toeplitz structure of the Hamiltonian and overlap matrices, this method scales independently of the system size (constant scaling), allowing studies of large systems. As a proof-of-concept example, we investigate the decay of surface effects in an armchair graphene nanoribbon, demonstrating the persistence of surface effects hundreds of atomic layers ($\sim$0.5 μm) away from a surface. We finally compare the surface-to-bulk transitions of finite and semi-infinite systems, finding that finite systems exhibit amplified surface effects.

12:03PM Q40.00005 Projecting the phase-space trajectory of multidimensional non-equilibrium systems onto a discrete set of states: a Projective Dynamics approach , KATJA SCHAEFER, M.A. NOVOTNY, Department of Physics and Astronomy, Mississippi State University — Phase-space trajectories, which are either continuous or possess small discontinuities, can be projected onto a discrete set of states with nearest neighbor coupling. The pointwise projection leads for non- equilibrium system to a non-Markovian process, even if the dynamics of the original system is Markovian. However, using time-averaged transition-rates a Markov process can be obtained, which has the same overall properties as the original dynamics of the system. The projected process defines a new dynamics, which only in the limit $t \to \infty$ obtains the property on the time-scale of the averaging procedure. We demonstrate the Projective Dynamics method in theory and applications to absorption processes, which in general are not describable through equilibrium or steady-state models. We show the discrete set of states $\{\zeta_k\}$ can be chosen arbitrarily (with slight restrictions) for all systems.

12:15PM Q40.00006 Finding lowest saddle point , QING LU, Department of Mechanical Engineering and Division of Materials Science and Engineering, Boston University, MINGHAI LI, Gustaf H. Carlson School of Chemsitry and Biochemistry, Clark University, AKIHIRO KUSHIMA, Department of Materials Science and Engineering, University of Pennsylvania, XI LIN, Department of Mechanical Engineering and Division of Materials Science and Engineering, Boston University — A history-penalized basin filling algorithm is presented in this work which identifies the lowest saddle point starting from any given initial state on any given potential energy hypersurface. The natural analogy of this algorithm is filling a barrel with water; by monitoring the location where leakage occurs one identifies the lowest opening on the wall of the barrel. The successful implementation of this algorithm relies on insightful choices of the penalty function, penalty function combination, and peak refinement. Several types of penalty functions are implemented to study two classical systems, the ad-cluster surface diffusion and supercooled binary Lennard-Jones liquid, and one quantum system of the topological soliton migration. The most efficient penalty function is found to be a triangle penalty function with uniform forces and large 3N+1-dimensional volume. The combination of penalty functions dramatically improves the computational efficiency. The lowest saddle point can be precisely located by the basin filling algorithm coupled with a few standard peak-refinement methods.

12:27PM Q40.00007 The Reaction of Carbon Dioxide with Water Clusters: an Ab Initio Metadynamics Study , GREGOIRE GALLET, FABIO PIETRUCCI, CECAM EPF Lausanne (CH), WANDA ANDREONI, CECAM and Institut de Théorie des Phénomènes Physique EPF Lausanne (CH) — Simulations are often invoked as aid to understand and optimize carbon capture and sequestration processes. The hydration of carbon dioxide (CO_2) offers an excellent test case for assessing the reliability of computational schemes. We present a density-functional-theory study of the reaction of CO_2 with water clusters. The first step was to validate DFT results in different approximations of the exchange and correlation functional with respect to quantum chemical methods for the structure, binding energies and vibrational frequencies of several isomers. Next, simulations of the reactions leading to the formation of carbonic acid were performed using metadynamics as accelerating procedure. This method allows us both to identify the reaction mechanisms and to obtain an estimate of the free energy barriers via the reconstruction of the free energy profiles. Comparisons were drawn with previous static calculations of the barriers. As reference, a similar calculation in liquid water will be presented.

12:39PM Q40.00008 Triplet Pairing and Odd-Electron Densities in Constrained-Pairing Mean-Field Theory , JASON K. ELLIS, Department of Physics and Astronomy and Department of Chemistry, Rice University, CARLOS A. JIMENEZ-HOYOS, Department of Chemistry, Rice University, GUSTAVO E. SCUSERIA, Department of Chemistry and Department of Physics and Astronomy, Rice University — Describing strong (also known as static or non-dynamical) correlation caused by degenerate or nearly degenerate orbitals near the Fermi level remains a theoretical challenge, particularly in molecular systems. Constrained-pairing mean-field theory (CPMFT) has been quite successful capturing the effects of static correlation in bond formation and breaking in closed- shell molecular systems. This method uses singlet electron entanglement to model static correlation at *mean field* cost. The present work extends the previous formalism to include triplet pairing, allowing a description of same-spin correlation and open-shell species. Additionally, a spin-orbital extension of the "odd-electron" formalism of Yamaguchi and co-workers is presented as a method for understanding triplet radical character in molecules. Results from representative systems are presented.

12:51PM Q40.00009 Dynamical Mean-Field Theory for Quantum Chemistry[1] , NAN LIN, Department of Physics, Columbia University, 538 West 120th Street, New York, NY 10027, USA, CHRIS MARIANETTI, Department of Applied Physics, Columbia University, New York, NY 10027, USA, ANDREW MILLIS, Department of Physics, Columbia University, 538 West 120th Street, New York, NY 10027, USA, DAVID REICHMAN, Department of Chemistry, Columbia University, 3000 Broadway, New York, NY 10027, USA — The dynamical mean-field concept of approximating an unsolvable many-body problem in terms of the solution of an auxiliary quantum impurity problem, introduced to study bulk materials with a continuous energy spectrum, is here extended to molecules, i.e. finite systems with a discrete energy spectrum. Application to chains and small clusters of hydrogen atoms yields ground state energies which are competitive with leading quantum chemical approaches at intermediate and large interatomic distances, and provides good approximations to the excitation spectrum. The method is a promising approach to the strong correlation problems of quantum chemistry.

[1]This work is supported by NSF-DMR-075847, NSF-CHE-0641523 and NYSTAR.

1:03PM Q40.00010 Constrained Active Space Unrestricted Mean-Field Approaches for Controlling Spin-Contamination , TAKASHI TSUCHIMOCHI, GUSTAVO E. SCUSERIA, Department of Chemistry, Rice University — We have recently shown that unrestricted Hartree-Fock (UHF) variationally reduces to high-spin restricted open-shell Hartree-Fock when constraints are imposed on the eigenvalues of the spin density matrix [T. Tsuchimochi and G. E. Scuseria, J. Chem. Phys. **133**, 141102 (2010)]. We here generalize these ideas and propose to control spin-contamination in UHF by releasing the constraints in an active space while imposing them elsewhere. If the active space is properly chosen, our constrained UHF (CUHF) method greatly benefits from a controlled broken-symmetry effect while avoiding the massive spin contamination arising in the traditional UHF. We apply Löwdin's projection operator to CUHF and obtain multireference wave functions with moderate computational cost. We report results on singlet-triplet energy gaps to show that our constrained scheme outperforms fully unrestricted methods. This constrained approach can be readily used in Kohn-Sham (KS) density functional theory with similar favorable effects, provided that spin-contamination is given by the KS orbitals as in UHF.

1:15PM Q40.00011 Nuclear quantum effects using selective mode excitation in water , SRIRAM GANESHAN, MARIVI FERNANDEZ-SERRA, Stony Brook university — Recently, Ceriotti et. al. [1] introduced a comprehensive framework to use a custom-tailored Langevin equation with correlated-noise in the context of MD simulations. One of the interesting applications of these thermostats is that, such a framework can be used to selectively excite normal modes whose frequency falls within a prescribed, narrow range [2]. The general idea of this work is to understand whether, the selective excitation of modes in some systems like water is enough to reproduce the necessary nuclear quantum effects at a given temperature. Ceriotti et. al has also implemented their colored noise thermostat (Langevin) to the PIMD of TIP4P/F model [3]. In this work we study how the TIP4P/f responds to the selective mode excitation using the delta-thermostats. We apply this delta thermostat to the molecular dynamics of TIP4P/F [4] water force field, a model explicitly fitted with the lack of zero point ionic vibrations. TIP4P/F provides us an ideal platform to study the effect of selective mode excitation on water. We address the question of whether selective mode excitations are enough to generate the nuclear quantum effects in water. This work will also provide a way to identify the dominant modes for which the quantum effects are important. [1] Chem. Theory Comput.6, 1170 (2010) [2] Proc. Comp. Sci. 1, 1601 (2010), [3] J. Chem. Phys. 131, 024501 (2009), [4] J. Chem. Phys 133, 124104 (2010).

1:27PM Q40.00012 *Ab Initio* Composite Methods , ANGELA WILSON, WANYI JIANG, GBENGA OYEDEPO, MARIE LAURY, University of North Texas — In this brief presentation, we highlight recent developments of the *ab initio* composite method, the correlation consistent Composite Approach (ccCA). Recent work has enabled ccCA to be utilized for 3d transition metals, as well as for species for which a multireference wavefunction is required. We overview the development, as well as applications of the method to the prediction of spectroscopic and thermodynamic properties of molecules.

1:39PM Q40.00013 Distortion of scanning-tunnelling-spectroscopy images of isolated molecules induced by electron correlation , MASSIMO RONTANI, DIMITRIOS TOROZ, STEFANO CORNI, CNR-NANO S3, Modena, Italy — Scanning tunnelling spectroscopy (STS) visualizes electron states in both extended systems and nano-objects, as quantum dots and molecules. Whereas bulk quantum states are insensitive to electron number fluctuations, an energy gap opens each time a new electron is injected by the STS tip into a sufficiently small system. This gap originates from the interaction of the next incoming electron with the others already present in the system. In this Coulomb blockade regime a fundamental question is whether the wave function of the "quasi-particle" added to the system -imaged by the STS tip- is sensitive to electron-electron interaction. Here we show that the STS images of single planar molecules with metal centres predicted by ab initio many-body calculations differ qualitatively from their uncorrelated counterparts. We find in the maps resolved at the Fermi energy that correlation significantly removes spectral weight from the metal atom, as well as the overall weight is remarkably reduced. This change may be measured and compared with STS images of molecules without the metal center, whose many-body and uncorrelated versions are alike.

1:51PM Q40.00014 Maximizing the hyperpolarizability poorly determines the potential , ROLFE PETSCHEK, TIMOTHY ATHERTON, JOSEPH LESNEFSKY, GREG WIGGERS, Case Western Reserve University — Increasing the non-linear response of materials to an electric field, characterized by quantities such as the first hyperpolarizibility β, is a mattter of importance for applications. We optimized the zero frequency β of a one-dimensional potential well containing a single electron by freely adjusting the shape of that potential. It is shown that with careful optimization the maximum hyperpolarizability converges quickly with increasing numbers of parameters in the potential to approximately 0.708951 of the proven upper bound. The Hessian of β at the maximum makes it clear that there is a very wide range of nearby, nearly optimal potentials: with several measures of differences between potentials, this Hessian has only two large eigenvalues with the others diminishing quickly. The optimum potentials are substantially different and more affected by small eigenvectors than the wavefunctions. Thus, wavefunctions are superior for describing the conditions that optimize the hyperpolarizability. Prospects for a concise description of the two important constraints on near-optimum potentials and wavefunctions are discussed.

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q41 DCP: Focus Session: Fundamental Issues in Interfacial Charge Transport for Energy Applications II A115/117

11:15AM Q41.00001 First principles simulations of materials and processes in photo- and electro-catalysis , ANNABELLA SELLONI, Princeton University — I shall discuss applications of electronic structure calculations and molecular dynamics simulations to understand materials properties and reaction mechanisms in photo- and electro-catalysis. Examples will include studies of the interface between water and titanium dioxide (TiO_2), a widely used photocatalyst capable of splitting water in $O_2 + H_2$, and the cycle of H_2 production from water by the active site of an enzyme of hydrogen-producing bacteria, the di-iron hydrogenase, linked to a pyrite electrode.

11:51AM Q41.00002 Theoretical studies on a new pattern of laser-driven systems: towards elucidation of direct photo-injection in dye-sensitized solar cells[1] , KENJI MISHIMA, KOICHI YAMASHITA, The University of Tokyo — We theoretically and numerically investigated a new type of analytically solvable laser-driven systems inspired by electron-injection dynamics in dye-sensitized solar cells. The simple analytical expressions were found to be useful for understanding the difference between dye excitation and direct photo-injection occurring between dye molecule and semiconductor nanoparticles. More importantly, we propose a method for discriminating experimentally dye excitation and direct photo-injection by using time-dependent fluorescence. We found that dye excitation shows no significant quantum beat whereas the direct photo-injection shows a significant quantum beat.

[1]This work was supported by Funding Program for World-Leading Innovative R&D on Science and Technology (FIRST) "Development of Organic Photovoltaics toward a Low-Carbon Society," Cabinet Office, Japan.

12:03PM Q41.00003 Investigation of the Potential Difference between C60 and TiOPc on Ag(111) by Local Probe Techniques , KRISTEN BURSON, YINYING WEI, WILLIAM CULLEN, JANICE REUTT-ROBEY, University of Maryland-College Park — One challenge for increasing efficiency of organic photovoltaics is to understand the barrier to exciton separation that exists at the interface between organic molecules. Here we report a local probe measurement of the potential barrier at the interface between submonolayer C60, a good electron acceptor, and honeycomb phase TiOPc, an organic with high hole mobility, on Ag(111). We employ UHV AFM (atomic force microscopy) and KPFM (Kelvin probe force microscopy) to obtain simultaneous images of the potential and topographic landscapes. This technique allows for high spatial resolution of both the potential and the topography. In addition to reporting the work function difference between C60 and TiOPc, we investigate the work function for C60 on Ag(111).

12:15PM Q41.00004 Ultrafast proton coupled charge transfer dynamics in photocatalysis , HRVOJE PETEK, University of Pittsburgh — In this talk I will present our experimental and theoretical studies on the nature of electron and hole acceptor states and their dynamics for protic solvent molecule (H_2O, CH_3OH) covered TiO_2 surfaces. Electron-hole pair generation by band gap excitation can introduce charges into protic solvent/TiO_2 interface, which can drive photocatalytic processes. By time resolved two-photon photoemission and DFT electronic structure calculations we identify the partially solvated or "wet" electron accepter states, and their proton-coupled electron transfer (PCET) dynamics. Because holes are through to be the primary reagents for photocatalysis on TiO_2, we also explore possible hole driven PCET dynamic pathways.

12:51PM Q41.00005 First-principles study on Ru(4,4',4"-tricarboxy-2,2':6',2"-terpyridine)$(NCS)_3$ sensitizer on TiO_2 anatase(101) surface: Adsorbed structures and electronic states for dye-sensitized solar cells[1] , KEITARO SODEYAMA, MASATO SUMITA, YOSHITAKA TATEYAMA, National Institute for Materials Science MANA — Dye-sensitized solar cells are expected as a cost effective solar-to-electricity energy conversion devices. The efficiency of the power conversion is greater than 10% when Ru(II) polypyridyl sensitizers are used. For further improvement of the efficiency, we need to understand the adsorbed structures at atomistic level in detail. In this study, we investigated the adsorbed structures of Ru(4,4',4"-tricarboxy-2,2':6',2"-terpyridine)$(NCS)_3$ sensitizer on TiO_2 anatase(101) surface. For four possible adsorbed structures (two candidates have one adsorbed carboxyl group(one-leg) and the others have two adsorbed groups(two-leg)), we found the adsorption energies are quite similar within 0.4 eV. This is attributed to the presence of the hydrogen bond between the hydrogen of carboxyl group and the oxygen of the surface in the one-leg structure. We also calculated the excited states of the four structures of the sensitizer by TDDFT and found that the UV spectrum shift depending on the structure differences.

[1]This work is supported by JST-CREST, PRESTO, and KAKENHI.

1:03PM Q41.00006 Reverse-engineering the atomic-scale structure of the TiO2/N3 interface in dye-sensitized solar cells using O1s core-level shifts , CHRISTOPHER PATRICK, FELICIANO GIUSTINO, Department of Materials, University of Oxford — Dye-sensitized solar cells employing mesoporous titania films sensitized with ruthenium-based dyes have shown consistently good performance over the past two decades. Understanding the process of charge injection in these devices requires accurate atomistic models of the interface between the light-absorbing dye and the semiconducting substrate. Despite considerable efforts devoted to the experimental and theoretical investigation of such interfaces, their atomistic nature remains controversial. In this work we pursue a novel computational approach to the study of the semiconductor/dye interface which does not rely on the calculated adsorption energies. In our approach we reverse-engineer photoemission data through the first-principles calculation of O1s core-level spectra for a number of candidate interface models. Our calculations allow us to discard some of the adsorption geometries previously proposed and point to an interface model which reconciles conflicting assignments based either on photoemission or infrared data.

1:15PM Q41.00007 Studies of Interfacial Electronic Processes in Nanoporous TiO2 Thin-Films[1] , VICTOR BATISTA, Yale University — Metal-oxide nanoparticles sensitized to visible light by covalent attachment of molecular adsorbates have attracted considerable attention in recent years due their central role in technologies for solar energy conversion, including dye-sensitized solar cells (DSSCs) and solar photocatalysis. However, the mechanisms of interfacial electron transfer and subsequent electron transport induced by photoexcitation of the molecular adsorbates remain only partially understood. We report recent progress in studies of nanoporous TiO2 thin-films functionalized with molecular adsorbates, with emphasis on interfacial electron injection, molecular rectification and the mechanism of electron transport through sintered TiO2 nanoparticles in thin-films relevant to DSSCs.

[1]The author acknowledges support from DOE (grants DE-FG02-07ER15909 and ANSER EFRC Award Number DE-PS02-08ER15944) and NSF (grants ECCS-0404191 and CHE 0911520).

1:51PM Q41.00008 Efficient adsorbate transport by electron wind: The role of resonant photoexcitation , KIRILL VELIZHANIN, DMITRY SOLENOV, Los Alamos National Laboratory — We study the surface electromigration force acting on an organic molecule at a conducting (metal) surface. The dominant contribution to the force comes from the scattering of metallic electrons off the molecule, as they tunnel to and from nearby molecular orbitals. When metal carries non-zero current, the net force is directed with the current flow. This force, however, is often too small for efficient transport of adsorbed molecules and only reveals itself through a contribution to the metal resistivity. We show that surface-molecule electron wind force can be substantially enhanced and controlled by exploiting appropriate resonances between molecular and metallic states activated by coherent light. This effect opens a path to new surface-molecule functionality, including high resolution spatially controlled force patterns, controlled molecule motion, etc.

2:03PM Q41.00009 Real-time observation of bond-by-bond interface formation during oxidation of H-terminated (111)Si by second-harmonic generation , BILAL GOKCE, North Carolina State University, ERIC J. ADLES, Johns Hopkins University, DAVID E. ASPNES, KENAN GUNDOGDU, North Carolina State University — Structure of solids is typically determined at the atomic level by techniques such as X-ray and electron diffraction, which are sensitive to positions of atomic nuclei. However, structure is determined by bonds between atoms, which are difficult to measure directly. We combine second-harmonic generation and the bond-charge model of nonlinear optics to probe, in real time, the dynamics of bond-by-bond chemical changes during the oxidation of H-terminated (111)Si, a surface that has been well characterized by static methods. Oxidation is activated by applied macroscopic strain, and exhibits anisotropic kinetics with one of the three equivalent back- bonds of on-axis samples reacting differently from the other two. This also leads to transient changes in bond directions. Strain is known to increase oxidation rate of Si for thermal oxides, however its affects at the microscopic scale has not been studied at the bond level. By comparing results for surfaces strained in different directions, we show that in-plane control of surface chemistry is possible. The use of nonlinear optics as a bond-specific characterization tool is readily adaptable for studying structural and chemical dynamics in many other condensed-matter systems.

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q42 DPOLY: Polymer Composites A302/303

11:15AM Q42.00001 Dispersion and composite processing of polymer coated graphene , SRIYA DAS, AHMED WAJID, JOHN SHELBURNE, ABEL CORTINAS, MICAH GREEN, Texas Tech University — Liquid phase exfoliation and dispersion of graphene, i.e. single layer graphite, is a critical challenge for bulk processing of graphene into advanced materials and devices. We demonstrate a suite of techniques for dispersing pristine graphene using polymer coatings for the purpose of liquid-phase nanocomposite processing. First, we illustrate a unique in situ polymerization technique to develop localized polymer coatings on the surface of dispersed pristine graphene sheets in solution. These polymer coatings do not disrupt the pristine structure or superior properties of the graphene sheets; instead, these coatings allow for stable, aggregation resistant graphene dispersions, as characterized through rheology, SEM, and AFM. We also demonstrate that certain polymers naturally wrap and stabilize pristine graphene in various organic solvents. We use this technique to prepare epoxy and PVA nanocomposites loaded with polymer-wrapped graphene as filler.

11:27AM Q42.00002 Fabrication of Graphene Oxide/Polypropylene Nanocomposites and Their Electrical Conductivity Study , JINYONG DONG, Institute of Chemistry, Chinese Academy of Sciences — Graphene oxide (GO) /polypropylene nanocomposites were fabricated via in situ polymerizing propylene monomer over a GO that had been treated with a Grignard reagent and $TiCl_4$ successively when GO was not only catalytically activated but also largely reduced to an almost O- free state. The polymerization led to the in situ formation of the PP matrix, which was synchronized by the nanoscale exfoliation of the reduced GO as well as its gradual dispersion. Morphological examination of the ultimate GO/PP nanocomposites by TEM and SEM techniques revealed effective dispersion in nanoscale of GO in PP matrix. High electrical conductivity was discovered with thus prepared GO/PP nanocomposites, e.g. at a GO loading of 4.9 wt%, σ_c was measured at 0.3 S·m^{-1}

11:39AM Q42.00003 Controlling nanorod self-assembly in polymer thin film composites , MIGUEL MODESTINO, University of California, Berkeley, JEFFREY URBAN, Molecular Foundry, Lawrence Berkeley National Laboratory, RACHEL SEGALMAN, University of California, Berkeley — Semiconducting nanorods are of particular interest for use in polymer composites due to their anisotropic physical properties; however such properties can only be harnessed in systems with orientational order. Here, we demonstrate control over nanorod self-assembly in solution which leads to arrays of vertically aligned nanorods in polymer thin films over large areas (>1 cm^2). Transmission electron microscopy and X-ray scattering techniques were used to determine the structure of composites and probe the nanorod self-assembly mechanism. This work demonstrates that strong interactions between alkane-covered colloidal nanorods can enable the formation of hexagonally packed arrays of nanorods in a wide range of polymer matrices. Kinetic effects during the casting process are shown to affect the final morphology of the composites, leading to reduced array sizes for systems with increasing polymer molecular weight and nanorod concentration. The results presented show that thin film confinement as well as surface segregation of the nanorod arrays enhance the orientational order of nanorods in composites.

11:51AM Q42.00004 Multi-Walled Carbon Nanotube Network Formation in Extruded High Density Polyethylene/MWNT Composites[1] , FRANK YEPEZ CASTILLO, BRIAN P. GRADY, DANIEL E. RESASCO, The University of Oklahoma — Multi-walled carbon nanotube (MWNT) / high density polyethylene (HDPE) composites with varying amounts of carbon nanotubes were investigated and the effect of MWNT weight fraction on their electrical conductivity, crystallinity and mechanical properties is presented here. Samples were prepared by melt dilution of a HDPE masterbatch containing 20 wt% MWNT with varying amounts of neat HDPE. Conductivity measurements on compression molded samples showed that electrical percolation occurs at 4.5 wt% MWNTs. The effect of processing conditions on the formation of a MWNT network in extruded samples was assessed by the addition of a low-shear annealing zone (shear rate 1-10 s^{-1}) before final extrusion through a die. The time in the low shear zone was varied from almost zero to 90 sec. Extruded samples above the compression-molded percolation threshold were tested, and electrical conductivity did not develop. However, a significant increase in electrical conductivity was observed in these samples when annealed for 5 minutes at the same temperature.

[1]This research was supported by grants from the Oklahoma State Regents for Higher Education and the Department of Energy (Grant ER64239 0012293).

12:03PM Q42.00005 Effect of Nanowire Size Dispersity on the Electrical Conductivity in Polymer Nanocomposites , ROSE MUTISO, MICHELLE SHERROTT, JU LI, KAREN WINEY, University of Pennsylvania — In this simulation study, we model the percolation threshold and electrical conductivity of three-dimensional networks containing finite, conductive cylinders with experimentally typical (Gaussian) and engineered (Bidisperse) distributions in their length and/or diameter. We have previously used this approach to explore the effects of cylinder orientation and aspect ratio. Preliminary results suggest that narrow Gaussian distributions do not affect the threshold concentration or electrical conductivity significantly in both isotropic and oriented networks, while the addition of a small fraction of longer rods in a bidisperse system can improve the electrical properties considerably. Additionally, polydispersity in the filler length has a more pronounced effect on the electrical percolation behavior than that in filler diameter. This implies that the separate effects of length and diameter should be decoupled from the overall filler aspect ratio when probing the effects of size dispersity in conducting polymer nanocomposites with elongated fillers.

12:15PM Q42.00006 Simulating the Effect of Flame Retardant Materials on Heat Diffusion in Polymers , JOSEPH ORTIZ, Stony Brook University, ARPON RAKSIT, Commack High School, DILIP GERSAPPE, Stony Brook University — Many commonly used polymers have low ignition temperatures, presenting the dangers of combustion and thermal degradation. Simulating the effect of flame retardants on the spread of heat throughout a polymer may provide a better understanding on how to effectively manipulate and make use of flame retardant materials. Using the lattice Boltzmann method, a simulation of heat diffusion from a heat source to sink was implemented in three dimensions. The polymer and flame retardant material were incorporated into the system by implementing ignition within the particles of the polymer and by adding heat absorbing microscale filler particles within the polymer matrix, while allowing for reduced-rate heat transfer between interspecies particles. Flame retardant particles were given various volume fractions and morphologies in order to simulate the addition of a variety of particles such as carbon nanotubes. By manipulating the flame retardant particles' ability to absorb heat, and their efficiency in removing heat from the system, different degrees of polymer heat transport were simulated while polymer systems ranged from single polymer systems to multi-component blends.

12:27PM Q42.00007 Diffusion of small molecules in polymer nanocomposites: relationship between local free volume dynamics and penetrant diffusivity , VICTOR PRYAMITSYN, VENKAT GANESAN, University of Texas at Austin — Polymer membranes are widely used as barrier or gas/vapors separation materials. Recent experiments have demonstrated that the barrier properties of the polymer nanocomposites (PNC) dramatically different from pure polymer. Usually such properties are quantified by the permeability P of the material to a penetrant which consists of two contributions: the penetrant solubility S and diffusivity D: $P = S\ D$ In present work we only discuss term D. We use the Bond Fluctuation Model, which allows us to model the diffusivity of the penetrant, the dynamics of the polymer and the dynamics of the polymer free volume in a single framework. We modeled PNC's at different particle load and the penetrant size and found that addition of nanoparticles increseses the penetrant diffusivity and selectivity to the penetrant size. This increase is attributed to the free volume increase and the acceleration of the free volume relaxation in PNC relatively to the pure polymer. We have compared the penetrant diffusivity in a rubbery and glassy PNC's and found than the effect of the PNC load on diffusivity and selectivity is much stronger for the glassy system which is due to rubbery system D is controlled by the rate of matrix free volume relaxation and in glassy regime it is controlled by the static free volume percolation, which is more sensitive to the PNC load.

12:39PM Q42.00008 Nanoparticle Size Dependence of a Polymer's Mechanical Properties[1] , JOSEPH MOLL, Columbia University, SHUSHAN GONG, The Pennsylvania State University, SANAT KUMAR, Columbia University, RALPH COLBY, The Pennsylvania State University — Nanoparticle size critically affects the properties of polymer nanocomposites. We use a silica/poly(2-vinyl) pyridine (P2VP) polymer nanoparticle composite to investigate these effects by varying the nanoparticle sizes from 2nm to a micron. Since silica and P2VP are miscible, we obtain uniform nanoparticle spatial distribution in all cases. Rheology is employed to measure the macroscopic mechanical properties. X-ray photon correlation spectroscopy is used to probe nanoparticle dynamics. We rationalize our search for an optimal nanoparticle size (with regards to composite mechanical properties) by using thermogravimetric analysis to determine particle bound layer thickness as a function of particle size.

[1]NSF DMR-1006659

12:51PM Q42.00009 Preparation and Characterization of Electrospun Poly(Methyl Methacrylate)-QDs NanoComposite Fibers[1] , SUYING WEI, Lamar University, JAYANTHI SAMPATHI, DAN RUTMAN, ASHWINI KUCKNOOR, ZHANHU GUO — In this talk, we describe the simple electrospinning method to fabricate PMMA-CdSe/ZnS Quantum Dots (QDs) nanocomposite fibers followed by property analysis using a variety of techniques. The parameters that affect the electrospinning process including concentration, feed rate, applied voltage and working distance between the needle tip and the fiber collector are investigated and optimized to acquire uniform and defect-free polymer nanocomposite fibers. The surface morphology of the fiber was characterized by scanning electron microscopy, while the fluorescence emission characteristics were analyzed with fluorescence microscopy. In addition, the PMMA-QDs nanocomposite is thermally more stable than the pristine PMMA fibers as determined by the thermal-gravimetric analysis technique. The glass transition temperature and the melting temperature of the polymer are also altered due to the incorporation of QDs. This can be attributed to the interaction between the included QDs and the polymer structure, as disclosed by the surface analysis techniques attenuated total reflectance-infrared spectroscopy (ATR-IR) and X-ray photoelectron spectroscopy (XPS).It showed new vibration bands in the composite fiber in the ATR-IR spectra while the binding energy of both C1s and O1s shifted in their corresponding high-resolution XPS spectra.

[1]the Welch Foundation (V-0004)

1:03PM Q42.00010 Improvement of the dispersion of silica nanoparticles in PMMA[1] , KEREM GOREN, OSMAN B. OKAN, LIMENG CHEN, LINDA S. SCHADLER, RAHMI OZISIK, Rensselaer Polytechnic Institute — Creating well-dispersed polymer nanocomposites is an important part of controlling composite properties. Nanoparticles have been shown to demonstrate quite beneficial electrical and thermo-mechanical properties when they are added to polymers. In the current study, the effects of foaming on de-aggregation of nanoparticles in silica/PMMA nanocomposites are investigated. It was found that the saturation of polymer nanocomposite with supercritical carbon dioxide and subsequent rapid de-pressurization is successful in improving the dispersion of nanoparticles in polymer matrix. In addition, by varying saturation pressure, the degree of dispersion improvement can be controlled. Controlled saturation pressure experiments demonstrated that a decrease in saturation pressure led to decreased improvement of nanoparticle dispersion in polymer matrix. By monitoring the inter-nanoparticle distance using transmission micrographs, a quantitative comparison via radial distribution function (RDF) was constructed for before and after each saturation pressure.

[1]Supported by the NSF (CMMI-0500324).

1:15PM Q42.00011 Dispersion of Magnetic Brushes in Polymer Melts , YANG JIAO, PINAR AKCORA, Stevens Institute of Technology — It is now known that polymer grafted amphiphilic spherical silica nanoparticles can self-assemble into anisotropic nanostructures. In this study, we will show how dipolar interactions can affect the self-assembly mechanism of magnetic nanoparticles in polymer composite melts. Hydrophobic iron oxide nanoparticles of 6nm in size are synthesized and then decorated with poly(styrene) by reversible addition fragmentation chain transfer (RAFT) polymerization at various grafting densities and brush lengths. Dispersion of these magnetic brushes are examined in poly(styrene) matrices in TEM. Structures obtained from the balance of attractive dipolar interactions and repulsive forces between polymer chains are investigated. The influence of grafting densities and grafted chain lengths on the dispersion of magnetic nanoparticles and formation of the "equilibrium" structures will be discussed.

1:27PM Q42.00012 Modeling nanoparticle aggregation in nanocomposites , TANYA CHANTAWANSRI, Army Research Laboratory, LEE TRASK, ERIC COCHRAN, Iowa State University, JAN ANDZELM, Army Research Laboratory — A hybrid self-consistent field theory model (H-SCFT) was utilized to model the morphology of nanocomposities composed of cylinder forming ABA triblock copolymer and large nanoparticles (radius on the order of 10 nm). In this system, the size of the nanoparticles is comparable to the cylindrical domains such that nanoparticle segregation into this otherwise compatible phase would cause a significant loss in conformational entropy. To reduce this loss, the nanoparticles could instead macrophase separate out to form aggregates. To capture this particle aggregation in the H-SCFT model, we incorporated a Lennard-Jones potential into the framework. The incorporation of this interaction into the model can significantly alter the observed phase morphology since aggregation can prevent the nanoparticles from swelling and distorting the compatible block copolymer domain. We will demonstrate how the morphology of this nanocomposite varies as a function nanoparticle volume fraction and functionalization. Results will be compared to experimental findings when available.

1:39PM Q42.00013 Effect of Silicon Dioxide Nanoparticles on the Morphology and Interphase Structure of Electrospun PET Nanofibers[1] , QIAN MA, BIN MAO, PEGGY CEBE, Department of Physics and Astronomy, Tufts University — Poly(ethylene terephthalate), PET, nanofibers containing silicon dioxide nanoparticles were electrospun from solutions in hexafluoro-2-propanol. Various fill fractions of silicon dioxide nanoparticles in PET were used, ranging from 0-2.0% by weight. The morphologies of both the electrospun (ES) nanofibers and the SiO2 powders were investigated by scanning and transmission electron microscopies. The phase structure of the non-woven, nanofibrous composite mats was investigated with differential scanning calorimetry and real-time wide-angle X-ray scattering. The amount of immobilized layer, the rigid amorphous fraction (RAF), was obtained based on measurement of the specific reversing heat capacity for both as-spun amorphous and isothermally crystallized PET/silica nanocomposite fibers. For the first time, existence of rigid amorphous phase in the absence of crystallinity was verified for electrospun nanocomposite fibers, and two locations of the rigid amorphous fraction are proposed. The effect of interaction between the filler and polymer matrix on the mechanical properties of single fiber is also investigated using atomic force microscopy.

[1]This research was supported by the National Science Foundation, through grant DMR-0602473.

1:51PM Q42.00014 Flexible Polymer Nanocomposite Hydrogen Sensors by Solution Processes[1] , HOWARD WANG, YAYONG LIU, LIWEI HUANG, KAIKUN YANG, LIANFENG ZOU, State University of New York, Binghamton, CHEOL PARK, National Institute of Aerospace — Using solution processes such as flow coating and inkjet printing, flexible hydrogen sensors arrays have been fabricated on thin polymer nanocomposite films containing dispersed palladium nanoparticles (Pd-NPs). Composite films were annealed at temperatures from 150 °C to 200 °C to allow Pd-NPs to sinter and form a conductive network. An optimal processing temperature is found to yield the most sensitive sensors due to a good balance between the electrical resistance and connectivity of the Pd-NP network. As-fabricated hydrogen sensors can detect a hydrogen level of ca. 200 ppm or lower with a response time of less than 1 second upon the exposure to hydrogen gas, and a recovery time of *ca*. 5 min upon the removal of hydrogen. The sensitivity, repeatability and linearity of sensor arrays are shown to depend on the processing history, the morphology of sensing films, and the geometry of sensor layout.

[1]NSF CMMI- 0928865 & 0928839

2:03PM Q42.00015 Thermal Properties of PEO-anatase nanocomposites , MIRCEA CHIPARA, The University of Texas Pan American, HE HUANG, University of New Orleans, KAREN LOZANO, The University of Texas Pan American, DAVID HUI, XU HAILAN, University of New Orleans, RAFAEL VILLEGAS, THOMAS MION, The University of Texas Pan American — Polyethylene-oxide (PEO) - anatase composites containing various amounts of anatase ranging between 0 and 20 % wt. have been prepared. The as obtained samples have been investigated by Thermogravimetric Analysis at different heating rates ranging from 5 to 40 K/min. This study was focused on the effect of nanofillers on the activation energy and overall reaction order as well as on the temperature at which the mass loss rate is maxim. The first derivative of the as obtained thermogram has been fitted by using an extended Wigner-Breit-Fano function. The effect of the concentration of anatase nanoparticles on the parameters of the Wigner-Breit-Fano are discussed in detail. Non-isothermal differential scanning calorimetry measurements have been performed in order to determine the effect of anatase nanoparticles on the melting and crystallization of PEO. Isothermal crystallization at various temperatures ranging from 303 to 320 K have been also performed. The study aimed to correlate isothermal crystallization data with non-isothermal results and to determine the effect of anatase nanoparticles on the melting and crystallization of PEO. The crystallization process has been investigated within Avrami and Ozawa approaches.

Wednesday, March 23, 2011 11:15AM - 2:03PM –

Session Q43 DPOLY DBP: Focus Session: Translocation through Nanopores I A306/307

11:15AM Q43.00001 A Coupled-Dynamics Model for Polymer Translocation , TIMO IKONEN, TAPIO ALA-NISSILA, Aalto University School of Science, Finland, ANIKET BHATTACHARYA, University of Central Florida, WOKYUNG SUNG, Pohang University of Science and Technology, South Korea — We study a coarse-grained model of driven translocation of biopolymers, which comprises coupled equations of motion for the translocation coordinate s and the spatial coordinates for the first and the last bead of the translocating chain. We use Langevin dynamics simulations to solve the equations of motion and to study the dynamics of translocation through a nanopore, including the residence time distribution of the individual monomers and the average translocation time. In addition, we consider the time evolution of the spatial coordinates of the first and last bead, which underline the asymmetry of the dynamical chain conformations on the cis and $trans$ sides.

11:27AM Q43.00002 A new approach to polymer translocation , JOHAN DUBBELDAM, Delt University of Technology, VAKHTANG ROSTIASHVILI, Max Planch Institute for Polymer Research, ANDREY MILCHEV, Bulgarian Academy of Sciences, THOMAS VILGIS, Max planck Institute for Polyme Research — Polymer translocation is ubiquitous in nature. It plays a role in phenomena like virus infections and in trafficking of proteins through pores in a cell membrane. Many theoretical models have been developed to explain scaling properties of simple polymer chains through tiny nanopores. This has not resolved the controversies in this field, however. In this paper we employ novel methods to shed light on the results that were obtained using the different models that are in use today. We use, for example fractional Brownian motion to explain the scaling of the variance in the translocation length with time and find good agreement between simulation results and theoretical predictions. An extension of the theory to nanopores with more complex geometries are discussed.

11:39AM Q43.00003 Stepping dsDNA through a solid-state nanopore one basepair at a time[1] , ANTHONY HO, JEFFREY COMER, ALEKSEI AKSIMENTIEV, Department of Physics, University of Illinois at Urbana-Champaign — Solid-state nanopores hold great promise for single-molecule detection and manipulation, including low-cost, high-speed DNA sequencing. In a typical experiment, single molecules of DNA are driven through a nanopore by applying an electric potential difference across the membrane. As DNA passes through the pore, it modulates the ionic current, which potentially can be used to determine the DNA sequence. However, the typical rate of DNA transport in experiment is too high for detection of DNA sequences by ionic current measurement. It has been shown that it is possible to slow and weakly trap dsDNA in solid-state nanopores with diameters smaller than that of dsDNA [Nanotechnology 21:395501]. Using all-atom molecular dynamics simulations, we demonstrate that such pores can be used not only to trap but also to displace dsDNA in discrete steps using nanosecond-long pulses of electric field. Specifically, we have identified the pore geometry and pulse profiles that impel dsDNA by one basepair when the pulse is on and retain dsDNA in the same position when the pulse is off. Such nanopore traps may offer new means for manipulating single molecules in biophysics experiments.

[1]Supported by the NSF through grants DMR-0955959 & PHY-0822613.

11:51AM Q43.00004 Universal and Non-Universal Translocation Dynamics of Coarse-Grained Biopolymers , TAPIO ALA-NISSILA, Aalto University School of Science — I will discuss recent progress on the dynamical scaling of coarse-grained models of (bio)polymers under spontaneous and forced translocation.

12:27PM Q43.00005 DNA translocation through grapheme nanopores , CHRISTOPHER A. MERCHANT, University of Pennsylvania, KEN HEALY, MENI WANUNU, VISHVA RAY, NEIL PETERMAN, JOHN BARTEL, MICHAEL D. FISCHBEIN, KIM VENTA, ZHENGTANG LUO, A.T. CHARLIE JOHNSON, MARIJA DRNDIC — We report on DNA translocations through nanopores created in graphene membranes. Devices consist of nanometer-thick graphene membranes with electron-beam sculpted nanopores. Due to the thin nature of the graphene membranes, we observe larger blocked currents than for traditional solid-state nanopores. Unlike traditional solid-state nanopore materials that are insulating, graphene is an excellent electrical conductor. Use of graphene as a membrane material opens the door to a new class of nanopore devices in which electronic sensing and control are performed directly at the pore.

12:39PM Q43.00006 Characterization of DNA Translocation and Detection in Functionalized Nanopores , YALING LIU, Lehigh University, ABHIJIT RAMACHANDRAN, QINGJIANG GUO — Functionalized nanopores have been used in selective detective of DNA. While the interaction between a bare nanopore and a DNA has been analyzed extensively, little is know for that of a functionalized nanopore. This work focuses on studying the DNA translocation dynamics and mechanism of DNA sequencing in a functionalized nanopore through a coarse-grained molecular dynamics model. Physical properties of chemically modified nanopores, i.e., the effective pore diameter under different bias voltages are characterized. The DNA translocation dynamics under different nanopore coatings and different bias voltages are studied. The simulation results reveal that molecular selective translocation larges lies on the flexibility and orientation of the coating molecules and their interaction with the translocating DNA. This research supports rational designs of DNA transportation- and manipulation-based diagnostic systems.

12:51PM Q43.00007 Direct observation of DNA motions into solid state nanopore under applied electrical potentials on conductive surface , YOSHITAKA HAYASHI, GENKI ANDO, ICHIRO IDUTSU, TOSHIYUKI MITSUI, Aoyamagakuin University — Solid state nanopore is one of emerging methods for rapid single DNA molecule detection because the translocation of the DNA though nanopore produces ionic current changes. One of issues in this method is clogging long DNA molecules. Once DNA molecules clogged, the molecules are rarely removed by varying or switching the polarity of applied bias voltages across the nanopore. We develop a modified nanopore by 50nm Au coating on top of the nanopore surface to be able to remove the clogged DNA molecules during the DNA translocation experiment. Fluorescence microscopy was implemented for observation of stained DNA molecules. The nanopores with diameters near 100 nm can be used initially. DNA translocation rates changes dramatically by tuning the applied electrical potentials on surface higher or lower than the potentials across the nanopore. Furthermore, the Au potentials modifies IV characteristic of the ionic current across the nanopore which is similar to the gate voltages controlling the SD current in FET. We will discuss the influence of surface potential on DNA motion and translocation and clogged DNA molecules. Finally, we will present the recent results of DNA translocation into the SiN-Au-SiO2 nanopore and discuss the effect of applied voltages on Au.

1:03PM Q43.00008 Polymer Translocation through a Nanopore in the Presence of a Viscosity Gradient[1] , HENDRICK W. DE HAAN, GARY W. SLATER, University of Ottawa — Of interest for both biological and technological applications, the translocation of a polymer across a membrane through a nanopore has been studied via simulations under a great variety of conditions. In this work, results will be presented from Langevin Dynamics (LD) simulations of polymer translocation where the viscosity on the cis side of the membrane is different from the viscosity on the $trans$ side - a scenario both applicable to biological instances of translocation and replicable with artificial nanopores. Starting with the polymer halfway through the pore, the establishment of a preferential direction for large viscosity differences is observed. To investigate the origin of this effect, a simple model of the system as a 1D biased random walker in a viscosity gradient is explored by Monte Carlo and LD simulations. Good agreement between the simple model and the full polymer simulations for both the preferential direction and mean first passage time indicate that the effects that a viscosity difference across the membrane may have on translocation arise in the general case of a particle at a viscosity interface.

[1]Funded by NSERC

1:15PM Q43.00009 Ionic Coulomb Blockade in Nanopores[1] , MATT KREMS, MASSIMILIANO DI VENTRA, University of California, San Diego — Understanding the dynamics of ions in nanopores is essential for potential applications in molecule detection, DNA sequencing, and other technologies [1]. We show both analytically and by means of molecular dynamics simulations that ion-ion interactions in nanopores leads to the phenomenon of ionic Coulomb blockade, namely the build-up of ions inside a nanopore with specific capacitance impeding the flow of additional ions due to Coulomb repulsion. This is the classical counterpart of electronic Coulomb blockade in mesoscopic systems. We discuss the analogies and differences with the electronic case as well as experimental situations in which this phenomenon could be detected.

[1] M. Zwolak, M. Di Ventra, Physical Approaches to DNA sequencing and Detection, Rev. Mod. Phys. 80, 141 (2008).

[1]Work supported by NIH.

1:27PM Q43.00010 Modeling polyelectrolyte translocation through protein channels , JYOTI MAHALIK, JING HUA, YANBO WANG, MURUGAPPAN MUTHUKUMAR, University of Massachusetts, Amherst — We will present results from Brownian Dynamics simulations of translocation of polyelectrolyte chains through alpha-hemolysin and MspA protein channels. Comparisons will be made between these two pores in terms of the various characteristics of translocation events. Specifically, we will discuss the distribution functions of blocked ionic current and translocation time. The critical roles played by the charge decorations and the geometries of these two protein pores will be presented. The sequence of the polymer will also be addressed.

1:39PM Q43.00011 Polyelectrolyte translocation through a spherical cavity with tunable charge , ALEXANDER ELISEEV, MURUGAPPAN MUTHUKUMAR, University of Massachusetts, Amherst — We will present theoretical results on the free energy barrier for a translocating polyelectrolyte through a charge-decorated hole from a confining spherical cavity. Our results are based on self-consistent-field theory for the combined system of polyelectrolyte chain, counterions, electrolyte ions, and the dielectric mismatch between the cavity and the enclosing space. The effects of degree of ionization of the polymer and the net charge of the hole on the translocation barrier will be presented.

1:51PM Q43.00012 Polymer translocation facilitated by Chaperones , ANIKET BHATTACHARYA, University of Central Florida, Orlando, TAPIO ALA-NISSILA, Aalto University School of Science, Finland, WOKYUNG SUNG, Pohang University of Science and Technology, South Korea — We study translocation of biopolymers through a nanopore in a membrane facilitated by attractive binding particles (Chaperones) using Langevin dynamics simulation. Specifically we study how the density and attractive strength of these bindings particles affect the chain conformations at the $trans$ side and mean first passage time (MFPT). We also consider model larger chaperone that can bind reversibly on the multiple units of the translocating chain. Finally, we consider translocation of heteropolymers and how a specific sequence affect the translocation process. We discuss relevance of our studies in biological translocation processes.

[1]R. Zandi, D. Reguera, J. Rudnick and W. M. Gelbart, Proc. Natl. Acad. Sci. USA **100** 8649 (2003).
[2]W. Sung and P. J. Park, Phys. Rev. Lett. **77**, 783 (1996).

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q44 DPOLY: Focus Session: Dynamics of Polymers-Phenomena due to Confinement

A309

11:15AM Q44.00001 The effect of pattern dimensions on the thermal decay of polymer patterns created by nanoimprint lithography , KENNETH KEARNS, Saginaw Valley State University, H.W. RO, HEATHER J. PATRICK, THOMAS A. GERMER, CHRISTOPHER SOLES, National Institute of Standards and Technology — Spectroscopic ellipsometry, combined with rigorous coupled wave modeling, is used to characterize the thermal decay of polymeric patterns prepared by nanoimprint lithography. When the residual layer is on the order of 10 nm, the pattern decay kinetics of patterns with a 420 nm periodicity near their glass transition temperatures are nearly an order of magnitude slower than patterns sitting on a thick residual layer. Pattern decay is not observed when the periodicity increased to 800 nm for the 10 nm residual layers. Polystyrene, poly(methyl methacrylate), and poly(4-t-butyl styrene) all show this behavior suggesting that changes in entanglement density are not important. The difference in the radius of curvature for the two different pattern periodicities is the likely origin for the pattern decay. The sensitivity of the technique to thin residual layers and nanoscale patterns is enhanced with an optical cavity of SiO_2 between the polymer and Si substrate. The SiO_2 layer enhances the changes in the ellipsometric parameters alpha and beta, which are related to psi and delta. The model dependent scatterometry data is corroborated by atomic force microscopy.

11:27AM Q44.00002 Capillary levelling as a probe of rheology in polymer thin films[1] , JOSHUA D. MCGRAW, NICK M. JAGO, KARI DALNOKI-VERESS, Department of Physics and Astronomy and the Brockhouse Institute for Materials Research, McMaster University — While measuring the rheology of bulk polymer systems is routine, when the size of a system becomes comparable to the molecular size, flow properties are poorly understood and hard to measure. Here, we present the results of experiments that are easily performed and can probe the rheological properties of polymer films that are mere tens of nanometres in thickness. We prepare glassy bilayer polymer films with height profiles well approximated by a step function. Upon annealing above the glass transition, broadening of the height profiles due to gradients in the Laplace pressure is observed. By validating the technique as a probe of the rheology with a range of molecular weights, we will show that this robust technique can be used to investigate the effects of confinement and interfaces on the rheology of ultrathin polymer films.

[1]Financial support from NSERC of Canada is gratefully acknowledged.

11:39AM Q44.00003 Direct evidence of heterogeneous dynamics within ultrathin polystyrene melt films[1] , TAD KOGA, NAISHENG JIANG, PETER GIN, MAYA ENDOH, Stony Brook University, SURESH NARAYANAN, Argonne National Laboratory, LARRY LURIO, Northern Illinois University, SUNIL SINHA, University of California San Diego — We report heterogeneous dynamics associated with cooperative motions of polymer chains within single polystyrene (PS) films at temperatures far above its glass transition temperature. The technique used was a marker x-ray photon correlation spectroscopy technique using "dilute" gold nanoparticles embedded in PS films in conjunction with resonance-enhanced x-rays scattering which intensifies the probing electrical field in the regions of interest within the films. We found that as the thickness decreased below around 60 nm, the diffusive motions of the markers were significantly suppressed both at the free surface and the center of the film relative to those for the thicker films (>100 nm thickness). It is attributed to the long-range effects on the polymer dynamics induced by an immobile layer at the substrate interface.

[1]This project was partially supported by NSF CAREER AWARD under funding number CMMI-0846267.

11:51AM Q44.00004 Anisotropic Dependence of Capillary Dynamics of Confined Polymer Liquid Films , YELING DAI, OLEG SHPYRKO, Department of Physics, University of California, San Diego, KYLE ALVINE, Pacific Northwest National Lab, SURESH NARAYANAN, ALEC SANDY, Argonne National Lab — We experimentally investigate the effect of highly anisotropic confinement on the capillary dynamics of polymer liquid films. Polystyrene films confined laterally within line-space silicon grating patterns of varying channel width represent a highly anisotropic liquid. The capillary fluctuation modes of such system can be expected to persist along the direction of the channels, while fluctuations perpendicular to the channels are likely to be suppressed. We utilized X-ray Photon Correlation Spectroscopy (XPCS) to access this capillary wave dynamics. In addition to the channel-width dependence of the capillary relaxation times, we also observe the anisotropic dependence of the capillary wave fluctuations on the confined polymer surface. I will discuss how XPCS can access the directional dependence of capillary dynamics and comment on the role played by interfacial pinning in suppressing capillary fluctuations.

12:03PM Q44.00005 Surface Dynamics of Macrocyclic Polystyrene Films , SHIH-FAN WANG, MARK D. FOSTER, Dept. of Polymer Science, The University of Akron, Akron OH 44325-3909, ZHANG JIANG, SURESH NARAYANAN, X-ray Science Division, Argonne National Laboratory, Argonne, IL 60439 — Thermally stimulated fluctuations of the surface of a melt of macrocyclic polymers have been studied for the first time. The surface fluctuations of macrocyclic polystyrene (cPS) of 2k, 7k, 17k, and 37k molecular weight (M) were probed using x-ray photon correlation spectroscopy (XPCS), a recently-developed technique that has already been applied to study surfaces of linear PS melts. The surface fluctuations for the cPS films are slower than those of linear chain analogs for all M. However, the glass transition temperatures (Tg) of the cyclic chains are higher than those of the linear analogs, with the discrepancy decreasing with increasing M. A continuum hydrodynamic theory of thermally stimulated capillary waves with a nonslip boundary condition is adequate to rationalize the behavior of the cPS films. When results from cPS of different M are plotted as a function of T/Tg the data nearly collapse to a single curve, indicating that Tg is a key parameter for the surface dynamics of macrocyclics in the temperature range studied. Acknowledgements: NSF CBET 0730692

12:15PM Q44.00006 Surface dynamics of micellar diblock copolymer films[1] , SANGHOON SONG, WONSUK CHA, HYUNJUNG KIM, Sogang University, ZHANG JIANG, SURESH NARAYANAN, Advanced Photon Source — We studied the structure and surface dynamics of poly(styrene)-b-poly(dimethylsiloxane) (PS-b-PDMS) diblock copolymer films with micellar PDMS surrounded by PS shells. By 'in-situ' high resolution synchrotron x-ray reflectivity and diffuse scattering, we obtained exact thickness, electron density and surface tension. A segregation layer near the top surface was appeared with increasing temperature Surface dynamics were measured as a function of film thickness and temperature by x-ray photon correlation spectroscopy. The best fit to relaxation time constants as a function of in-plane wavevectors were analyzed with a theory based on capillary waves with hydrodynamics with bilayer model Finally the viscosities for the top segregated layer as well as for the bottom layer are obtained at given temperatures

[1]This work was supported by National Research Foundation of Korea (R15-2008-006-01001-0), Seoul Research and Business Development Program (10816), and Sogang University Research Grant (2010).

12:27PM Q44.00007 Polymer Transport Near Rough Surfaces , MOSES BLOOM, Northwestern University, JONATHAN WHITMER, University of Illinois, ERIK LUIJTEN, Northwestern University — The rheology of dilute polymer solutions under confinement is important in biology, medicine, microfluidic device design, synthetic polymer processing, and even geologic porous media. However, the solution's specific interactions with the confining surface are poorly understood. This situation is exacerbated for composite nanoparticles, such as polymer/metallic hybrids. Using multi-particle collision dynamics, we find a rich array of transport regimes depending on small-scale surface roughness and the specific surface/solute interactions. These factors couple to hydrodynamic conditions, including flow strength and confinement geometry in unexpected ways. Our findings may be relevant to transport phenomena in certain rough-walled capillaries, such as the distribution of various nanoconjugates in vivo.

12:39PM Q44.00008 Molecular dynamics simulation study of slip flows over surfaces with periodic and random anisotropic textures , NIKOLAI PRIEZJEV, Michigan State University — The influence of surface patterns on slip flow of a Lennard- Jones fluid is investigated using molecular dynamics simulations. We consider a situation when the typical pattern size is smaller than the channel width. First, anisotropic slip lengths are reported at low shear rates for flows over periodic stripes of different wettability when the shear flow direction is misaligned with respect to the stripe orientation. The results of MD simulations are compared with continuum predictions. Second, in case of random chemical patterning, the slip length depends sensitively on the total area of wetting texture. Finally, we found that at sufficiently high shear rates the slip length is anisotropic even for atomically flat crystalline surfaces; and, in particular, the slip length is enhanced when the shear flow is oriented along the crystallographic axis of the wall lattice. The simulation results indicate that the onset of the nonlinear regime between the slip length and shear rate is determined by the diffusion of fluid monomers within the first layer.

12:51PM Q44.00009 Glass Transition Dynamics and Surface Layer Mobility in Unentangled Polystyrene Films , ZHAOHUI YANG, Boston University, YOSHIHISA FUJII, F.K. LEE, C.H. LAM, DONGDONG PENG, OPHELIA TSUI — Most polymers solidify into a glassy amorphous state, accompanied by a rapid increase in the viscosity when cooled below the glass transition temperature (Tg). There has been an ongoing debate on whether the Tg changes with decreasing polymer film thickness and the origin of the changes. We measured the viscosity of unentangled, short-chain polystyrene (2.4kg/mol) films on silicon at different temperatures and found that the transition temperature for the viscosity decreases with decreasing films thickness, in agreement with the changes in the Tg of the films observed by thermal expansion measurements. By applying the hydrodynamics equations to the films, we are able to explain the data fully by assuming that a highly mobile layer is present within the top 2.3 nm thick region of the films and follows an Arrhenius dynamics while the remaining of the films is bulk-like.

1:03PM Q44.00010 Fingering Instability of Debonding Soft Elastic Adhesives , ELIE RAPHAEL, CNRS ESPCI — We study the crack-front fingering instability of an elastic adhesive tape that is peeled off a solid substrate. Our analysis is based on an energy approach using fracture mechanics and scaling laws and provides simple physical explanations for (i) the fact that the wavelength depends only on the thickness of the adhesive film and (ii) the threshold of the instability, and (iii) additionally estimates the characteristic size of the fingers. The scaling laws for these three observables are in agreement with existing experimental data.

1:39PM Q44.00011 Effect of molecular weight on surface mobility of polystyrene films , DONGDONG PENG, ZHAOHUI YANG, OPHELIA TSUI, Boston University — There have been mounting experimental results showing that a two-layer model is appropriate for describing the dynamics of polymer films. The model postulates that a surface mobile layer exists at the free surface and can modify the dynamics of the entire film. In a recent study, we measured the viscosity of unentangled, short-chain polystyrene (Mw=2.4kg/mol) films supported by silicon at different temperatures including the bulk Tg, and found that the data could be fully explained by assuming a surface mobile layer with a constant thickness exists and sits atop a bulk-like layer. In this talk, I will report the result we obtained by measuring the viscosity of polystyrene films with a wide range of molecular weights from 6.4 to 2316 kg/mol supported by silicon. Our result shows that the same two-layer model is applicable in describing the data if the mobility of the surface layer assumes a molecular weight dependence that differs from either the Rouse or Reptation model.

1:51PM Q44.00012 Scaling of confined and interacting comb polymers , CATHERINE YEH, PHILIP PINCUS, University of California, Santa Barbara — We study the scaling of polymer chains grafted to a line, i.e. a 1-D brush or comb polymer, on a repulsive plane in good solvent using classical molecular dynamics. The grafting density is large enough to cause chain stretching. The confined comb geometry is motivated by intermediate filaments where the unstructured monomer c-termini form annular rings that can be modeled as a confined comb bent into a ring. We find that the scaling of brush size as a function of the number of monomers per chain is the same for a comb with and without confinement by a repulsive plane. We also consider the transition of a line of parallel interacting combs to the planar brush geometry as they are compressed from isolated combs; we present results for the dependence of brush height on the distance between combs.

2:03PM Q44.00013 Geometry and molecular architecture effects in nanobubble inflation measurements , SHANHONG XU, Texas Tech University, SYLVIE CASTAGNET, Laboratoire de Mecanique et Physique des Materiaux, Poitiers, France, GREGORY MCKENNA, Texas Tech University — Confinement effects on the mechanical properties of ultrathin polymer films were investigated by a bubble inflation technique developed in our lab. Prior studies of ultrathin films of poly(vinyl acetate) (PVAc) and linear polystyrene (PS) were performed on circular bubbles of different diameters. Here the creep behaviors of ultrathin films of linear PS were investigated on rectangular bubbles. The modulus of the thin film rectangular bubbles was analyzed by approximation methods. The inflation of rectangular bubbles was simulated by finite element analysis (FEA). The mechanical properties of the thin films with the same thickness for circular and rectangular bubbles are compared and we find that the rubbery plateau compliance is geometry independent. We also investigated the creep behaviors of ultrathin films of 3-arm star PS on circular bubbles. We find the rubbery plateau compliance is molecular architecture independent.

Wednesday, March 23, 2011 11:15AM - 2:15PM –

Session Q45 DAMOP: Non-equilibrium Physics with Cold Quantum Gases II A310

11:15AM Q45.00001 Quenched dynamics in interacting one-dimensional systems: Appearance of current carrying steady states from initial domain wall density profiles[1] , JARRETT LANCASTER, New York University, EMANUEL GULL, Columbia University, ADITI MITRA, New York University — Dynamics arising after an interaction quench in the quantum sine-Gordon model is studied for the case of a system initially prepared in a spatially inhomogeneous domain wall state. The time-evolution of the density, current and equal time correlation functions are studied using the truncated Wigner approximation (TWA) to which quantum corrections are added in order to set the limits on its validity. For weak to moderate strengths of the back-scattering interaction, the domain wall is found to spread out ballistically with the system within the light cone reaching a non-equilibrium steady-state characterized by a net current flow. A steady state current is also found to exist for a quench at the exactly solvable Luther-Emery point. The magnitude of the current decreases with increasing strength of the back-scattering interaction. The two-point correlation function of the variable canonically conjugate to the density reaches a steady state which is spatially oscillating at a wavelength which is inversely related to the current.

[1]This was was supported by NSF-DMR (Award no. 1004589).

11:27AM Q45.00002 Quantum quenches and off-equilibrium dynamical transition in the infinite dimensional Bose Hubbard model , GIULIO BIROLI, BRUNO SCIOLLA, IPhT CEA Saclay — We study the off-equilibrium dynamics of the infinite dimensional Bose Hubbard Model after a quantum quench. The dynamics can be analyzed exactly by mapping it to an effective Newtonian evolution. For integer filling, we find a dynamical transition separating regimes of small and large quantum quenches starting from the superfluid state. This transition is very similar to the one found for the fermionic Hubbard model by mean field approximations.

11:39AM Q45.00003 Optimal control for unitary preparation of many-body states: application to Luttinger liquids[1] , ARMIN RAHMANI, CLAUDIO CHAMON, Boston University — Many-body ground states of local Hamiltonians can be prepared via unitary evolution in cold atomic systems. Given the initial state and a fixed time for the evolution, how close can we get to a desired ground state if we can tune the Hamiltonian in time? Here we study this optimal control problem focusing on Luttinger liquids with tunable interactions. We show that the optimal protocol can be obtained using the simulated annealing method. Rather surprisingly, we find that in the Luttinger liquid case the interaction strength in the optimal protocol can have a *non-monotonic* time-dependence. We find a marked difference in the behavior of the system when the ratio τ/L of the preparation time to the system size exceeds a critical value around 1/8. In this regime, the optimal protocol can prepare the states with almost perfect accuracy. Finally, we argue that the time-scale of the optimal evolution defines a dynamical measure of distance between quantum states.

[1]DOE Grant DE-FG02-06ER46316

11:51AM Q45.00004 Dissipative Transport of Trapped Bose-Einstein Condensates through Disorder , SATYAN BHONGALE, George Mason University, PAATA KAKASHVILI, NORDITA, CARLOS BOLECH, University of Cincinnati, HAN PU, Rice University — After almost half a century since the work of Anderson [Phys. Rev. **109**, 1492 (1958)], at present there is no well established theoretical framework for understanding the dynamics of interacting particles in the presence of disorder. Here, we address this problem for interacting bosons near $T = 0$, a situation that has been realized in trapped atomic experiments with an optical speckle disorder. We develop a theoretical model for understanding the hydrodynamic transport of *finite-size* Bose-Einstein condensates through disorder potentials. The goal has been to set up a simple model that will retain all the richness of the system, yet provide analytic expressions, allowing deeper insight into the physical mechanism. Comparison of our theoretical predictions with the experimental data on large-amplitude dipole oscillations of a condensate in an optical-speckle disorder shows striking agreement. We are able to quantify various dissipative regimes of slow and fast damping. Our calculations provide a clear evidence of reduction in disorder strength due to interactions. The analytic treatment presented here allows us to predict the power law governing the interaction dependance of damping. The corresponding exponents are found to depend sensitively on the dimensionality and are in excellent agreement with experimental observations.

12:03PM Q45.00005 Mesoscopic Transport of Ultracold Atoms in Optical Lattices[1] , MARTIN BRUDERER, WOLFGANG BELZIG, Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — Transport of quantum gases is attracting considerable attention, both on a theoretical and experimental level, in part because ultracold atoms confined to optical lattices can be coherently manipulated and detected on microscopic scales. In particular, substantial technological progress has opened the way for a bottom-up approach to mesoscopic transport in optical lattices, in which case the coherence in certain parts of the system is deliberately destroyed. We show based on a specific setup, namely two incoherent atomic reservoirs connected by a short optical lattice, that mesoscopic phenomena such as, e.g., phonon assisted transport, coherent suppression of tunneling and non-adiabatic quantum pumping can be realized with ultracold atoms. For our analysis in the tight-binding regime we use the non-equilibrium Green's functions formalism extended to include the time dependence of the reservoirs.

[1]Supported by the Swiss National Science Foundation (Project No. PBSKP2/130366).

12:15PM Q45.00006 Detecting Paired and Counterflow superfluidity via dipole ocsillations , ANZI HU, LUDWIG MATHEY, Joint Quantum Institute, University of Maryland and National Institute of Standard and Technology, Gaithersburg, MD 20899, IPPEI DANSHITA, Department of Physics, Faculty of Science, Tokyo University of Science, Shinjuku-ku, Tokyo 162-8601, Japan, CARL WILLIAMS, CHARLES CLARK, Joint Quantum Institute, University of Maryland and National Institute of Standard and Technology, Gaithersburg, MD 20899 — We study the dynamic response of the paired superfluid (PSF) and counterflow superfluid (CFSF) states in a binary mixture of ultra-cold bosonic atoms following an abrupt displacement of the trapping potential. In the PSF and CFSF states, the pairing and anti-pairing orders lead to novel transport properties and distinctive dynamic responses to the abrupt displacement. The findings provide a clear experimental procedure to detect these orders and give an intuitive insight into the dynamics of paired and counterflow superfluidity.

12:27PM Q45.00007 ABSTRACT WITHDRAWN –

12:39PM Q45.00008 Adiabatic Quantum Transport of Bosonic Atoms in Double Well Optical Lattices[1] , YINYIN QIAN, CHUANWEI ZHANG, Department of Physics and Astronomy, Washington State University, Pullman, Washington, 99164 USA — Quantum charge pump, where the amount of pumped charges is controlled precisely through the quantized adiabatic charge transport in periodic crystals, has many important applications in electronics. The quantum pump of cold neutral atoms may play a similar significant role in atomtronics. Neutral atoms can be bosons, and their transport properties can be very different from electrons (fermions). We study the adiabatic quantum transport of bosonic atoms in double well optical lattices where the lattice parameters are adiabatically and periodically tuned. The effects of the interaction between atoms on the transport properties are characterized. In the strong interacting regime, the bosonic atoms behave similarly as fermions with quantized atom transport. In the weak interacting regime, the atom transport depends strongly on the paths in the lattice parameter space and the quantized transport may be destroyed. The effects of harmonic traps and disorder potentials are also studied. The investigation is based on the numerical simulation of the exact quantum dynamics of cold atoms in double well optical lattices using the time evolving block decimation algorithm.

[1]This work is supported by the ARO (W911NF-09-1-0248).

12:51PM Q45.00009 Schwinger-Keldysh approach to the Bose-Hubbard model with time varying hopping[1] , MALCOLM P. KENNETT, Simon Fraser University, DENIS DALIDOVICH, Perimeter Institute; Simon Fraser University — Cold bosonic atoms confined in an optical lattice potential give a realization of the Bose Hubbard model, and it is possible to study the phase transition between a superfluid and a Mott insulator as the depth of the optical lattice is varied. We study the real time dynamics of the Bose Hubbard model at zero and finite temperature in the presence of time-dependent hopping using the Schwinger-Keldysh technique. Using a strong-coupling approach, we determine the effective action in the vicinity of the zero-temperature transition between superfluid and Mott insulating phases. We then study the solutions of the resulting saddle-point dynamical equations as the hopping is varied to sweep across the phase transition from the superfluid to insulating phase.

[1]Supported by NSERC

1:03PM Q45.00010 Optimal loading for a Tonks-Girardeau gas , CLAUDIA DE GRANDI, ANATOLI POLKOVNIKOV, Boston University — We analyze the process of loading a one-dimensional system of hard-core bosons, i.e. a Tonks-Girardeau gas, into a commensurate optical lattice. We consider different loading protocols (e.g. linear, quadratic or sudden ramp in time, or cyclic loading). We discuss possible ways of optimization to minimize the heating and the excitations rate of the system due to the loading process. Combining analytical and numerical methods we analyze the problem under experimentally realistic conditions and we compare the results with earlier scaling predictions.

1:15PM Q45.00011 Weakly interacting bosons in a periodic optical lattice[1] , QINQIN LU, KELLY R. PATTON, DANIEL E. SHEEHY, Louisiana State University — We study an interacting boson gas in a periodic optical potential, with the goal of understanding the properties of such a gas away from the Mott insulating regime at large optical lattice depth. In particular, we analyze the density dependence of the transition temperature as a function of optical lattice depth and the response to a dynamical modulation of the optical lattice.

[1]This work was supported by the Louisiana Board of Regents

1:27PM Q45.00012 Pairsuperfluid in Dynamically Constraint Bose-Hubbard Models , LARS BONNES, University of Stuttgart, STEFAN WESSEL — We consider ultra-cold atoms loaded into a two-dimensional optical lattice with strong three-body losses, i.e. three bosons sharing one lattice site scatter inelastically and dissipate from the system. This process dynamically stabilizes a three-body on-site repulsion in analogy to the quantum Zeno effect. The system studied here is described by a Bose-Hubbard model on a square lattice with on- site attraction. The maximal number of particles per lattice site is restricted to two in order to take the three-body repulsion into account. Field theoretical considerations and numerical simulations using Matrix Product States in one dimension suggest the existence of a dimer superfluid phase for small tunneling rates that is effectively described by the condensation of boson pairs and the absence of an atomic condensate. In this work we explore the ground state and finite-temperature phase diagram for our model using large-scale quantum Monte- Carlo simulations. Our main emphasis is the detection of the dimer superfluid phase and we address the issue of extrapolating our finite-temperature data to the thermodyanmic limit at $T = 0$. Furthermore, we explore the possibility of adding an explicit dimer hopping term that drastically changes the behavior of our system.

1:39PM Q45.00013 Beyond mean-field dynamics in open Bose-Hubbard chains[1] , HOLGER HENNIG, Max Planck Institute for Dynamics and Self-Organization (MPIDS), Goettingen, Germany and Department of Physics, Harvard University, Cambridge (USA), DIRK WITTHAUT, MPIDS, Goettingen, Germany, FRIEDERIKE TRIMBORN, Institute for Theoretical Physics, University of Hannover, Germany, GEORGIOS KORDAS, Institute for Theoretical Physics and Center for Quantum Dynamics, University of Heidelberg, Germany, THEO GEISEL, MPIDS, Goettingen, Germany, SANDRO WIMBERGER, Institute for Theoretical Physics and Center for Quantum Dynamics, University of Heidelberg, Germany — We investigate the effects of phase noise and particle loss on the dynamics of a Bose-Einstein condensate in an optical lattice. Starting from the many-body master equation, we discuss the applicability of generalized mean-field approximations in the presence of dissipation and methods to simulate quantum effects beyond mean-field by including higher-order correlation functions. It is shown that localized particle dissipation leads to surprising dynamics, as it can suppress decay and restore the coherence of a Bose-Einstein condensate. These effects can be applied to engineer coherent structures such as stable discrete breathers and dark solitons.

[1]We acknowledge support by the DFG via Forschergruppe 760 (grant no. WI 3426/3-1), HGSFP (grant no. GSC 129/1) and grant no. WI 3415/1-1.

1:51PM Q45.00014 Strong local-field effect on dynamics of a dilute atomic cloud irradiated by two counterpropagating optical fields: beyond standard optical lattices[1] , GUANGJIONG DONG, JIANG ZHU, WEIPING ZHANG, State Key Laboratory of Precision Spectroscopy, East China Normal University, Dongchuan Rd. 500, Shanghai, 200241, China, MIKHAIL SHNEIDER, MAE Department, Princeton University, NJ 08544 — We study a recent experiment (K. Li et al., Phys. Rev. Lett. 101, 250401 (2008)) on diffracting a Bose-Einstein condensate by two counterpropagating optical fields. Including the local field effect, we explain asymmetric momentum distribution and self-imaging of the BEC in a self-consistent way, and find that the self-imaging is not dependent on the intensity difference of the two optical fields, but on the light-condensate interaction time. We show further that the local field effect leads to deformation of an optical lattice, and thus is essential for getting better quantitative analysis of other current optical lattice experiments of cold atoms. Moreover, intensity imbalance of the two optical fields could be applied as a new means to tailor both cold atom dynamics and optical propagation.

[1]This work was supported by the National Natural Science Foundation of China under Grants Nos. 10588402, 10474055, 10874045 and 11034002, the National Basic Research Program of China (973 Program) under Grant No. 2011CB921604.

2:03PM Q45.00015 Quenched dynamics in a spin-1/2 chain prepared in a sharp domain wall state , LEA SANTOS, Yeshiva University, ADITI MITRA, New York University, EMIL PRODAN, Yeshiva University — Using exact diagonalization and Expokit, we study the time evolution of current, magnetization and correlation functions in an isolated spin-1/2 chain initially prepared in a domain wall state. The domain wall consists of spins pointing up in the first half of the chain and down in the other half. Integrable and nonintegrable regimes are reached by adjusting the parameters of the Hamiltonian, which allows for the comparison of behaviors in both limits. In a chain with nearest- neighbor couplings, chaos is induced by adding on-site disorder or by adding next-nearest-neighbor couplings. The magnitude of the current decreases with interaction for the clean integrable system and for the chaotic disordered case. For the chaotic clean system with next-nearest-neighbor couplings, a non- monotonic behavior in the current is found as the interaction strength is increased.

1:00PM - 1:00PM –
Session S1 APS: Poster Session III (1:00pm - 4:00pm) Hall D

S1.00001 POLYMERS AND SOFT MATTER II –

S1.00002 Scaffolding of peptides using a coarse-grained representation of residues with side chain and backbone nodes[1] , RAS PANDEY, University of Southern Mississippi, BARRY FARMER, Air Force Research Laboratory — Monte Carlo simulations are performed to study scaffolding of peptides (KSL) on a cubic lattice. A residue is represented by three backbone nodes (C-terminal, C-alpha, N-terminal) and a side node connected to the central C-alpha node each connected by fluctuating bond. A peptide is a chain of residues. A solvent constituent is represented by a particle of the same size as that of a node. Peptides and solvent are distributed randomly in the cubic box with concentration C_p and C_w respectively. Each residue interacts with other residues and solvent particles via its side chain with the Lennard-Jones (LJ) potential where a knowledge-based interaction matrix is used for the residue-residue interaction. We examine local and global physical quantities such as mobility and energy of each residue, radial distribution function, and structure factor. We find that the scaffolding of peptides depends on the interaction strength and concentration of the solvent. The structure factor shows multi-scale structure of the aggregates.

[1]This work is supported by the Air Force Research Laboratory.

S1.00003 Ion tunable of rheology of supramolecular metallogels , NIGEL CLARKE, JONATHAN STEED, MARC-OLIVER PIEPENBROCK, Durham University — A bis(pyridylurea) ligand forms metallogels in methanol in the presence of up to 0.5 equiv of copper(II) chloride. The addition of further copper(II) chloride gives an unusual crystalline 4:3 coordination polymer, whereas in the presence of 0.5 equiv of copper(II) nitrate, a 2:1 crystalline coordination polymer arises. The latter represents a possible model for supramolecular gelators and highlights key interactions with counteranions that suggest a means to tune gel properties using anion binding. The influence of chloride and acetate anions on the rheological properties of the copper(II) chloride metallogels are investigated [1]. The rheology of the anion-containing mixtures shows complex behavior with the gel structure evolving over time. We also observe shear-induced gelation [2], where vigorous shaking, rather than sonication, transforms a weak jelly like aggregate into a robust gel, exhibiting clear structural changes within the gel fibres. Reversible anion tuning allows these compounds to as responsive soft materials.

[1] Piepenbrock, M.M.; Clarke, N.; Steed, J.W.; Langmuir, 25, 8451, 2009.
[2] Piepenbrock, M.M.; Clarke, N.; Steed, J.W.; Soft Matter, 6, 3541, 2010.

S1.00004 Amine-sulfonyl hydrogen bonding forms β-strand mimics , JUSTIN BARONE, KATHERINE HARVEY, Virginia Tech — Ethyl vinyl sulfone (EVS)-substituted amino acids have the ability to form β-strand mimics that can then continue to aggregate into larger structures such as sheets. The β-strand forms from a sulfonyl-amine hydrogen bond. Here, we show that EVS-substituted lysine forms β-structures similar to protein β-structures as measured with x-ray diffraction. The β-structures can aggregate into macroscopic sheets with the ability to roll under the influence of the amino acid chirality. Microtubules form from sheets rolling left (L-lysine) or right (D-lysine).

S1.00005 Relationship between Hydrophilicity of PEO-PPO-PEO Copolymers and Their Ability to Protect Liposomes from Peroxidation , JIA-YU WANG, The Univeristy of Chicago, CHI-YUAN CHENG, SONG-I HAN, University of California, Santa Barbara, KA YEE LEE, The University of Chicago, THE UNIVERISTY OF CHICAGO COLLABORATION, UNIVERSITY OF CALIFORNIA, SANTA BARBARA COLLABORATION — It is known that PEO-PPO-PEO triblock copolymers interact with lipid membranes but can have opposing effects on membrane integrity - they can behave either as membrane sealants or as permeabilizers depending on their architecture. To understand the origin of their biomedical functionality, interactions between PEO-PPO-PEO triblock copolymers and biomimetic phospholipid vesicles were investigated by evaluating the effect of hydrophilicity of the triblock copolymers on their ability to protect liposomes from oxidative stress, a stress source used to disrupt lipid vesicles. Our results show that while highly hydrophilic triblock copolymers exhibit no apparent insertion into lipid membranes, they are most effective in protecting liposomes from oxidation, indicating that the protective effect of triblock copolymers comes from their physical adsorption onto, rather than their insertion into the membrane. Gaining a better understanding of polymer-membrane interactions could lead to a better design of polymeric cell membrane sealants.

S1.00006 The effect of ion beam sculpted nanopore size and shape on DNA translocation[1] , RYAN ROLLINGS, University of Arkansas, EDWARD GRAEF, University of Texas at Dallas, DENIS TITA, SANTOSHI NANDIVADA, MOURAD BENEMARA, JIALI LI, University of Arkansas — Solid state nanopore based devices can sense single biomolecules in their native environment. Nanopore thickness plays a crucial role in the signal to noise ratio of current blockades caused by biomolecule translocation and ultimately limits the spatial resolution of the nanopore device when discriminating small features on DNA and protein molecules. Low energy ion beam irradiation can create nanometer size pores in very thin membranes 10-20 nm thick, but to date ion beam sculpted nanopores have shown current blockades smaller than predicted from pores of this thickness. We use electron energy loss spectroscopy and energy filtered transmission electron microscopy to study ion beam sculpted nanopore geometry in detail and determine its effect on conductance blockades and I-V curves. Current blockades from pores thinned by chemical etching and ion beam sputtering will also be presented.

[1]We acknowledge the funding support provided by NHGRI/NIH R21HG00477 and NSF/MRSEC 080054

S1.00007 Detection of SPM tip-attached DNA molecules with solid state nanopores[1] , CHANGBAE HYUN, ZHEXUE LU, BRADLEY LEDDEN, JIALI LI, University of Arkansas — Using an apparatus that combines solid-state nanopores with a scanning probe microscope (SPM), we studied ionic current reduction due to the SPM tip. The experiment was performed at different KCl concentrations, SPM tip probing heights, and several bias voltages. The same experiment was also performed with DNA molecules attached to the SPM tip. The current blockage signal through solid-state nanopores with and without luDNA molecules attached to the SPM tip was analyzed. We also present the current blockage and electrical field profile simulation using finite element analysis software (Multiphysics, COMSOL Inc).

[1]We acknowledge the funding support provided by NHGRI/NIH R21HG00477 and NSF/MRSEC 080054

S1.00008 Micro-phase assembly of active sites in a coarse-grained model of chromatin by Monte Carlo simulation[1] , YANG ZHANG, DIETER HEERMANN, University of Heidelberg, Germany, BARRY FARMER, Air Force Research Laboratory, RAS PANDEY, University of Southern Mississippi — A coarse-grained model is used to study the self-assembly of active sites in a DNA (chromatin) chain. The chromosome is described by a bond-fluctuating chain of two types of nodes A (interacting) and B (non-interacting), distributed randomly with concentration C and $1-C$ respectively. Active nodes interact with a Lennard-Jones (*LJ*) potential and execute their stochastic motion with the Metropolis algorithm. The depth of the *LJ* potential (f), a measure of interaction strength and the concentration (C) of the active sites are varied. A number of local and global physical quantities are studied such as mobility (M_n) profile of each node, their local structural profile, root mean square (RMS) displacement (R), radius of gyration (R_g), and structure factor $S(q)$. We find that the chain segments assemble into microphase of blobs which requires higher concentration of active sites at weaker interaction. These findings are consistent with that of a dynamic loop model of chromatin on global (large) scale but differ at small scales.

[1]This work is supported in part by the Alexander von Humboldt foundation and AFRL.

S1.00009 Single-molecule studies of DNA self-diffusion in entangled linear and circular DNA blends , COLE D. CHAPMAN, UCSD, MICHAEL HARLANDER-LOCKE, University of San Diego, DOUGLAS E. SMITH, UCSD, RAE M. ROBERTSON-ANDERSON, University of San Diego, UCSD PHYSICS TEAM, USD PHYSICS TEAM — Here, we use single-molecule fluorescence and particle-tracking to measure self-diffusion coefficients of single DNA molecules in varying blends of entangled linear and circular DNA. We have previously shown that the self-diffusion of entangled circular and linear DNA differ from each other and are strongly dependent on the topology of the background DNA. This phenomenon can be attributed in part to the tendency of linear polymers to thread their circular counterparts, leading to constraint release, as well as reptation. Previous rheological studies have shown a complex relationship between the ratio of linear to circular polymers and viscosity, however, conflicting results have been reported and the molecular dynamics that lead to this behavior remain unclear. Using single-molecule methods, we can directly measure self-diffusion coefficients for individual DNA molecules within concentrated solutions of linear and circular DNA, and thus determine for both topologies the dependence of self-diffusion on: the ratio of linear and circular species, the overall solution concentration, and the molecular length.

S1.00010 Dual-Function Epi-fluorescence Optical Tweezers to Characterize Single Polymer Interactions in Complex Polymeric Fluids , KENT LEE, USD, COLE D. CHAPMAN, UCSD, RAE M. ROBERTSON-ANDERSON, USD, USD TEAM, UCSD TEAM — Intermolecular interactions within entangled polymeric fluids are highly complex and not well understood. Previously, we investigated these interactions on a single-molecule level by using optical tweezers and fluorescence microscopy to measure interaction forces between DNA molecules and self-diffusion of DNA, respectively. To better characterize these interactions, we have developed an epi-fluorescence optical tweezers which combines an epi-fluorescence microscope with a dual-trap, force-measuring optical tweezers. One of the optical traps is moveable enabling different DNA lengths to be stretched across the two traps. Forces on both traps are measured allowing us to probe the force exerted on a trapped DNA molecule by surrounding entangling DNA. Fluorescence capabilities allow us to directly visualize polymer interactions and dynamics while take force measurements. By fluorescently-labeling either the trapped DNA or a select number of surrounding DNA, we can determine both the conformational changes that the measured force induces on the DNA as well as the various molecular configurations that produce each force. These studies will provide a much needed link between single-molecule dynamics and conformations and intermolecular forces in complex polymeric fluids.

S1.00011 Dynamics of a linear polymer in a microchannel creeping flow[1] , PRASENJIT BOSE, MIRON KAUFMAN, PETRU FODOR, Cleveland State University — An understanding of the dynamics of a polymer in a microchannel could be used to design the technology for high throughput molecular analysis and manipulation. We simulate the motion of a linear polymer advected by a fluid in a rectangular microchannel. We consider the creeping laminar flow, i. e. zero Reynolds number. The model polymer is made up of beads connected by elastic springs. The dynamics of this nonlinear mechanical system is studied as a function of model parameters: the spring equilibrium distance, the mass of a bead, and the spring constant.

[1]This work was supported by the Cleveland State Summer Undergraduate Research Program.

S1.00012 Glassy dynamics in thin layers of polystyrene and polyisoprene[1] , EMMANUEL URANDU MAPESA, MARTIN TRESS, FRIEDRICH KREMER, University of Leipzig — Broadband Dielectric Spectroscopy (BDS), Spectroscopic vis-Ellipsometry (SE), X-Ray Reflectometry (XRR), Alternating (ACC) and Differential Scanning Calorimetry (DSC) are combined to study glassy dynamics and the glass transition temperature in nanometric thin ($\geq$5 nm) layers of polystyrene (PS) having widely varying molecular weights (27,500 to 8,090,000 g/mol). For the dielectric measurements two sample geometries are employed, the common technique (capped) using evaporated electrodes and a recently developed approach (uncapped) taking advantage of highly-insulating silica nanostructures as spacers. *All* applied methods deliver the concurring result that deviations from glassy dynamics and from the glass transition temperature of the bulk never exceed margins of $\pm$3K *independent* of the layer thickness and the molecular weight, indicating that the length scale of interfacial interaction is restricted to less than 5 nm. We also show preliminary BDS results where thin layers of cis-1,4-polyisoprene (PI) are measured in both geometries; there are indications that the confinement-induced mode is absent when the layers are uncapped.

[1]Financial support from DFG (SPP 1369) is gratefully acknowledged.

S1.00013 Dynamics of Silica Particles Grafted with Polymer Brush in Polystyrene Matrix , TAIKI HOSHINO, MORIYA KIKUCHI, JST, ERATO, DAIKI MURAKAMI, JST,ERATO, KOJI MITAMURA, JST, ERATO, YOSHIKO HARADA, JST,ERATO, KIMINORI ITO, YOSHIHITO TANAKA, RIKEN SPring-8 Center, SONO SASAKI, Graduate School of Science and Technology, Kyoto Institute of Technology, MASAKI TAKATA, RIKEN SPring-8 Center, ATSUSHI TAKAHARA, JST, ERATO, Institute for Materials Chemistry and Engineering, Kyushu University — Nanoparticles (NPs) in soft materials near the glass transition temperature sometimes show fast diffusive behavior, called hyperdiffusion. In this study the dynamics of polystyrene (PS)- grafted silica NPs in PS matrix have been investigated by X-ray photon correlation spectroscopy (XPCS). XPCS system was setup at 27-m-long undulator beamline BL19LXU, SPring-8 (Japan). Detectors, a direct-illuminated CCD camera with a pixel size of 20$\times$20 μm^2 and a two-dimensional hybrid pixel array detector PILATUS, whose pixels were covered with a mask with $\sim$50 μm diameter holes for enhancement of the spatial resolution, were located about 3.2 m downstream of the sample. By XPCS measurements, autocorrelation functions, expressed by $g(q,t) = \exp(-2(\Gamma t)^{\beta}) + 1$ were obtained. At much higher temperature than the glass transition of PS matrix, g(q,t) with $\beta \leq 1$ were observed, but at decreased temperature, $beta > 1$ were observed. These behaviors can originate from hyperdiffusion. The detail of the measurements and the results will be presented.

S1.00014 New methods to characterize the confinement effects in epoxy nanocomposites[1] , LIYUN REN, MICHAEL GOODMAN, RAHMI OZISIK, Rensselaer Polytechnic Institute — Properties of epoxy can be improved/controlled via the addition of nanofillers. However, use of nanofillers leads to confinement and interfacial effects and the exact nature of these two effects on the properties are not yet clearly understood. In this study, the glass transition temperature of epoxy nanocomposites was investigated. The changes in the glass transition temperature were analyzed as a function of nanofiller content (confinement) and epoxy-nanofiller interface. In addition to these, the distribution and dispersion of nanoparticles also influences the properties. We applied two different methods to characterize the interparticle distance and compare the dependence of glass transition temperature on the nanofiller content and interparticle spacing. We found that our model provides a new understanding of the effect of interparticle spacing on glass transition phenomenon in polymeric nanocomposites.

[1]This work is supported by a grant from IBM.

S1.00015 Defect structures and coarsening in spherical shells of asymetric block copolymer systems , NICOLÁS GARCÍA, LEOPOLDO R. GÓMEZ, ALDO D. PEZZUTTI, DANIEL A. VEGA, Dep. de Fisica-IFISUR- Universidad Nacional del Sur. Conicet, MARCELO A. VILLAR, Dep. de Ing. Química-PLAPIQUI- Universidad Nacional del Sur. Conicet — We use a Brazovskii model to numerically investigate the defect structures and coarsening process of spherical shells of asymmetric block copolymers. It was found that the configurations of defects are dictated by the ratio between the radius of the spherical shell and the average lattice constant. For small system sizes most configurations of defects are in good agreement with the results for the Thomson problem and simply exhibit 12 well ordered disclinations. As the size of the system increases, in addition to the 12 disclinations the structure of defects is characterized by a varying number of dislocations arranged in grain boundary scars.

S1.00016 Nanoconfinement Effect on Polymerization , MAITRI VADDEY, SINDEE SIMON — Ring-opening metathesis polymerization of endo-dicyclopentadidene (DCPD) with second generation Grubbs catalyst is carried out under nanoscale constraint. Differential scanning calorimetry is used to study the polymerization reaction both in the bulk and in the nanopores of controlled pore glass as a function of heating rate; the Tg of the resulting reaction product is also determined. In 110 nm-diameter pores, DCPD undergoes incomplete polymerization followed by the reverse Diels-Alder reaction to form pentadiene. Decreasing the heating rate shifts both reactions towards lower temperatures but does not avert the side reaction. In the bulk unconfined case, the reverse Diels-Alder reaction only occurs in the absence of catalyst. The glass transition temperature of the nanoconfined polymerization product is 164 $^{\circ}$C, approximately 20 $^{\circ}$C higher than the polymer prepared under bulk conditions. Reaction kinetics in bulk and nanoconfined cases will also be discussed.

S1.00017 Molecular Dynamics Simulations of Grafted Layers of Bottle-Brush Polyelectrolytes[1] , DANIEL RUSSANO, JAN-MICHAEL CARRILLO, ANDREY DOBRYNIN, Department of Physics, University of Connecticut — Using molecular dynamics simulations, we study the effect of the brush grafting density and degree of polymerization of the side chains on conformations of brush layers made of charged bottle-brush macromolecules. The thickness of the brush layer first decreases with increasing brush grafting density; then, it saturates and remains constant in the wide interval of the brush grafting densities. The brush layers consisting of the bottle-brush macromolecules with longer side chains have a larger layer thickness. The elongation of the side chains of the bottle-brush macromolecules decreases with increasing brush grafting density. This contraction of the side chains is due to counterion condensation inside the volume occupied by bottle-brushes. Our simulations showed that counterion condensation is a multiscale process reflecting different symmetries of the bottle-brush layer.

[1]NSF: DMR-1004576

S1.00018 Influence of Ionic Strength on Chain Dimension in Polyelectrolyte Brushes at Aqueous Solution Interface[1] , KOJI MITAMURA, MOTOYASU KOBAYASHI, JST, ERATO & Kyushu Univ., MAYUMI TERADA, JST, ERATO, NORIFUMI L. YAMADA, KEK, ATSUSHI TAKAHARA, JST, ERATO & Kyushu Univ. — Polyelectrolyte brush on a solid surface in water generally has a swollen structure and provides high lubricity on the surface. Previously, we have reported that friction force on a cationic poly(2-(methacryloyloxy)ethyltrimethylammonium chloride) (PMTAC) brush in an aqueous medium increased with NaCl concentration, of which reason was not clear but probably due to a shrinkage of the swollen brush with the addition of salt. In this study, we investigated the salt concentration dependency of the chain dimension in PMTAC brush at the aqueous solution interfaces by neutron reflectometry. We also estimated how polydispersity in molecular weight of the brush influences the chain dimension.

[1]The present work was supported in S-type research project in KEK (2009S08).

S1.00019 Densely grafted brushes of gradient copolymers: an effective Flory-Huggins parameter approach[1] , SERGEY VENEV, IGOR POTEMKIN, Department of Physics, Moscow State University, Moscow 119992, Russian Federation; Department of Polymer Science, University of Ulm, 89069 Ulm,Germany — Manufacturing of gradient copolymers becomes cheaper and easier nowadays. There is a wide spectrum of experimental applications for such polymers. In this work, densely grafted gradient copolymer (monomers distribution function $g(n)$ along the chain is assumed to be a power law) brushes in a selective solvent are considered. Equilibrium thermodynamic properties of the system are investigated within the frames of a simple mean-field approach and an effective Flory-Huggins parameter $\chi_{eff}(n)$ approximation. Constructed profiles for polymer concentration demonstrate non-linear behavior, however the brush thickness varies in direct proportion to the molecular weight of copolymer. Coil-Globule transition properties in such a system are investigated as well.

[1]The financial support of the Ministry of Education and Science (Russian Federation), the Deutsche Forschungsgemeinschaft within SFB 569 is gratefully acknowledged

S1.00020 Fast Lattice Monte Carlo Simulations of Inhomogeneous Polymers , QIANG WANG, Department of Chemical and Biological Engineering, Colorado State University, PENGFEI ZHANG, Institute of Physics, Nankai University, XINGHUA ZHANG, DELIAN YANG, Department of Chemical and Biological Engineering, Colorado State University, BAOHUI LI, Institute of Physics, Nankai University — Fast lattice Monte Carlo (FLMC) simulation with multiple occupancy of lattice sites and Kronecker δ-function interactions gives orders of magnitude faster/better sampling of the configurational space of multi-chain systems than conventional lattice MC simulations with self- and mutual- avoiding walks and nearest-neighbor interactions.[1] It also enables direct comparisons with the corresponding polymer field theories based on the same Hamiltonian (thus without any parameter-fitting) to unambiguously and quantitatively reveal the effects of fluctuations and correlations neglected or treated only approximately in the theories. Here we present our FLMC simulations of inhomogeneous polymeric systems including grafted and confined polymers, as well as the comparisons with lattice self-consistent field theory and Gaussian fluctuation theory to quantitatively reveal the consequences of approximations in these theories.

[1]Q. Wang, **Soft Matter, 5**, 4564 (2009).

S1.00021 Structure and Swelling Behavior of Weak Polyelectrolyte Brushes , CHAITRA DEODHAR, ERICK SOTO-CANTU, University of Tennessee, DAVID UHRIG, JOHN ANKNER, S. MICHAEL KILBEY II, Oak Ridge National Laboratory — In this work we describe the structure and swelling behavior of polyelectrolyte brushes consisting of poly(methacrylic acid) (PMAA) homopolymer brushes and random copolymer brushes made by a surface initiated copolymerization to create poly(MAA-co-2-hydroxyethyl methacrylate) brushes P(MAA-co-HEMA). To create dense polyelectrolyte brushes and alleviate problems with polymerization of the reactive electrolytic form of the monomer MAA, these brushes were made by chemical conversion of neutral, precursor brushes comprised of t-butyl methacrylate (tBMA). Neutron reflectivity (NR) was used to investigate the chemical conversion to "deprotected" form. Insight into the swelling behavior of PtBMA and PMAA brushes was obtained by ellipsometry and neutron reflectometry measurements. The responsive behavior of PMAA-containing brushes in different pH environments is evident from in situ ellipsometry and neutron reflectometry measurements, which in particular show significant sensitivity to the amount of water present in the layer as pH is changed. Current efforts to manipulate responsiveness through copolymerization to make P(MAA-co-HEMA) brushes will also be described.

S1.00022 Molecular dynamics simulations of interactions and friction between bottle-brush layers[1] , DANIEL RUSSANO, JAN-MICHAEL CARRILLO, ANDREY DOBRYNIN, University of Connecticut — Experiments on tethered polyelectrolyte bottle-brush-like macromolecules consisting of glycoproteins display fascinatingly low friction properties of biological tissues such as cartilage. To understand the role of the electrostatic interactions in lubricating properties of brush layers we have performed MD simulations of charged and neutral bottle-brush macromolecules tethered to substrates. In the case of charged bottle-brush layers the compression force per unit area F between two brush layers in salt-free solutions increases with decreasing the distance D between substrates as $F \propto D^{-2}$. A stronger dependence of the compression force F on the surface separation D was observed for neutral bottle-brushes, $F \propto D^{-4.7}$, in the same interval of compression forces. This strong dependence of the compression force F on the distance D is due to excluded volume interactions between monomers belonging to two overlapping bottle-brush layers. The weaker dependence observed in polyelectrolyte bottle-brushes is due to interaction between counterion clouds surrounding the bottle-brush layers. The charged bottle-brush layers have lower friction coefficient than neutral layers at the same interval of the compression and shear forces.

[1]NSF: DMR-1004576

S1.00023 Surface Dynamics of Partially Tethered Polymer Films , JIN KUK LEE, Dept. of Polymer Science, The University of Akron, Akron, OH 44325, BULENT AKGUN, NIST Center for Neutron Research, NIST, Gaithersburg, MD 20899, ZHANG JIANG, SURESH NARAYANAN, X-ray Science Division, Argonne National Laboratory, Argonne, IL 60439, SUSHIL SATIJA, NIST Center for Neutron Research, NIST, Gaithersburg, MD 20899, MARK D. FOSTER, Dept. of Polymer Science, The University of Akron, Akron, OH 44325 — The surface dynamics of "partially tethered" thin films have been studied using X-ray photon correlation spectroscopy (XPCS). Polystyrene (PS) chains have been grafted to substrates with low grafting densities, untethered deuterated PS (dPS) chains spun cast on the tethered chains and the films annealed to create layers containing both tethered and untethered chains. The extent of mixing between the tethered PS and untethered dPS chains has been measured by neutron reflectivity. The relaxation of surface height fluctuations for these films depends on the density of grafting, molecular weight of tethered chains, and extent to which tethered chains extend into the layer. When the tethered chains are able to stretch to the top surface, the relaxation time is slowed most remarkably.

S1.00024 A mechanistic study of a thermo-responsive polymer in a liquid crystal solvent , TIMOTHY BUNNING, MICHAEL MCCONNEY, JENNIFER HURTUBISE, VINCENT TONDIGLIA, TIMOTHY WHITE, Materials and Manufacturing Directorate, Air Force Research Laboratory — Thermo-responsive polymers are highly promising for a variety of applications including tailored drug release, gene delivery, and chromatography. Typical swelling/de-swelling polymer phase transitions involve isotropic liquids and disordered polymers. Here, we present a unique swelling/de-swelling polymer transition involving structured polymers and ordered liquids crystals. The polymers in this study have a degree of order that is imparted by polymerizing in the presence of a liquid crystal. The study focuses on helicoidal structured polymers templated by cholesteric liquid crystals because the optical properties are a simple indicator of the material structure properties. The mechanism of the swelling/de-swelling transition of this unique system were studied with differential scanning calorimetry, polarized optical microscopy, white light interferometery and visible/near-infrared spectroscopy. Differences in the dynamic optical changes with polymer structure are explored.

S1.00025 Formation of Liquid Crystal Elastomer Microparticles , CHANJOONG KIM, HUAN YAN, SOUPTIK MUKHERJEE, PAUL LUCHETTE, PETER PALFFY-MUHORAY, Liquid Crystal Institute and Chemical Physics Interdisciplinary Program, Kent State University, Kent, OH 44242, USA — Liquid crystal elastomer (LCE) combines the properties of rubber elasticity and anisotropic properties of liquid crystalline materials. In particular, LCE has a potential to exhibit interesting properties like electric polarization, ferroelectricity and piezo-electricity. Thin films, fibers and even balloons of LCE using techniques such as spin coating, electro-spinning and in cells have been reported by many groups before. Using microfluidics technique followed by photo-polymerization, we produce uniform spherical LCE microspheres with diameter of 20 - 85 μm. Compression of the LCE microspheres generates a characteristic director configuration. The elastomers may also reveal interesting magnetic and electrical properties due to the intrinsically anisotropic nature of liquid crystalline materials.

S1.00026 Coupling of Smectic Liquid Crystalline Order of iPP to Carbon Nanotube Alignment under Melt-Shear[1] , GEORGI GEORGIEV, Assumption College, ROBERT JUDITH, Tufts University, ERIN GOMBOS, MICHAEL MCINTYRE, Assumption College, PEGGY CEBE, Tufts University, ASSUMPTION/TUFTS TEAM, ASSUMPTION/TUFTS COLLABORATION — Carbon nanotubes (CNTs) exhibit liquid crystalline order and their nematic director couples to the one of low molecular weight liquid crystals. Here we explore the interactions between CNTs and the smectic liquid crystal phase of a polymer and the possibility for a similar coupling in this system. The pure iPP and iPP/CNT films were sheared in the melt state at 200 °C and 1Hz. The sheared samples were analyzed using polarized optical microscopy, Two Dimensional Microscopic Transmission Ellipsometry (2D-MTE) and Two Dimensional Wide Angle X-Ray Scattering (2D-WAXS). During shearing we detected a sudden increase of birefringence at 151 °C in the samples, higher than the iPP crystallization temperature, indicating liquid crystalline ordering. We measured anisotropic 2D-WAXS patterns of the samples that contained CNTs, indicating strong ordering of the crystals. Our results indicate that CNTs couple to the smectic phase of iPP, improve its order upon shearing and the crystals created after the formation of the oriented smectic phase are strongly aligned parallel to the direction of shearing.

[1]Assumption College / NSF

S1.00027 Magnetic fields for the long-range ordering of amphiphilic block copolymers and surfactant mesophases[1]

, PAWEL MAJEWSKI, MANESH GOPINADHAN, CHINEDUM OSUJI, Yale University — We present a diamagnetic interactions-based approach to impose long range order in self-assembled soft materials. We discuss two chemically different systems which have been successfully aligned with the use of a magnetic field. The orientation and the degree of alignment are quantified by small-angle X-ray scattering, polarized optical microscopy and electrical impedance spectroscopy. We focus on Li ion-conducting liquid crystalline diblock copolymers. Our technique allows us to control the orientation of hexagonally packed PEO channels within a non-conducting liquid crystalline matrix that is responsive to the field. The electrical conductivity of the cylindrical samples with PEO domains aligned perpendicular to electrodes is an order of magnitude greater than for samples featuring randomly orientated domains. Our second system consists of non-ionic surfactants forming lamellar or cylindrical mesophase in water. The method which we term "rotational annealing", is successfully used to obtain highly ordered mesophases which can be further utilized as a template for nanomaterials synthesis.

[1]This work is funded by the NSF under DMR-0847534.

S1.00028 Morphology and Proton Conductivity of Ionic Liquid Containing Sulfonated Block Copolymers

, SUNG YEON KIM, MOON JEONG PARK, POSTECH — Proton exchange membrane fuel cells (PEMFC) offer the prospect of supplying clean electrical power for a wide variety of systems such as portable electronic devices and vehicles. Although, significant effort has been devoted to improvement of the transport properties of PEMs which is operated relatively lower temperature below 80°C, it suffers from a CO poisoning at Pt catalysis, complexity of water and heat management in the system. Herein, we report unique block copolymer electrolyte membrane systems containing ionic liquid. Due to the nonvolatile property of ionic liquid the systems exhibit effective proton transport above 100°C without humidification. In present study, sulfonated block copolymers, i.e., poly(styrenesulfonate-b-methylbuthylene) (SnMBm), are utilized for matrix materials by varying the ion contents and molecular weight. Imidazolium based ionic liquids are selectively incorporated into polystyrenesulfonate phases, which results in various morphological transitions as a function of the amount of the ionic liquid. The effect of counter ions on the observed morphologies is significant yielding concurrently different values of conductivity. Small angle x-ray scattering and transmission electron microscopy have been employed to determine various morphologies of the ionic liquid containing sulfonated block copolymer membranes and impedance spectroscopy is used for the conductivity measurements.

S1.00029 The Role of Neutralizing Ion Type on the Dynamics of Sulfonated Polystyrene Ionomers

, ALICIA CASTAGNA, The Pennsylvania State University, WENQIN WANG, KAREN I. WINEY, University of Pennsylvania, JAMES RUNT, The Pennsylvania State University — Sulfonated polystyrene (SPS) ionomers neutralized with Na, Cs, and Zn were investigated using scanning transmission electron microscopy (STEM), X-ray scattering, and dielectric relaxation spectroscopy. The role of the neutralizing ion on the structure and molecular dynamics will be discussed as a function of sulfonation level. STEM and X-ray scattering revealed the presence of spherical aggregates 2 nm in diameter. Successful fitting of the scattering data to the Kinning-Thomas modified hardsphere model provides additional information on aggregate size, number density and radius of closest approach. The dynamics of these materials, as revealed by DRS, are highly sensitive to the neutralizing ion, in particular, the character of the segmental relaxation, i.e. relaxation time, breadth and number of relaxations. Additionally, the relaxation time of the Maxwell-Wagner-Sillars interfacial polarization process at high temperatures is also highly dependent on neutralization and ion character.

S1.00030 Mixed-salts effect on the ionic conductivity of PEO-containing block copolymers

, WEN-SHIUE YOUNG, ALLEN SCHANTZ, THOMAS EPPS, University of Delaware — Salt-doped poly(ethylene oxide)-based block copolymers have attracted significant interest, as nanoscale ordered structures offer ideal platforms for the design of electrolytes for lithium battery membranes. However, the room temperature conductivities of these polymer electrolyte membranes are too low for many applications due to the crystallization of the PEO or the PEO:salt complex. In this study, a mixed-salt system, $LiClO_4$/LiTFSI, was adopted to decrease the crystallinity of PEO:salt complex and improve the relative conductivity at room temperature. Small-angle X-ray scattering and transmission electron microscopy were used to determine the microstructures of the copolymer electrolytes, while differential scanning calorimetry and AC impedance studies were used to examine the crystallinities of PEO:salt complexes and ionic conductivities of electrolyte membranes. Our results show that the 50%-50% $LiClO_4$/LiTFSI-doped PS-PEO with [EO]:[Li]=6:1 has no crystalline phase above room temperature and exhibits a higher conductivity than corresponding $LiClO_4$-doped and LiTFSI-doped PS-PEOs at low temperatures.

S1.00031 Time Scales of Ion Transport in Imidazolium-based Polymers

, U. HYEOK CHOI, Penn State University, YUESHENG YE, Drexel University, MINJAE LEE, HARRY GIBSON, Virginia Polytechnic Institute and State University, YOSSEF ELABD, Drexel University, JAMES RUNT, RALPH COLBY, Penn State University — We synthesize and characterize ionic polymers with imidazolium cations covalently attached to the polymer chain and various ionic liquid counterions for ionic actuators. The imidazolium cations are attached to the polymers with flexible alkyl spacer chains and also have a variety of alkyl and alkyl ether termini. The anionic counterions are also varied; tetrafluoroborate (BF_4), hexafluorophosphate (PF_6) and bis(trifluoromethanesulfonyl)imide (TFSI) were mainly used in this study. Dielectric relaxation spectroscopy (DRS) is utilized to measure the dielectric constant and conductivity, as a function of temperature. The 1953 Macdonald model is applied to estimate the number density of conducting ions and their mobility, from electrode polarization at low frequencies in DRS. The 1988 Dyre model is used to determine ion hopping times from the frequency-dependent conductivity at higher frequencies. The consequence of polymer structural variations will be elucidated for these vital characteristics.

S1.00032 Ionic Aggregation and Microphase Separation in Sulfonated Polyester Multiblock Copolymers and Ionomers

, MICHAEL O'REILLY, University of Pennsylvania, GREGORY TUDRYN, RALPH COLBY, Pennsylvania State University, KAREN WINEY, University of Pennsylvania — Polyethylene oxide (PEO) has been copolymerized with polytetramethylene oxide (PTMO) using a sulfonated phthalate ionic linker between blocks. The product is a linear multiblock copolymer, which is neutralized with lithium and sodium. We used X-ray scattering to investigate the morphology from 25 °C to 200 °C. The results show that this copolymer exhibits three distinct morphology characteristics. First, microphase separation exists between the PEO and PTMO phases. Second, ionic aggregates occur in the PEO microdomains. Finally, the appearance of better defined ionic aggregates occurs in the PTMO microdomains. Ion aggregation and microphase separation are studied as functions of temperature and copolymer molar composition. DRS analysis confirms that ionic aggregation is independent of copolymer composition.

S1.00033 Ion Conduction in Perfectly Aligned Block Copolymer-Ionic Liquid Mixtures

, JAE-HONG CHOI, Department of Materials Science and Engineering, University of Pennsylvania, YOSSEF A. ELABD, Department of Chemical and Biological Engineering, Drexel University, KAREN I. WINEY, Department of Materials Science and Engineering, University of Pennsylvania — Our earlier work to correlate the transport measurements in diblock copolymer-ionic liquid mixtures was limited by our bulk samples that have only partial alignment. Here, thin films with perfect alignment of lamellar microdomains from mixtures of a poly(methyl methacrylate-*b*-styrene) diblock copolymer and an ionic liquid, 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide, have been studied. The morphologies will be characterized by cross-sectional transmission electron microscopy. Ion conduction will be presented within and through the thin film.

S1.00034 Modification of Aqueous Peptide-based Block Copolymer Morphologies through Addition of Ionic Liquid , ASHLEY JOHNSON, JACOB RAY, SANDEEP NAIK, LAURA BULLOCK, DANIEL SAVIN, School of Polymers and High Performance Materials — The self assembly of block copolymers in aqueous solution is a synthetically tunable behavior. Varying composition and the size of the block lengths, a range of morphological structures can be obtained each having diverse characteristics. Polypeptide blocks incorporate pH responsiveness due in part to the helix-coil transition. In these studies, we use light scattering to explore the morphology and pH responsiveness of PPO-P(Lys) diblock and triblock copolymers. While these materials have limited solubility for pH>8, the addition of a small amount of ionic liquid extends the phase range to pH above 10. Similar behavior is observed in Pluronic copolymers, which are solubilized in the presence of ionic liquid. Through use of dynamic light scattering (DLS), transmission electron microscopy (TEM), circular dichroism (CD), and Fourier Transform IR (FTIR), we seek to obtain a molecular-level understanding of the peptide interactions in water/ionic liquid solutions and how this translates to pH responsiveness.

S1.00035 Phase behavior of the blend of rod-coil block copolymer with the corresponding coil homopolymer , CHIA-SHENG LAI, National Tsing Hua University, CHUN-CHIH HO, WEI-FANG SU, National Taiwan University, HSIN-LUNG CHEN, National Tsing Hua University — We investigated the self-assembly behavior of the blends of a rod-coil block copolymer DEH-PPV-*b*-PMMA with the PMMA homopolymers (h-PMMA) with various molecular weights to clarify how the rigidity and self-organization of the rod block would affect the morphologies and the phase behavior comparing with those of coil-coil block copolymer blending. SAXS/WAXS along with TEM were used to reveal the nanostructure in detail. In the case of the blends with h-PMMA with lower molecular weight, the morphology was strongly dependent on the interplay between microphase separation and nematic interaction. The h-PMMA tended to localize into the middle of PMMA nanodomain and formed a lamellar structure irrespective of the volume fraction of h-PMMA. At high volume fraction of h-PMMA, a sponge phase was found to coexist with the lamellar structure. The interdomain spacing increased with the overall PMMA content. Macrophase separations became dominate in the blends with h-PMMA of high molecular weight. WAXS studies of the blends indicated the amorphous h-PMMA reduced the correlation of the rod-rod ordered packing. Upon heating, the lamellar structure transformed into a disordered state, and the T_{ODT} was found to be reduced by adding h-PMMA with lower molecular weight.

S1.00036 Threaded molecular wires as building blocks for advanced polymer blends: WPLEDs, ultra-broadband optical amplifiers, multi color lasers , SERGIO BROVELLI, MARTA MROZ, GIUSEPPE SFORAZZINI, TERSILLA VIRGILI, FRANCO MEINARDI, ALBERTO PALEARI, HARRY L. ANDERSON, GUGLIELMO LANZANI, FRANCO CACIALLI — The ability to produce semiconducting polymer blends with white emission spectra, large emission cross sections and broad optical gain is critical to their application in white PLEDs, lasers and broadband amplifiers. Cyclodextrin-encapsulation is an effective means of suppressing detrimental intermolecular interactions, and energy transfer (ET) channels in polymer blends, thus enabling fabrication of white-PLEDs. We show that all such properties combine into a high impact photonic application: ultra-broad optical gain and two-color lasing in a binary polyrotaxane blend. We study the ultrafast photophysics of a blend of a conventional and an encapsulated polyfluorene. The morphology is investigated by microRaman imaging, AFM, and fluorescence lifetime microscopy. We ascribe the ultra-broad optical gain (>850 meV), and the simultaneous ASE for both constituents, to the dual effect of reduced polaron formation and suppressed ET. Our results demonstrate that polyrotaxanes could realistically represent the building blocks for advanced polymer blends with highly controlled optical properties, for applications in solid state lightning, lasers and photovoltaic technologies.

S1.00037 Measurements of Thermally Stimulated Luminescence in Gamma-Irradiated Ultra-High Molecular Weight Polyethylene in the Presence of Vitamin E[1] , DEREJE ABDI, MUHAMMED JAHAN, BENJAMIN WALTERS, University of Memphis — Thermally stimulated luminescence (TSL) was detected in medical grade ultra-high molecular weight polyethylene (UHMWPE) GUR 1020 (Ticona) after gamma irradiation at room temperature (22°C) in air or nitrogen and subsequent heating from 22°C to 399°C using a commercial TSL apparatus (Thermec). A typical TSL glow curve exhibits two major glow peaks near 116°C and 200°C with a weak shoulder near 250°C. Additional glow peak is observed near 140°C in GUR 1020E (UHMWPE containing 0.1% vitamin E (alpha-tocopherol (α-T)). Full-width-at-half-max (FWHM) and activation energy for each peak were found as follows. 116°C: 40°C, 1.2 eV; 140°C: 40°C, 1.3 eV; 200°C: 64°C, 1.0 eV; 250°C: 56°C, 1.5 eV. The glow peaks seem to follow a kinetic order of 1.5. While the 116-°C glow is produced in all irradiated samples, the 200°- and 250-°C peaks are produced when irradiation is performed in air, suggesting that these latter glow peaks are associated with the oxygen-centered species and the former (at 116°C) with polyethylene (PE) radicals. The 140-°C peak could result from thermal breakdown of vitamin E radical (α-T-O*). Irradiation dose, 30, 65 or 100 kGy, simply changes the TSL intensity without affecting the TSL characteristic. Vitamin E, which is used as an antioxidant, does not seem to affect the TSL in UHMWPE.

[1]NSF Center for Biosurfaces and the University of Memphis.

S1.00038 Confocal Raman Microscopy on in-situ Structural Evolution of Polyolefin Blends[1] , WANSOO CHANG, BYUNGHO JEON, JONG-WON LEE, CHANG Y. RYU, Rensselaer Polytechnic Institute — Polyolefins account for more than half of world-wide consumption of plastic materials, and are typically blended with fillers and other types of polymers in applications. In particular, understanding the miscibility and phase behaviors of polyolefin blends is important for the advancement of a wide array of new applications in medicine, packaging, and other fields. We have used Confocal Raman Microscopy to take the advantages of it capability to locally probe the transformation of physical states in polymeric materials and to characterize morphology of polyolefin blends in-situ for lateral and in-depth imaging with a micron-scale spatial resolution. Upon distinct changes of Raman spectra associated with the melting of semicrystaline polyolefins, we report the in-situ morphological changes upon heating and cooling of polyethylene-polyethylene and polypropylene-polyethylene using confocal Raman microscopy with heating stage.

[1]NSF MRI-0722563

S1.00039 Polymer Blends for Proton Exchange Membranes[1] , TINA LOVATO, National Technical Institute for the Deaf, RIT, KELLY MCNABB, RIT, Mechanical Eng, JASON MEYERS, National Technical Institute for the Deaf, RIT, GABER RUPNIK, Gallaudet, Chemistry, QIAN MA, Tufts, Physics, MENG ZHAO, JINGJING PAN, JOEL WALKER, THOMAS SMITH, RIT, Chemistry, PEGGY CEBE, Tufts, Physics — In the present research, the crystal structure of PVDF in semicrystalline composite films composed of poly(vinylidene fluoride) (PVDF) and poly[4(5)-vinylimidazole/vinylimidazolium trifluoro-methyl-sulfonyl-imide] (PVIm/VIm$^+$ TFSI$^-$) were studied. In these composites, conditions such as choice of solvent, drying conditions, and thermal treatment can affect the crystal phase, crystallite size and degree of crystallinity of PVDF as well as the distribution of the minor component, poly[4(5)-VIm/VIm$^+$ TFSI$^-$]. Such composites may have potential in fuel cells as high-temperature proton-exchange membranes. PVDF imparts mechanical strength to the blend, and because of its high crystal melting point ($T_m > 160^\circ$C), should improve the high temperature stability of resulting fuel cell membranes. The long range goal is to make a thin, high strength membrane that will exhibit substantial proton conductivity at high temperature and low relative humidity. Thin PVDF/PVIm-PVIm$^+$ composite films have been fabricated and the nature of the PVDF crystalline polymorph and % crystallinity have been evaluated as a function of the HTFSI content.

[1]Research was supported by the National Science Foundation, through grant DMR-09-06455

S1.00040 Diffusion Studies of Compatibilizers in Immiscible Polymer Blends , CANDICE HALBERT, JOHN ANKNER, JAMES BROWNING, Oak Ridge National Laboratory, HASKELL BECKHAM, DAVID BUCKNALL, Georgia Institute of Technology — Much is known about how linear polymers and oligomers modify polymer interfaces, and this knowledge forms the basis for some very important commercial processes and products, including impact modifiers and immiscible blend compatibilizers. However, little is known about cyclic polymers at interfaces, despite evidence that indicates that loops are far better at improving interfacial fracture toughness than linear chain entanglements. Generally, polymer films strongly adhere to one another when there is efficient chain interpenetration and entanglement at the interface. When such reinforcement does not exist, as with immiscible polymers, the interfacial fracture toughness is rather weak (< 20 J/m^2), but even in these cases the adhesion strength can be correlated with interfacial entanglements. Neutron reflectivity measurements have been used to correlate the interfacial width of homopolymer interfaces with fracture toughness measurements. We have performed NR experiments to elucidate the interfacial activity of linear versus cyclic poly(oxyethylene). During our experiments at SNS we studied the effect of surface segregation in poly(methyl methacrylate) films as well as the effects of interfacial segregation in PMMA/polystyrene films. The results from these diffusion studies will be presented.

S1.00041 Synthesis of Functional Nanoparticles by Amphiphilic Star-like Block Copolymer as Template , XINCHANG PANG, ZHIQUN LIN, NANOFM TEAM — New strategies for materials fabrication are of fundamental importance in the advancement of science and technology. Organometallic and other organic solution phase synthetic routes have enabled the synthesis of functional inorganic nanoparticles (NPs). However, much research needs to be done to find a simple and unified approach to synthesize nanoparticles with different chemistry and properties. Here we report a novel approach to produce a variety of nanoparticles with different chemistry, properties and controllable diameters, including metallic NPs, ferroelectric NPs, superparamagnetic ion oxide nanoparticle (SPION), semiconducting NPs. These NPs capped with polymer as surface ligand are synthesized using a series of amphiphilic star-like diblock copolymer (forming single component NPs) and triblock copolymer (forming core/shell NPs) as templates.

S1.00042 Low temperature electrical conductivity of low-density polyethylene/carbon black composites , TAREK TAWALBEH, NMSU, SUBHI SAQ'AN, SHADI YASIN, AWWAD ZIHLIF, GIUSEPPE RAGOSTA — The study deals with the electrical characteristics of carbon black/low-density polyethylene (CB/LDPE) composites of various CB filler concentrations (10, 15, and 20% wt.). DC-electrical conductivity was studied as a function of filler concentration in the low temperature range 25–285K. It was found that the composites exhibit a negative temperature coefficient of resistivity (TCR) at low temperatures and a high enhancement in electrical conductivity with both temperature and carbon black concentration. The observed increase of conductivity with the filler concentration was interpreted through percolation theory. The dependence of the electrical conductivity of the given composites on temperature (25–285 K) was analyzed in terms of a formula consistent with the Mott hopping mechanism.

S1.00043 Effect of Grain Size on the AC Electrical Properties of Kaolinite/Polystyrene Composites , LINA ABDALLAH, NMSU, AWWAD ZIHLIF — Impedance spectroscopy has been used to study the effect of kaolinite grain sizes on the AC electrical properties of kaolinite/polystyrene composites under different temperatures and applied frequencies. Impedance measurements were performed on prepared composites containing 20% kaolinite mineral of grain sizes 63, 106, 212, and 300 μm in addition to neat polystyrene. The measured electrical quantities such as impedance, phase angle, dielectric constant and loss, AC conductivity, and thermal activation all showed a temperature and frequency dependence. The dielectric constant and loss increases with both grain size and temperature. The AC conductivity increases with decreasing kaolinite grain sizes. The 63 μm grain size composite has higher electrical conduction under applied frequencies and temperatures. A statistical model is presented to explain the dependence of the AC electrical properties on the filler grain size. The study concludes that the overall electrical behavior is influenced by some processes such as electron hopping, ion diffusion, and space charge polarization that take place in the composite microstructure.

S1.00044 Domain Structure Formation in Swollen Side-Chain Liquid Crystal Elastomers[1] , CHRISTOPHER GRABOWSHI, PAUL LUCHETTE, PETER PALFFY-MUHORAY, Liquid Crystal Institute - KSU — Liquid crystal elastomers (LCEs) are soft materials consisting of a crosslinked polymer network that incorporates mesogenic groups, allowing for orientational order in a solid rubber. Maintaining uniaxial strain on a swollen nematic polymer gel will fix the direction of average orientation of mesogens along the strain axis, yielding a monodomain LCE. Failure to strain the swollen gel within $\sim$30 minutes of formation will produce an opaque polydomain LCE that possesses no long-range nematic order unless stretched. Polarized laser light scattering has been previously employed to monitor the size of liquid crystal domains in fully-formed LCEs; however, no studies have focused on the initial stages of domain formation. We have recorded the time evolution of the far-field scattering patterns produced by swollen polymer gels under varying levels of applied strain. These scattering patterns provide dynamical information of domain behavior during synthesis and processing of monodomain and polydomain LCEs.

[1]This work was supported by the NSF under grant DMR 0606357.

S1.00045 Molecular Alignment and Temperature Effects on Photodriven, Mulitidimensional Oscillation of Azobenzene Liquid Crystalline Polymer Networks[1] , KYUNG MIN LEE, MATTHEW SMITH, HILMAR KOERNER, RICHARD VAIA, TIMOTHY BUNNING, TIMOTHY WHITE, Air Force Research Laboratory — The photodriven oscillation of uniaxially aligned monodomain azo-LCNs was investigated as a function of molecular alignment and temperature spanning a range of +/- 40 of the glass transition temperature (T_g). Monodomain azo-LCNs were synthesized between glass slide cells coated with Elvamide with an anti-parallel rubbing direction. In this work, multidimensional oscillations that include in plane bending and out of plane twisting are observed when the orientation of the axis is at intermediate angles to the long axis of the cantilever. The added dimensionality to the previously reported in plane oscillation is a result of a photoinduced shear gradient that causes twisting. The degree of twisting is shown to be dependent on both the polarization of the illuminating 442 nm light, and the orientation of the director to the cantilever geometry. Comparatively, rubbery azo-LCNs (e.g. systems heated $> T_g$) show higher amplitude than glassy azo-LCN cantilevers. The relationship between the critical laser intensity and the concentration of azobenzene monomer for the photodriven oscillation behavior of azo-LCNs will also be discussed.

[1]Authors acknowledge support from AFRL/RX and AFOSR

S1.00046 The role of uniaxial deformation on microstructure and dynamics of a bulk-polymerized polyurea[1] , JAMES RUNT, TAEYI CHOI, The Pennsylvania State University, DANIEL FRAGIADAKIS, C. MICHAEL ROLAND, Naval Research Laboratory — Polyureas, formed by the rapid reaction between isocyanates and diamines are attractive for various applications due to their outstanding mechanical properties, which can be tuned by varying component chemistry, molecular weight and stoichiometry. Polyureas synthesized from a modified methylene diphenyl diisocyanate (Isonate 143L) and polytetramethylene oxide-di-p-aminobenzoate (Versalink P1000) are widely utilized and investigated for energy absorbing applications such as impact mitigation and ballistic protection. In order to develop a more complete understanding of their mechanical response, we explore the effect of uniaxial strain on the phase separated microstructure and molecular dynamics. We utilize wide- and small-angle X-ray scattering to investigate amorphous segment and hard domain orientation and broadband dielectric spectroscopy for interrogation of the dynamics Uniaxial deformation was found to significantly perturb the phase separated microstructure and chain orientation, and result in a considerable slowing down and broadening of the polyurea soft phase segmental relaxation.

[1]This work is supported by Office of Naval Research

S1.00047 Characterization of a Poly(styrene-block-methylacrylate-random-octadecylacrylate-block-styrene) Shape Memory ABA Triblock Copolymer , PENGZHAN FEI, KEVIN CAVICCHI — A new ABA triblock copolymer of poly(styrene-block- methylacrylate-random-octadecylacrylate-block-styrene) (PS-b- PMA-r-PODA-b-PS) was synthesized by reversible addition fragmentation chain transfer polymerization. The triblock copolymer can generate a three-dimensional, physically crosslinked network by self-assembly, where the glassy PS domains physically crosslink the midblock chains. The side chain crystallization of the polyoctadecylacrylare (PODA) side chain generates a second reversible network enabling shape memory properties. Shape memory tests by uniaxial deformation and recovery of molded dog-bone shape samples demonstrate that shape fixities above 96% and shape recoveries above 98% were obtained for extensional strains up to 300%. An outstanding advantage of this shape memory material is that it can be very easily shaped and remolded by elevating the temperature to 140°C, and after remolding the initial shape memory properties are totally recovered by eliminating the defects introduced by the previous deformation cycling.

S1.00048 Structure and dynamics of of solution polymerized polyureas[1] , TAEYI CHOI, YOUMI JEONG, JAMES RUNT, The Pennsylvania State University — Polyureas consisting of alternating soft and hard (urea containing) segments exhibit physical properties that are closely related to their microphase separated structure, which consist of rigid (high Tg and sometimes crystalline) hard domains embedded in a matrix dominated by flexible polyether segments. Polyurea properties can be controlled over a rather broad range by varying the chemical structures, molecular weight of the components, and reaction stoichiometry. In the present study, we focus primarily on linear polyureas synthesized using methylene diphenyl diisocyanate and polytetramethylene oxide-di-p-aminobenzoate using a solution polymerization method. Soft segment (diamine) molecular weights were varied from 460 to 860 to 1200 g/mol and characterize their morphology, hydrogen bonding, mechanical behavior and dielectric properties upon varying molecular weight of diamines. This presentation will focus on our latest findings, particularly details of the microphase separated morphology and molecular dynamics as measured using dielectric relaxation spectroscopy

[1]This work is supported by Office of Naval Research

S1.00049 The elastic Maier-Saupe-Zwanzig model and some properties of nematic elastomers[1] , DANILO LIARTE, SILVIO SALINAS, CARLOS YOKOI, University of Sao Paulo — We introduce a simple mean-field lattice model to describe the behavior of nematic elastomers. This model combines the Maier-Saupe-Zwanzig approach to liquid crystals and an extension to lattice systems of the Warner-Terentjev theory of elasticity, with the addition of quenched random fields. We use standard techniques of statistical mechanics to obtain analytic solutions for the full range of parameters. Among other results, we show the existence of a stress-strain coexistence curve below a freezing temperature, analogous to the P-V diagram of a simple fluid, with the disorder strength playing the role of temperature. Below a critical value of disorder, the tie lines in this diagram resemble the experimental stress-strain plateau, and may be interpreted as signatures of the characteristic polydomain-monodomain transition. Also, in the monodomain case, we show that random-fields may soften the first-order transition between nematic and isotropic phases, provided the samples are formed in the nematic state.

[1]Financial support of the Brazilian agency CNPq.

S1.00050 The Effect of Multiple Parallel Bonds on the Self-healing of Labile Crosslinked Nanogel Networks , ISAAC G. SALIB, GERMAN V. KOLMAKOV, CHET N. GNEGY, Chemical Engineering Department, University of Pittsburgh, KRZYSZTOF MATYJASZEWSKI, Department of Chemistry, Carnegie Mellon University, ANNA C. BALAZS, Chemical Engineering Department, University of Pittsburgh — We develop a hybrid computational approach to examine the mechanical properties and self-healing behavior of nanogel particles that are crosslinked primarily by highly reactive bonds that can break and readily remake (labile bonds). The individual nanogels are modeled via the lattice spring model (LSM). The crosslinks between the nanogels are simulated via a modified Hierarchical Bell Model (HBM), which allows us to capture both the rupturing and reforming of multiple, parallel bonds due to an applied force. Using our hybrid HBM/LSM, we simulate the behavior of the crosslinked nanogels under a tensile deformation. In these simulations, each labile linkage between the nanogels contains at most N parallel bonds. We reveal that while numerous parallel bonds within a linkage enhance the strength of the material, these bonds diminish the ductility and the ability of the material to undergo the structural rearrangements that are necessary for self-repair.

S1.00051 Characterization of hybrid hydrogel with different shape of particles after gamma-ray radiation , DONGHYUN KIM, HOIK LEE, HYEMI PARK, DAEWON SOHN, Department of Chemistry, Hanyang University, Seoul 133-791, Korea — Due to high specific surface area and the ability to absorb organic molecules, inorganic particles such as silica particle (spherical), imogolite (rodlike), and clay (fan shape) could be used as precursors for hydrogels. The hydrogel which had 3-D network structure was directly prepared by polymerization with acrylic acid (AA) on hydroxide surface of inorganic particles that was irradiated by gamma-ray at ambient condition. Surface of inorganic particles was used as sites of initiator and cross-linker to make hydrogel, so we don't need any additional additives to make hydrogel. The properties of hydrogel were characterized by small angle x-ray scattering (SAXS), universal testing machine (UTM), and Raman spectroscopy. By changing the inorganic particles/monomer ratio, the mechanical strength was significantly changed. The synthesized hydrogel can be elongated maximum 1800%. 2D SAXS pattern was different depending on the shape of inorganic particles. And the hydrogel swelled only in basic solutions at pH $>$ 7.

S1.00052 A State-of-Ease Analysis of Shape Memory Elastomers[1] , CHRISTOPHER LEWIS, JIAHUI LI, MITCHELL ANTHAMATTEN, University of Rochester — A state-of-ease model is developed to predict the time-dependent mechanical behavior of a shape memory elastomer. The model assumes continuous mechanical equilibrium between applied stress and stresses of entropic origin arising from a permanent network and a second, independent network composed of reversible bonds. Bonds forming the reversible network are assumed to rearrange at a constant rate, and newly formed bonds are created in a stress-free state. This gives rise to a time-dependent distribution of bond ages and corresponding stresses, and both are accounted for in the model using a delay integral approach. The model is capable of describing creep, stress relaxation, and shape memory responses. The model will be fit to experimental data for a poly(butyl acrylate) shape memory elastomer, and results will be compared to a simpler dashpot-spring model.

[1]Support provided by the NSF (DMR-0906627).

S1.00053 Real time small angle X-ray scattering from cyclically stretched nanoparticle-filled siloxane elastomers , ARTHUR K. SCHOLZ, University of California, Santa Barbara, CA, HUAN ZHANG, ESPCI Paris Tech, Paris, France, ELAINE R. CHAN, ALEXANDER HEXEMER, Advanced Light Source, Lawrence Berkeley Labs, Berkeley, CA, EDWARD J. KRAMER, University of California, Santa Barbara, CA — The origin of the cyclic softening and hysteresis (the well known "Mullins effect") observed in nanoparticle-filled elastomers is still debated. To probe this question we used synchrotron-based, time resolved, small angle x-ray scattering (SAXS) to observe changes in the structure of silica-filled siloxane elastomers with different filler loading and surface treatments under step cycle tensile deformation. We perform reverse Monte Carlo (RMC) simulations using graphical processing units (GPUs) to infer the real space configuration of the filler network that gives rise to the SAXS pattern and we compute the scattering invariant to quantify any void formation. We observe that the deformation is non-affine on length scales corresponding to the filler particles. The particles collect in "rafts" perpendicular to the tensile axis such that most of the deformation occurs in the elastomer-rich regions between rafts. At the largest deformations a scattering streak appears in a direction normal to the tensile axis at very small diffraction vectors (0.01 nm-1) which we attribute to the formation of elliptical voids whose long axis lies in the tensile direction.

S1.00054 Investigating Heterogeneous Microenvironments in Hydrogels by Single Quantum Dot Tracking , CHEOL HEE LEE, TODD EMRICK, ALFRED CROSBY, RYAN HAYWARD — Single particle tracking provides a powerful means to locally characterize physical properties within heterogeneous media. We have employed CdSe/ZnS core/shell quantum dots (QDs) as probes to characterize the heterogeneous microstructures within covalently- crosslinked polyacrylamide (PAAm) hydrogels. For appropriate gel compositions, the QDs show periods of caged motion within trapping sites, interspersed by nearly free diffusion. We analyze the trajectories of single QDs using a variety of statistical approaches to elucidate the distribution of trapping site strengths within gels of different average pore size.

S1.00055 Effects of AC Electrical Field on the Dielectrophoresis Force of Dielectric Elastomers and Blends , ANUVAT SIRIVAT, RUKSAPONG KUNANURUKSAPONG, The Petroleum and Petrochemical College, Chulalongkorn University — The effects of frequency and amplitude of AC electric field on the deflection and the dielectrophoresis force of an acrylic elastomer (AR71), styrene copolymers (SAR and SBR), and the blends of doped PPP and AR71 are investigated. The dielectrophoresis forces of the dielectric elastomers and blends were measured by using a vertical cantilever fixture at various frequencies (0.3 to 60 Hz) and at AC electric field strengths of 200-800 V_{pp}/mm. The effects of the thicknesses of the specimens and the particle concentration are studied. The doped PPP particles are embedded in the AR71 with concentrations of 1, 10, and 20 %vol. The dielectrophoresis forces and deflection distance of the dielectric elastomers and blends generally increase with increasing amplitude but slightly decrease with increasing frequency; and they dramatically drop at the cut-off frequency. The cut-off frequencies are 7.84, 1.45, and 0.74 Hz for AR71, SAR, and SBR, respectively, at E of 800 V_{pp}/mm and a thickness of 0.7 to 0.8 mm. After blending the AR71 with doped PPP, the cut-off frequencies of the 1 %vol, 10 %vol and 20 %vol of doped PPP are 18.51, 15.28, and 10.67 Hz, respectively, at an E of 800 V_{pp}/mm and a thickness of 0.2 to 0.3 mm. The conductive polymer particles are shown here to improve the electromechanical responses at high frequency.

S1.00056 Effects of Annealing on the Photovoltaic Performance of All-Conjugated Poly(3-alkylthiophene) Diblock Copolymer , MING HE, WEI HAN, YULIANG YANG, FENG QIU, ZHIQUN LIN — The effects of thermal annealing and solvent annealing on the photovoltaic performance of all-conjugated poly(3-butylthiophene)-b-poly(3-hexylthiophene) diblock copolymer, [6,6]-phenyl-C_{71}-butyric acid methyl ester (P3BHT:$PC_{71}BM$) based devices were investigated using the single diode model. Thermal annealing placed a better balance between the crystallization of P3BHT chains and the nanoscale phase separation with $PC_{71}BM$ domains, while solvent annealing under chloroform vapor induced a significant improvement in the crystallinity of P3BHT as well as enlarged P3BHT crystalline domains, thereby leading to unbalanced charge transport and increased charge recombination in the blend films. The physical meanings of the parameters in the equivalent single diode model were also discussed in terms of crystallinity and phase separation to gain the fundamental understanding of the mechanism that account for the annealing effects.

S1.00057 Role of Succinonitrile in a Poly(ethylene oxide)/LiTFSI membrane for lithium batteries , MAURICIO ECHEVERRI, THEIN KYU, Dept. of Polymer Engineering, University of Akron, Akron, Ohio — In designing novel flexible lithium battery membranes, high conductivity, peel strength and processability are the main targets for a successful product. Crystallinity of poly(ethylene oxide) (PEO) and lithium salts represent an obstacle to accomplish each of these specifications. We present a systematic study of ternary phase diagrams of PEO, bis(trifluoromethane) sulfonimide (LiTFSI) and succinonitrile (SCN) (i.e., solid plasticizer/co-solvent) mixtures by using DSC and polarized optical microscopy and map out various coexistence regions bound by the liquidus and solidus lines. The eutectic phase diagram of PEO/SCN system was calculated self-consistently using Flory-Huggins theory in conjunction with Landau-type phase field free energy for crystal solidification. Specific interactions such as hydrogen bonding were examined by FTIR. In lieu of PEO, poly(ethylene glycol) diacrylate (PEGDA) were used to completely eliminate all crystals. Further, photopolymerization of PEGDA affords a solid network containing LiTFSI and SCN that shows promising improvements with a conductivity value of 10^{-4}S/cm at 25°C.

S1.00058 Synthesis and Photovoltaic Properties of a New Class of Donor-Acceptor Alternating Copolymers Containing Pechmann-Dye Derivatives , JAE WOONG JUNG, WON HO JO, Department of Materials Science and Engineering, Seoul National University — Over the last decade, various low bandgap copolymers that exhibit over 5% power conversion efficiency have been developed. However, the synthesis of most low-bandgap polymers is complicated with relatively long synthetic routes and low yield. In this work, a new series of novel alternating copolymers composed of thiophene and Pechmann-dye derivatives were synthesized and used as an electron donor material of bulk heterojunction polymer solar cells. Two Pechmann-dye derivatives, 5,5'-bis-(3-octyl-thiophen-2-yl)-[3,3']bifuranylidene-2,2'-dione and 3,7-bis-(3-octyl-thiophen-2-yl)-pyrano[4,3-c]pyran-1,5-dione which have high molar absorption coefficient, strong electron-deficient core, and planar structure, were easily synthesized via simple three steps with high yield. The use of the Pechmann-dye derivatives as a building block for copolymers results in promising optical, electrochemical, and photophysical properties. Morphology, charge transport, and photovoltaic characteristics of the new copolymers will be discussed.

S1.00059 Nanostructured photovoltaic materials using conjugated block copolymer assemblies

, SARAH E. MASTROIANNI, THOMAS H. EPPS, III, University of Delaware, Chemical Engineering Department — Block copolymers containing a conjugated block offer attractive possibilities for creating nanostructured organic photovoltaic (OPV) devices. Current OPV materials suffer from efficiency losses primarily due to a size-scale discrepancy between exciton diffusion length and domain sizes; excitons that do not reach the interface between electron and hole-conducting materials recombine, preventing charge carrier separation. The inherent nature of block-copolymers to self-assemble into well-defined nanoscale structures with domain spacings on the order of exciton diffusion length offers a potential solution for reducing exciton recombination. In this work, allyl-terminated poly(3-hexyl thiophene) or poly(3-decyl thiophene) acting as electron donors are incorporated into the block copolymer chain via a coupling reaction with poly(styrene) or poly(isoprene-*b*-styrene) derivatives synthesized by anionic polymerization. The resulting block copolymer morphologies are characterized by small angle X-ray scattering and transmission electron microscopy.

S1.00060 Structure-performance analysis of donor/acceptor low band gap polymers: Effect of different acceptors

, LOUIS PEREZ, JAMES ROGERS, KRISTIN SCHMIDT, GUILLERMO BAZAN, EDWARD KRAMER, Materials Department UC-Santa Barbara, MATERIALS DEPARTMENT UC-SANTA BARBARA COLLABORATION — A well established method of designing low band gap polymers for bulk heterojunction solar cells employs what is known as a 'donor-acceptor' (D/A) motif. A D/A polymer is an alternating copolymer consisting of a covalently bound electron deficient unit as an electron acceptor and an electron rich component as an electron donor group. A notable D/A polymer, poly[2,6-(4,4-bis-(2-ethylhexyl)-4H-cyclopenta[2,1-b;3,4-b']-dithiophene)-alt-4,7-(2,1,3-benzothiadiazole)], (PCPDTBT) was the first to achieve device efficiencies over 5%. Device performance is predicted to improve by changing the acceptor to tune the energy level offsets between the polymers and the fullerene derivative to increase the driving force for exciton dissociation and the internal potential, (Voc). If the BT acceptor is changed to benzooxadiazole (BO) the Voc increases, however the current drops significantly, producing devices with efficiencies less than 2%. In order to understand the current drop, GIWAXS, NEXAFS, DSIMS, and TEM have been employed to elucidate structural and composition differences.

S1.00061 PCBM Functionalized Block Copolymer films for Photovoltaic Applications[1]

, ABUL M.A. HUQ, MANISH M. KULKARNI, ALAMGIR KARIM, Department of Polymer Engineering, University of Akron, USA — For efficient charge separation we examine block copolymer thin films as model nanoscale templates that can be utilized for OPV applications. If one can incorporate acceptor and donor in two different blocks, efficient charge separation can be possible. Microphase separation in block-copolymer (BCP) systems, a result of chemical incompatibility of the constituent polymer blocks can be used to control the nanoscale domain sizes. Here, Polystyrene-b-Polyethyleneoxide (PS-PEO) block copolymer, with the PEO being the cylinder forming phase was used because of its robust structural nature to form vertical nanomorphology of cylinders. The acceptor material, PCBM was incorporated into the block-copolymer at different concentration levels up to high levels (∼30%). Both TEM and AFM study showed that PCBM was well dispersed at up to 3:10 (PCBM:PS-PEO) in the block copolymer matrix. This amount is close to percolation threshold of PCBM at which independent donor and acceptor path is expected to be achieved. Further investigations by neutron scattering methods for possible numerous electronic applications including OPV are underway.

[1]Funding from Department of Energy Grant # DE-SC0005364.

S1.00062 Mixing Behavior of a Molecular Acceptor and Polymeric Donors in Organic Solar Cell Blends

, M.A. BRADY, N.D. TREAT, L.A. PEREZ, J.E. COCHRAN, UCSB, M.F. TONEY, Stanford Synchrotron Radiation Lightsource, C.J. HAWKER, M.L. CHABINYC, E.J. KRAMER, UCSB — Organic photovoltaics represent potentially low-cost, solution-processable materials for sustainable energy generation. The concept of a bulk heterojunction relies on the belief that separated domains of donor and acceptor exist to maximize interfacial area for exciton dissociation, while pathways are retained for charge transport to each electrode. Although phase-pure domains are believed to exist due to phase separation of acceptor (PCBM) and donor (P3HT) components, our results suggest otherwise. In this work, the rapid interdiffusion of PCBM and P3HT is investigated using dynamic secondary ion mass spectrometry and grazing-incidence wide angle X-ray scattering, illustrating the significant miscibility of PCBM within P3HT amorphous regions, especially at temperatures (150 °C) at which devices are often annealed to improve performance. The solubility of PCBM in the P3HT-rich phase decreases at lower temperatures. This mixing behavior is contrasted with that of PCBM with PBTTT, a poly(thiophene) of reduced side chain density.

S1.00063 Photophysical Study of Novel Perylene Analogues for Biophysical Applications[1]

, JORGE PALOS-CHÁVEZ, MARK PENICK, GEORGE NEGRETE, LORENZO BRANCALEON — Perylene and perylene derivatives have been shown to be useful in a variety of photoinitiated applications, such as molecular dyes, organic solar cells, etc. Recently we started the characterization of novel 3,9-perylene analogues which could potentially lead to the synthesis of novel molecules with improved ability to separate charges. We have characterized the basic photophysical properties of these molecules, and we are currently investigating the photochemistry that leads to photoproducts in chlorinated compounds. Spectroscopic measurements show the substantial changes in photophysical parameters consistent with the conversion of the original compounds into photoproducts. SEM and AFM imaging show that these photoproducts form ordered particles. Mass spectrometry studies have confirmed the presence of these photoproducts as well. Additional studies are underway concerning the use of these novel perylene analogues in binding to biological structures such as proteins. It is hoped that these compounds will prove useful for biophysical applications, specifically in studying the manipulation of protein conformation via physical methods.

[1]Supported by NIH/NIGMS MBRS RISE GM-60655.

S1.00064 Synthesis and Characterization of Quinoxaline-Based Low-Bandgap Copolymers for Bulk Heterojunction Solar Cells

, YOONKYOO LEE, WON HO JO, Department of Materials Science and Engineering, Seoul National University — A series of low-bandgap alternating copolymers consisting of quinoxaline derivatives and electron-donating carbazole or fluorene were synthesized via the Suzuki coupling reaction. For the purpose to improve the molecular packing of polymer chains and to enhance the charge carrier mobility in the packing direction, a new quinoxaline derivative, 5,8-dithien-2-yl-dibenzophenazine which has perfectly planar polycyclic structure, was synthesized and introduced as a new building block for alternating copolymers instead of frequently-used 5,8-dithien-2-yl-2,3-diphenylquinoxaline. The use of planar quinoxaline derivative exhibited better optical, electrochemical, and structural properties of the resulting copolymers as compared to those of polymers with less planar quinoxaline derivatives. Charge transport and photovoltaic properties of these two classes of copolymers are compared and discussed.

S1.00065 PL enhancement in MEH-PPV stretched films by suppression non-radiative relaxations

, JUI-HUNG HSU, Dept. of Materials & Opt-electronic Science, National Sun Yat-sen University, JONATHON DAVID WHITE, Dept. of Photonics Engineering, Yuan Ze University, ARNOLD C.-M. YANG, Dept. of Materials Science & Engineering, National Tsing-Hua University — Due to the strong electro-phonon coupling, excitation in conjugated polymer is easily relaxed through non-radiative decay channels, and the luminescence yield is lowering. It would be crucial to reduce the non-radiative relaxations for the high performance light-emitting applications. We report the study of stretched MEH-PPV blending films by fluorescence lifetime imaging microscopy. Polymer in the stretched region is fully aligned, and the emission yield is improved by 40%. The improvement is well-agreed with the lifetime studies. Our results indicate that the PL enhancement is due to the suppression of non-radiative relaxations while stretching. Comparing the lifetime imaging and the morphology by AFM, molecular strain distribution is provided. The investigation would be useful in the device application and the basic understanding of electronic excitation relaxation in conjugated polymers.

S1.00066 Classification of Semiconducting Polymeric Mesophases to Optimize Device Post-Processing , CHAD SNYDER, RYAN NIEUWENDAAL, LEE RICHTER, R. JOSEPH KLINE, DEAN DELONGCHAMP, NIST, MARTIN HEENEY, IAIN MCCULLOCH, Imperial College of London — Semiconducting polymers form a variety of phases and mesophases that respond differently to post-deposition solvent or thermal treatments. Here it is shown that classification of these materials into their appropriate mesophases can be a useful tool to optimize their post-deposition treatments. Calorimetry is used to quantify differences between very similar materials, using a well-established framework based on the kinetics and thermodynamics of phase changes. By way of example, this classification scheme is used to identify differences in three polymers, poly(3-hexylthiophene) and two isomeric bithiophene-thiophene copolymers (pBTTT and pATBT). It is demonstrated that poly(3-hexylthiophene) is a conformationally disordered (condis) crystal, and that the two bithiophene copolymers are liquid crystals. The condis state is used to help explain the wide range of reported values for poly(3-hexythiophene), as two separate glass transitions are clearly resolved. The diverse phase structure is notable in light of the molecular similarity of the three polymers, and it has impact on optimum post-processing conditions for maximum electrical performance in thin film transistor devices.

S1.00067 Solution processed organic microarray with inverted structure[1] , PATRICK TOGLIA, JASON LEWIS, EVAN LAFALCE, XIAOMEI JIANG, Department of Physics University of South Florida — We have fabricated inverted organic microarray using a novel solution-based technique. The array consists of 60 small (1 square mm) solar cells on a one inch by one inch glass substrate. The device utilizes photoactive materials such as a blend of poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl-C61-butyric acid methyl ester (PCBM). Manipulation of active layer nanomorphology has been done by choice of solvents and annealing conditions. Detailed analysis of device physics including current voltage characteristics, external quantum efficiency and carrier recombinations will be presented and complimented by AFM images and glazing angle XRD of the active layer under different processing conditions. The procedure described here has the full potential for use in future fabrication of microarrays with single cell as small as 0.01 square mm for application in DC power supplies for electrostatic Microelectromechanical systems (MEMS) devices.

[1]This work was supported by New Energy Technology Inc. and Florida High Tech Corridor Matching Fund (FHT 09-18)

S1.00068 Subpicosecond photonic switching based on bacteriorhodopsin , PAL ORMOS, LASZLO FABIAN, ZSUZSANNA HEINER, Institute of Biophysics, Biological Research Centre, Hung. Acad. Sci., MARK MERO, HAS Research Group of Laser Physics, MIKLOS KISS, Department of Optics and Quantum Electronics, University of Szeged, ELMAR WOLFF, Institute for Applied Biotechnology and System Analysis at the University of Witten/Herdecke, KAROLY OSVAY, Department of Optics and Quantum Electronics, University of Szeged, ANDRAS DER, Institute of Biophysics, Biological Research Centre, Hung. Acad. Sci. — All-optical data processing is the most promising approach for further improvement in data trafficking. We present a subpicosecond photonic switch where the active role is performed by the chromoprotein bacteriorhodopsin. The changes in the refractive index that accompany the steps of the photocycle of bacteriorhodopsin are used for all optical switching in appropriate integrated optical devices. We use grating coupled planar waveguides and the coupling is modulated by the light induced refractive index changes of bacteriorhodopsin. The switching is demonstrated in ultrafast pump-probe experiments. Different transitions of the photocycle are explored for switching applications. We show that by using the bR to I transition subpicosecond switching can be readily achieved. The approach is a basis for protein-based integrated optical devices, eventually leading to a conceptual revolution in telecommunications technologies.

S1.00069 Efficient blue PhOLEDs using host materials of lower triplet energy than the emitter , JAMES SWENSEN, EVGUENI POLIKARPOV, AMBER VONRUDEN, LIANG WANG, ASANGA PADMAPERUMA, Pacific Northwest National Laboratory — It is a commonly held view that the host material for a phosphorescent emitter in an organic light emitting device (OLED) must have a triplet energy higher than that of the phosphorescent emitter in order to obtain high quantum efficiencies. We show that a combination of HTL, ETL and host with appropriate energy levels can provide high external quantum efficiency (EQE), even with a host triplet energy smaller than that of the emitter. Specifically, we report results for a new host material, 4-(di-p-tolylamino)phenyl)diphenylphosphine oxide, with a triplet energy lower than FIrpic that demonstrate improved OLED performance. Our results suggest modified design rules for the development of new, high performance host materials. Molecular design strategies, device design and OLED data will be discussed.

S1.00070 Simulation of DNA Electrophoresis by Coarse-Grained Hybrid Molecular Dynamics Approach[1] , RONG WANG, Department of Polymer Science and Engineering, Nanjing University — Simulation of DNA electrophoresis facilitates the design of DNA separation devices. Various methods have been explored for simulating DNA electrophoresis and other processes using implicit and explicit solvent models. Explicit solvent models are highly desired but their applications may be limited by high computing cost in simulating large number of solvent particles. In this work, a coarse-grained hybrid molecular dynamics (CGH-MD) approach was introduced for simulating DNA electrophoresis in explicit solvent of large number of solvent particles. CGH-MD was further applied to the simulation of DNA electrophoresis in polymer solution and in a well-studied nanofluidic device. Simulation results are consistent with observations and reported simulation results, suggesting that CGH-MD is potentially useful for studying electrophoresis of macromolecules and assemblies in nano-fluidic, micro-fluidic, and microstructure array systems that involve extremely large number of solvent particles, non-uniformly distributed electrostatic interactions, bound and sequestered water molecules.

[1]This work is supported by NNSFC (No. 20874046 and 21074053) and NBRPC(No. 2010CB923303).

S1.00071 Examining Adsorbed Polymer Conformations with Fluorescence Imaging , MARIA PARKES, Student Graduate, MOURAD CHENNAOUI, JANET WONG, TRIBOLOGY GROUP, DEPT. OF MECHANICAL ENGINEERING TEAM — The conformation of adsorbed polymers can have significant impact on their properties such as dynamics and elasticity as well as their ability to take part in reactions with other molecules. Experimental research to determine adsorbed polymer conformation has relied mainly on atomic force microscopy (AFM) studies. During an AFM scan, the contact between the scanning probe and the polymer could affect the polymer conformation, particularly where parts of the polymer might have formed projected loops and tails. In this work, conformations of model polymers are examined with total internal reflection fluorescence microscopy (TIRFM). The advantage of TIRFM over AFM is that TIRFM is a non contact technique. Lambda DNA labelled along its length with fluorescent probes was adsorbed in a projected 2D – 3D state. With TIRFM, the relationship between intensity and depth was used as a basis to determine how the conformation of the adsorbed polymers evolved with time using our custom algorithm.

S1.00072 Study of pluronic F68 molecules on silicon with Atomic Force Microscopy (AFM) , M.J. RETAMAL, U.G. VOLKMANN, Pontificia Univ. Catolica de Chile, V.D. SAMITH, Univ. Andres Bello, Chile — The triblock copolymer pluronic F68 belongs to a class of amphiphilic nonionic surfactants, relevant for applications in medicine, which includes transport of drugs to selective targets in the human body. In the present work, pluronic F68 films have been deposited on Si/SiO2 substrates. Previous to deposition, Si/SiO2 substrates were cleaned in acid and afterwards rinsed with ultra pure water. This cleaning method leaves intact the silicon oxide layer and provides a hydrophilic surface. The aliquots were prepared from aqueous solutions, obtaining different concentrations, which were deposited on the substrates and dried at room temperature. Each of these dispersions is in the range from 0.5 x 10-4 M to 10.0 x 10-4 M. Atomic force microscopy (AFM) shows changes in the morphology of the films, caused by the gradual increase of concentration. These changes occur in a narrow range of concentrations, attributed to the critical micelle concentration (CMC). Supramolecular structures (clusters) coexist at the CMC and above, forming 3D structures such as "dendritics." The percentage of F68 coverage on the substrate depends on the increase in molar concentration. In a "coverage vs. molar concentration" plot we obtain a curve with an inflection point that coincides with the CMC reported for a variety of techniques and conditions.

S1.00073 Hierarchical self-assembly of spider silk-like block copolymers , SREEVIDHYA KRISHNAJI, WEN-WEN HUANG, PEGGY CEBE, DAVID KAPLAN, Tufts University — Block copolymers provide an attractive venue to study well-defined nano-structures that self-assemble to generate functionalized nano- and mesoporous materials. In the present study, a novel family of spider silk-like block copolymers was designed, bioengineered and characterized to study the impact of sequence chemistry, secondary structure and block length on assembled morphology. Genetic variants of native spider dragline silk (major ampullate spidroin I, Nephila clavipes) were used as polymer building blocks. Characterization by FTIR revealed increased ?-sheet content with increasing hydrophobic A blocks; SEM revealed spheres, rod-like structures, bowl-shaped and giant compound micelles. Langmuir Blodgett monolayers were prepared at the air-water interface at different surface pressures and monolayer films analyzed by AFM revealed oblate to prolate structures. Circular micelles, rod-like, densely packed circular structures were observed for HBA6 at increasing surface pressure. Exploiting hierarchical assembly provide a promising approach to rationale designs of protein block copolymer systems, allowing comparison to traditional synthetic systems.

S1.00074 Tunable surface properties from bioinspired polymers , WENDY VAN ZOELEN, ADRIANNE ROSALES, HANNAH MURNEN, University of California, Berkeley, RONALD ZUCKERMANN, Lawrence Berkeley National Laboratory, RACHEL SEGALMAN, University of California, Berkeley — Anti-fouling properties can be derived from patterned or "ambiguous" surfaces displaying multiple surface properties. Biological polymers with precisely controlled chain shapes and self-assembled structures are attractive materials for these applications, in which tunability is of great importance. We have investigated the surface properties of polypeptoids, a class of non-natural biomimetic polymers based on an N-substituted glycine backbone, that combine many of the advantageous properties of bulk polymers with those of synthetically produced proteins. Polypeptoids are of particular interest as they can be made in a sequence controlled fashion with functionalities already known to impart fouling-resistance (ethers, zwitterions, hydrophobicity, and nanoscale patterning). We demonstrate their surface stability and processibility from the standpoint of coating performance and also discuss controlled self-assembly of these materials. Used strategies include mediation of crystallization by incorporating chain defects and specific interactions.

S1.00075 Synthesis and Characterization of Thermally Responsive Polysaccharide Nanoparticles , KRISTA FREEMAN, SEAN SHERIDAN, IMAAN BENMERZOUGA, JOHN MCKENNA, KIRIL STRELETZKY, Cleveland State University — Environmentally-manipulable nanoparticles (microgels) have been synthesized from the amphiphilic polymer hydroxypropyl-cellulose and characterized using dynamic and static light scattering spectroscopies. Careful synthesis studies have revealed dependences of microgel size and structure on polymer molecular weight, polymer concentration, salt concentration, and crosslinker density. An understanding of these dependences has allowed the synthesis of stable, largely spherical, and relatively small (about 100nm) and monodisperse microgels. The synthesized microgels exhibit a volume phase transition between temperatures of 40 and 41C, under which particles undergo a reversible 15-50-fold change in volume. The microgel structure, dynamics, and longevity have been systematically studied by light scattering both below and above the transition temperature.

S1.00076 Uniform Yeast Cell Assembly Based on Microfluidic Microgels , YA-WEN CHANG, PENG HE, Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX, MANUEL MARQUEZ, YNano LLC, 14148 Riverdowns South Dr., Midlothian, Virginia 23113-3796, ZHENGDONG CHENG[1], Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX, SAMANTHA M. MARQUEZ, Maggie L. Walker Governor's School for Government and International Studies, Richmond, VA — We present a novel microgel templated Yeastosome® (Yeast-Celloidosome®) based on self-assembly of yeast cells onto liquid-gel interfaces. To organize living cells onto the surface of the gel particles, strong positive charges were first introduced via LbL (layer by layer) polyelectrolyte decoration on monodisperse agarose microgel templates fabricated with a microfluidic flow focusing device. Native yeasts, bearing negative surface charges can then be driven electrostatically to form a monolayer shell around the gel core. Surface coverage/packing density of the yeast biofilm on varying microgel-to-yeast size ratio assemblies is evaluated with optical microscopy. Mechanical properties of the corresponding shells are characterized with buckling or collapse behavior during drying-hydrating cycle. We demonstrate the capability to fabricate narrow size distribution Yeastosome® with a soft hydrogel core. The combination of microfluidic fabrication with cell assembly offers excellent control over inner core properties and could enable further hierarchy bio-structures.

[1]Material Science and Engineering Program, Texas A&M University, College Station, TX 77832

S1.00077 Clay platelets in a matrix of amino acids (of a clay binding peptide M1) homopolymer: binding, unbinding, dispersion, and self-assembly by a coarse-grained Monte Carlo simulation[1] , BARRY FARMER, LAWRENCE DRUMMY, SHARON JONES, RICHARD VAIA, RAJESH NAIK, Air Force Research Laboratory, HENDRIK HEINZ, University of Akron, RAS PANDEY, University of Southern Mississippi — Monte Carlo simulations are performed to study binding and distribution of a stack of clay platelets in a matrix of homo-polymers of residues. The set of residue monomers is selected from a clay binding peptide $(M1)$[1]. The length of homopolymer is same as that the peptide $M1$. Clay platelet and amino acid polymer (AAP) are described by a bond-fluctuation model[2] where specificity of each residue interaction is incorporated. Each node (of clay platelets and AAP) performs their stochastic motion via Metropolis algorithm subject to steric and excluded volume constraints. We examine the mobility of AAP and platelets and their density profiles. We find that dispersion and binding of each AAP is unique and differ from that of the clay platelets in peptide $M1$ matrix.

[1]This work is supported by the Air Force Research Laboratory.

S1.00078 Diffusion-driven looping provides a consistent framework for chromatin organization , DIETER HEERMANN, MANFRED BOHN, University of Heidelberg — Chromatin looping seems to play a dominant role both in transcriptional regulation as well as in chromatin organization and has been assumed to be mediated by long-range interactions in many polymer models. However, it remains a crucial question which mechanisms are necessary to make two chromatin regions become co-located, i.e. have them in spatial proximity. We demonstrate that the formation of loops can be accomplished solely on the basis of diffusional motion. The probabilistic nature of temporary contacts mimics the effects of proteins, e.g. transcription factors, in the solvent. We establish testable quantitative predictions by deriving scale-independent measures for comparison to experimental data. In this Dynamic Loop (DL) model, the co-localization probability of distant elements is strongly increased compared to linear non-looping chains. The model correctly describes folding into a confined space as well as the experimentally observed cell-to-cell variation. Most importantly, at biological densities, model chromosomes occupy distinct territories showing less inter-chromosomal contacts than linear chains. Thus, dynamic diffusion-based looping, i.e. gene co-localization, provides a consistent framework for chromatin organization in eukaryotic interphase nuclei.

S1.00079 Synthesis of a novel photopolymerized nanocomposite hydrogel for the treatment of acute mechanical damage to cartilage , KATHRYN SCHLICHTING, Department of Materials Science and Engineering, Iowa State University, TRISHELLE COPELAND-JOHNSON, Department of Chemical Engineering, University of South Florida, MATTHEW GOODMAN, Department of Materials Science and Engineering, Iowa State University, ROBERT LIPERT, Institute for Combinatorial Discovery, Iowa State University, TODD MCKINLEY, JAMES MARTIN, Department of Orthopaedic Surgery and Rehabilitation University of Iowa, SURYA MALLAPRAGADA, Department of Chemical and Biological Engineering, Iowa State University, ZHIQUN LIN, Department of Materials Science and Engineering, Iowa State University — Posttraumatic osteoarthritis is caused by a cascade of pathobiologic and pathomechanical events starting with intraarticular fractures in the cartilage. Currently, treatment of fractures is completely focused on restoration of the macroanatomy of the joint. The premise is that restoring the macroanatomy will prevent ongoing stresses and in turn prevent cartilage degeneration. However, current treatment ignores acute mechanical damage sustained by cartilage at the time of injury. This study describes the initial development of a novel nanocomposite photopolymerizing copolymer that has potential to restore local structural integrity to acutely injured cartilage, and subsequently act as a carrier for chondrocyte-enhancing bioactive agents.

S1.00080 Car–Parrinello Molecular Dynamics Study of Base-Catalyzed Hydrolysis Reactions[1] , SUFIAN ALNEMRAT, IGOR VASILIEV, HAOBIN WANG, NMSU — We apply the first principles metadynamics simulation technique implemented in the Car-Parrinello molecular dynamics package to study the base-catalyzed hydrolysis of N-methylacetamide in aqueous solution. Our calculations are carried out in the framework of density functional theory combined with the hybrid BLYP exchange-correlation functional The free energy surfaces and hydrolysis reaction pathways for N-methylacetamide are examined in the presence of a hydroxide ion, and 4, 32, and 64 water molecules. We find that at least 32 water molecules must be explicitly included in metadynamics simulations to accurately describe the mechanism of the hydrolysis reaction of N-Methylacetamide. Our theoretical estimate for the dissociation energy of N-Methylacetamide is in good agreement with the results of previous experimental and theoretical studies.

[1]Supported by LANL-NMSU MOU.

S1.00081 Silica-Based Janus Nanoparticles at the Water-Decane Interface[1] , HENG FAN, ALBERTO STRIOLO, The University of Oklahoma, School of Chemical, Biological and Materials Engineering — It is well known that solid particles adsorb at water-oil interfaces to reduce the contact area between the two immiscible phases. Stable emulsions are obtained when the particles strongly adsorb at the interfaces. We report herein all atom molecular dynamics simulation results for silica-based nanoparticles functionalized with hydrophobic moieties at the decane-water interface. The simulation results are quantified in terms of contact angle at the water-nanoparticle-decane interface, mobility of the nanoparticles, association of multiple nanoparticles at the interface, and free-energy landscapes that dictate the nanoparticle adsorption at the interface. The results are discussed based on the chemical features of the nanoparticle surface. Comparison with experimental data, including but not limited to TEM and cryo-TEM images of water-oil emulsions, are provided.

[1]Research supported by the National Science Foundation.

S1.00082 Synthesis of stable Au-PEG nanocomposite chains in a single step precursor free method and its formation mechanism and Di-electric behavior[1] , RAJESH KUMAR NEOGY, RAJIB NATH, S.N.Bose Centre, GAUTAM BASU, Bose Institute, ARUP KUMAR RAYCHAUDHURI, S.N.Bose Centre — We report a simple and effective one step and one-pot synthesis of stable assembly of Au nanoparticles (diameter 8-10nm) into chains in an Ethylene Glycol medium(MEG), using only a solid metallic Au target and a pulsed excimer laser. No use any external precursor, reducing agent or surfactant so it is a chemistry free synthesis route. The Au-PEG nanocomposite chains (with unbroken lengths often more than few microns) formed in liquid medium are mechanically and thermally stable and can be transferred unchanged into a solid substrate which can span a large surface area. The nanochains show a broad optical absorption near to visible spectrum. Hybrid of Au nanochains and separated nanoparticles can also be formed using a proper choice of the laser fluence and MEG/DI water concentration. The Au-PEG nanocomposite chains in the medium shows enhanced low frequency dielectric constant & electrical conductivity. NMR shows that due to the formation of dimer/trimers of MEG molecules that formed by the ablation process, attach to the Au nanoparticles and facilitate the nanocomposite chain formation.

[1]DST is acknowledged for financial support.

S1.00083 Assembly of carbon nanotube/polymer hybrids at liquid/liquid interface , WENDA WANG, ERIC LAIRD, Graduate Student, CHRISTOPHER LI, Associate Professor — Carbon nanotube (CNT)-templated polymer crystallization has led to controllable patterns on individual CNTs. Previous work has demonstrated that crystalline block copolymers (BCP) can be uniformly patterned on CNTs and the mechanism was attributed to CNT-induced BCP phase separation. Herein, we report that at liquid/liquid interface, CNTs can be bent into nanoscale rings. The structure and morphology of these intriguing CNT rings were investigated using electron microscope and Raman spectroscopy. Furthermore, these CNT rings were used as a template for polymer crystallization. Homopolymer, BCP and gold nanoparticles have been successfully patterned on sub-200 nm CNT rings. These unique hybrids are of great interest in various areas of nanoelectronics and single-electron devices.

S1.00084 Nucleation and Growth of Hydroxyapatite on Hierarchically Ordered Polymer Nanofibers , XI CHEN, BIN DONG, Drexel University, BINGBING WANG, CHRISTOPHER LI, Drexel University — The hierarchically ordered polymer nanofibers, named as nanofiber shish kebabs (NFSKs), were constructed via combination of electrospinning polycaprolactone (PCL) (shish polymer) and controlled crystallization of polycaprolactone-b-poly acrylic acid (PCL-b-PAA) (kebab polymer). These NFSKs were then employed as a template to control the nucleation and growth of hydroxypatite nanocrystals. Electron microscopy and diffraction technique were used to characterize this novel hybrid structure. The growth of minerals starts on the surface of single crystal kebabs and eventually covers the surface of NFSKs. The formation mechanism of hydroxyapatite on NFSKs is of great interest because of the NFSKs' potential application as bone scaffold materials.

S1.00085 Direct nanoparticle assembly in block copolymer based supramolecules containing liquid crystal , MYUNG IM KIM, University of California, Berkeley, CLAYTON E. MAULDIN, JEAN M.J. FRECHET, TING XU, University of California, Berkeley — Block copolymer (BCP)-based supramolecules which combine the nanoscopic assembly of BCPs and molecular ordering can generate hierarchical structure with built-in functionality. Here, we investigated the phase behavior of BCP-based supramolecules containing cholesteric liquid crystal (LC) moieties and achieved directed assembly of nanoparticles. In bulk, we found that BCP-based supramolecules formed a cylinder-in-lamellar structure after solution casting. Upon heating, the order-order transition from cylinder-in-lamella to lamella-in-cylinder was observed. In thin films, supramolecules forming a parallel cylinder-in-lamella structure on silicon substrates were induced by solvent-annealing in chloroform vapor. In addition, we could achieve directed nanoparticle assembly in BCP-based LC supramolecules in bulk and in thin films with control of nanoparticle spatial distribution.

S1.00087 PS-*b*-PDMS Block Copolymer Thin Film: Pattern Formation and Phase Behavior , I-FAN HSIEH, STEPHEN Z.D. CHENG, DEPARTMENT OF POLYMER SCIENCE, THE UNIVERSITY OF AKRON TEAM — Recently, block copolymer thin films attract great attention due to their potential applications in surface nano-lithography. In our work, PS-*b*-PDMS with cylinder morphology is chosen due to extremely large χ value between two blocks. Besides, PS-*b*-PDMS can be transformed into silicon oxide under UV/O_3 exposure and a layer of silicon oxide with the self-assembled block copolymer patterns can be made. By utilizing the PGMEA as solvent, we can easily obtain sphere morphology in cylindrical composition block copolymer by preserved block copolymer solution morphology during film formation. Furthermore, in thermal annealing process, the phase behavior of the PS-*b*-PDMS thin film is strongly affects by molecular weight, film thickness and annealing temperature. In larger-molecular-weight PS-*b*-PDMS, we only observed spherical domains rearrangement and without morphology transition between sphere and cylinder due to high energy barrier, whereas, in the case of smaller-molecular-weight polymer, depending on the film thickness and annealing temperature, its thin film morphology transits between sphere and cylinder alternatively, which is similar to what we found in solvent annealing.

S1.00088 Directing morphology development in Triblock copolymers: A Self-Consistent Field Theory Study , MOUGEH MOHAGHEGHI, BAMIN KHOMAMI, Mrail — Using combinatorial screening method based on self-consistent-field theory for multicomponent polymers, we study ABC block copolymers melt confined between two parallel neutral walls separated by distance L in which the backbone consists of A and B and C is the graft. We analyze the behavior of the system as a function of film thickness. It is shown that confining walls can direct the assembly of thin films of block copolymers. Moreover, by judicious select of film thickness and the position of the graft point, a number of novel morphologies that have not been experimentally realized to date can be created. Overall, These results demonstrate a promising strategy for fabrication of complex nanostructure materials for a variety of important applications such as organic photovoltaic materials.

S1.00089 How Fast Liposomes Diffuse in the Extracellular Matrix , JAMES KUO, BO WANG, SUNG CHUL BAE, STEVE GRANICK, UIUC — Single-particle tracking is used to compare the diffusivity of soft spheres (liposomes) with that of hard spheres of the same size, when they are embedded within gels whose mesh size is smaller than the particle size. The comparison is made in model systems and also in cell extracts of closer biological relevance. In both environments, the diffusivity of liposomes is systematically faster than that of hard spheres.

S1.00090 COMPLEX STRUCTURED MATERIALS III —

S1.00091 Preparation and Magnetic Properties of Co2Z Hexaferrite From Annealed Mixtures of BaM and Co2Y Hexaferrite Precursor Powders , MARC DOYLE, Drexel University, BRIAN KELLY, THOMAS EKIERT, KARL UNRUH, University of Delaware — The transformation of fine mixtures of BaM and Co2Y hexaferrite powders to Co2Z hexaferrite has been studied by scanning electron microscopy (SEM), x-ray diffraction (XRD), and vibrating sample magnetometry (VSM) measurements. The precursor hexaferrites were prepared by a solution-phase auto-combustion method and subsequently mixed in a low energy rolling mill. The BaM/Co2Y mixtures were annealed at temperatures between 800 and 1300 $^\circ$C in air for 2 hours. Over this temperature range a rapid decrease in the measured coercivity from a value of about 4 kOe, characteristic of the hard BaM component of the mixture, to a value of about 50 Oe, characteristic of the magnetically soft Co2Z phase, was observed. The coercivity reduction was accompanied by a modest increase in the saturation magnetization to a value of about 60 emu/g.

S1.00092 A High Energy X-Ray Diffraction Study of the Atomic-Scale Structure of Novel Vitreous Rare Earth Phosphates[1] , ERANDI S. GUNAPALA, G.K. MARASINGHE, Department of Physics and Astrophysics, University of North Dakota, Grand Forks, ND 58202, CHRIS J. BENMORE, Advance Photon Source, Argonne National Laboratory, Argonne, IL 60439 — The magneto-optical properties of rare earth phosphate glasses make them good candidates for numerous potential applications including high-energy/high power ($\sim 10^{15}$ watt) lasers. Because, properties of these materials depend heavily on their atomic structure, a detailed study can facilitate development of additional applications. A series of $(Pr_2O_3)_x(P_2O_5)_{1-x}$ glasses where $0.05 \leq x \leq 0.25$ had been characterized by high energy X-ray diffraction. Coordination parameters for nearest coordination neighbors were obtained by Gaussian fitting. The P-O coordination number, N_{PO}, and the P-O, O-O, P-P distances were found to be insensitive to the Pr_2O_3 content. Coordination numbers N_{PrO} decreased from $\sim$ 8.0 to $\sim$ 7.5 with increasing Pr_2O_3 content from 0.12 to 0.23. Pr-O distance did not seem to vary with Pr_2O_3 content in the x range that we studied.

[1]This research is funded by ND EPSCoR Infrastructure Improvement Program-Doctoral Dissertation Assistantship.

S1.00093 ABSTRACT WITHDRAWN —

S1.00094 Characterizing the Structure and Porosity of Organic Molecules of Intrinsic Microporosity by Molecular Simulations and Experiment[1] , LAUREN J. ABBOTT, AMANDA G. MCDERMOTT, Penn State University, ANNALAURA DEL REGNO, University of Manchester, KADHUM J. MSAYIB, MARIOLINO CARTA, RUPERT TAYLOR, NEIL B. MCKEOWN, Cardiff University, FLOR R. SIPERSTEIN, University of Manchester, JAMES RUNT, CORAY M. COLINA, Penn State University — Organic molecules of intrinsic microporosity (OMIMs) are amorphous, glassy solids that contain interconnected pores of sizes smaller than 2 nm. The philosophy behind OMIMs is similar to that of polymers of intrinsic microporosity (PIMs); rigid, awkwardly shaped molecules frustrate packing and form low density materials with intrinsically porous structures. Atomistic simulations were performed on OMIMs using our recently developed packing and compression procedure to study the effect of structure on packing behavior. The structure and porosity of the simulated samples were characterized, such as by surface areas and structure factors, and compared to experimental results. The presented computational procedure will further understanding of structure-property relationships and aid in the design of novel materials with high surface areas.

[1]Supported by NSF/Materials World Network/EPSRC.

S1.00095 Long-Range Potential Fluctuations in GST Chalcogenide Glasses , RAJEEV GUPTA, Department of Physics and Materials Science Programme, IIT Kanpur, India, CH. BAPANAYYA, Materials Science Programme, IIT Kanpur, India, S.C. AGARWAL, Department of Physics, IIT Kanpur, India — Ge-Sb-Te (GST) alloys are widely used for data recording based on the rapid and reversible amorphous to crystalline phase transformation that is accompanied by an increase in the optical reflectivity and electrical conductivity. However, their application in advanced memory technology is limited by their endurance; $Ge_2Sb_2Te_5$ (GST225) switch has the longest life. Search for more efficient materials has been on, but has not been fully successful so far. This is primarily because one does not know the algorithm to prepare such a material. In this paper, electrical transport properties - electrical conductivity and thermopower of GST alloys are studied and the widths of long-range spatial potential fluctuations present in thin films are estimated. The study shows that amorphous GST225 has the smallest potential fluctuations among all the alloys studied. This finding is correlated to the performance of the phase change materials. The presence of potential fluctuations increases the minimum free energy of the amorphous phase. This deteriorates the switching ability after a few cycles. This suggests that the material with smaller potential fluctuations is likely to be better suited as a switch with a longer life.

S1.00096 Extended X-ray Absorption Fine Structure (EXAFS) Analysis of Novel High Laser Media[1]

ARANWELA HEMANTHA, G.K. MARASINGHE, University of North Dakota, CARLO SEGRE, Illinois Institute of Technology, RICHARD BROW, Missouri University of Science and Technology — Rare earth-doped phosphate glasses are useful for a variety of optical and optoelectronic applications including high energy/high power ($\sim 10^{15}$ watt) Lasers. Binary $(R_2O_3)_x(P_2O_5)_{1-x}$ glasses can be prepared in the compositional range $0 \leq x \leq \sim 0.30$. Atomic-scale structure, especially the coordination environment of R^{3+} ions, play a major role in determining optical/physical characteristics. We have investigated the R^{3+} local environment of Praseodymium and Neodymium ultraphosphate and meta phosphate(REMP) glasses using extended X-ray absorption fine structure technique. For both Nd and Pr phosphate glasses, nearest neighbor (oxygen) coordination decreases with increasing RE concentration. For the first oxygen shell the RE-O distance ranges between 2.38-2.40 Å and 2.39-2.46 Å for Nd and Pr respectively. The second co-ordination shell around the RE ions consists of phosphorus ions, with RE-P distance about 3.4-3.5 Å and co-ordination numbers ranging from 1.5 to 3. There exists an Oxygen shell (third shell) about 4.1 Å from RE ion for both Nd and Pr phosphate glasses.

[1]Support was provided by the NSF (UND) and DoE (Argonne Natl. Lab).

S1.00097 Dynamics of endohedral hydrogen in C_{60}: Infrared study[1]

MIN GE, U. NAGEL, D. HUVONEN, T. ROOM, Nat. Inst. of Chem. Phys. Biophys., Tallinn, Estonia, S. MAMONE, M.H. LEVITT, M. CARRAVETTA, Southampton Uni., UK, Y. MURATA, K. KOMATSU, Kyoto Uni., Japan, J.Y.-C. CHEN, N.J. TURRO, Columbia Uni., NY10027 — Infrared spectra of endohedral hydrogen isotopomers H_2, D_2, and HD were measured in the temperature range from 6 to 300 K. A model of a vibrating rotor in a spherical potential together with the translational motion induced dipole moment theory was used to explain the positions and intensities of IR absorption lines. By measuring spectra of a *para* enriched sample of $H_2@C_{60}$, we confirmed the assignment of lines to *ortho*- and *para*-H_2. Inside C_{60} cage the rotation of hydrogen is unhindered and the translation is quantized and coupled to the rotation. The isotropic and translation-rotation coupling part of the potential are anharmonic and depend on the vibrational states of hydrogen. The analysis of the isotopic effect on the IR transition intensities and interaction potential in the C_{60} cage is presented.

[1]Support by the Estonian Ministry of Education and Research grant SF0690029s0 and SF grants ETF7011, ETF8170 and JD187 is acknowledged.

S1.00098 Interplay between structural and electronic properties of various fullerene derivatives, and their absorption spectra

SORA PARK, JEUNG SUN AHN, YOUNG-KYUN KWON, Kyung Hee University — Using density functional theory (DFT), we investigate the geometrical structures and electronic properties of various fullerene derivatives formed by attaching several kinds of addends on C_{60} through [2+2] cycloaddition. Various forms of such derivatives are modeled by considering different kinds, different positions and different numbers of addends to study how structural configurations will affect their electronic structures. Our results reveal that some derivatives with certain symmetries determined by the configuration of addends may have wider energy gap than that of pristine C_{60}. This suggests that absorption properties could be adjusted by controlling the addends configurations. To describe the excited state properties, such as absorption spectra, of various C_{60} derivatives more accurately, we performed time-dependent (TD) DFT calculations. We find the position and the intensity of the peak of absorption spectra of derivatives are affected by the specific symmetry of the derivatives defined by the configurations of the addends. To explore such peculiar effects, we analyze the charge distribution and orbital mixing characters.

S1.00099 Effective Shear Strain in Helical Rippled Carbon Nanotubes: A Unifying Concept for Understanding Electromechanical Response

TRAIAN DUMITRICA, DONG-BO ZHANG, University of Minnesota — Despite its importance, little is known about how complex deformation modes alter the intrinsic electronic states of carbon nanotubes. Here we consider the rippling deformation mode characterized by helicoidal furrows and ridges and elucidate that a new intralayer strain effect rather than the known bilayer coupling and σ-π orbital mixing effects dominates its gapping. When an effective shear strain is used, it is possible to link both the electrical and the mechanical response of the complex rippled morphology to the known behavior of cylindrical tubes. In combination with objective molecular dynamics, this concept may be useful for understanding the electromechanical characteristics of large scale carbon nanotube assemblies and other individual nanoscale forms of carbon.
Reference: D.-B. Zhang and T. Dumitrică, ACS Nano (2010) DOI: 10.1021/nn1019658.

S1.00100 Spin-dependent Tunneling through a Potential Barrier on a Nanotube

YONATAN ABRANYOS, GODFREY GUMBS, Hunter College at the City University of New York, PAULA FEKETE, United States Military Academy, West Point, New York — The electron spin effects on the surface of a nanotube have been considered through the spin-orbit interaction (SOI), arising from the electron confinement on the surface of the nanotube. This is of the same nature as the Rashba-Bychkov SOI at a semiconductor heterojunction. We estimate the effect of disorder within a potential barrier on the transmission probability. Using a continuum model, we obtained analytic expressions for the spin-split energy bands for electrons on the surface of nanotubes in the presence of SOI. First we calculate analytically the scattering amplitudes from a potential barrier located around the axis of the nanotube into spin-dependent states. The effect of disorder on the scattering process is included phenomenologically and induces a reduction in the transition probability. We analyzed the relative role of SOI and disorder on the transmission probability which depends on the angular and linear momentum of the incoming particle, and its spin orientation. We demonstrated that in the presence of disorder perfect transmission may not be achieved for finite barrier heights.

S1.00101 A First-Principles Study of SiGe Nanotubes[1]

PRABATH WANAGURU, ASOK K. RAY, Department of Physics, University of Texas at Arlington, Arlington, TX 76019 — A systematic study of the electronic structures of three types of SiGe armchair nanotubes from (3, 3) to (11, 11) using periodic boundary conditions has been performed. Geometries of the tubes have been optimized using the hybrid functional B3LYP, the double-zeta LANL2DZ basis set and the GAUSSIAN 03/09 software. Variations of the cohesive energies, band gaps, bond lengths, and Mulliken charges, among others, with the tube diameters will be presented in detail. The cohesive energies of all tubes, in general, increase as the diameters increase and appear to saturate at about 2.98eV for (11, 11) tubes. However, band gaps indicate an oscillatory pattern, with type 2 tubes, in general, with smaller band gaps. Results will be compared with previous results for SiGe tubes using the cluster approximation.[2]

[1]This work is supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525).
[2]S. Rathi and A. K. Ray, Chem. Phys. Lett. 466, 79 (2008).

S1.00102 Gas molecule adsorption on silicene nanoribbons: Conductance modulation and contact effects[1]

TIM OSBORN, AMIR FARAJIAN, Mechanical and Materials Engineering: Wright State University — We investigate the effects of adsorption of gas molecules on the quantum conduction of silicene nanoribbons with and without silver contacts, using ab initio methods and Green's function formalism. The adsorption positions and orientations are determined through energy calculations and structure optimizations for NO_2,CO_2, and CO gas molecules. The conduction change upon gas molecules adsorption is studied for isolated silicene nanoribbons and for silicene nanoribbons on silver side contacts for potential applications as ultrasensitive nanoelectrochemical sensors.

[1]This project is supported by the National Science Foundation grant ECCS-0925939.

S1.00103 A first principles study of the localized electronic states of noble metal atoms doped in Si nanocrystals , CEDRIC L. MAYFIELD, University of Texas at Arlington, M. SAIF ISLAM, University of California-Davis, MOWAFAK M. AL-JASSIM, National Renewable Energy Laboratory, MUHAMMAD N. HUDA, University of Texas at Arlington — The quest for a efficient energy conversion material has necessitated a detail study of semiconductors. Silicon is already playing important roles in many useful nano-applications. To optimize these nano-applications, electronically tailored nano-materials are needed. A number of semiconductor nanomaterials are synthesized using metal as catalysts contributing to various impurities into the nanomaterials. The solubility of a metal in nanomaterials is significantly higher than that in bulk materials. In this presentation, electronic and structural properties of noble metal atoms doping in silicon nano-crystals will be explored using density functional theory. The pristine nanocrystals are based on three different isomers of bulk silicon. We have identified the lower energy isomer and doped it with noble metals. Characterization of the structural changes is accomplished by studying the bonding near the impurity as a function of dopant site. Furthermore, energetic of these nano-structures, both doped and un-doped, such as binding energies, formation energies, and HOMO LUMO gaps will be compared along with their charge densities to identify localizations with respect to impurity site. Magnetism and surface terminations will also be addressed.

S1.00105 Anisotropic Electrical Properties of Nanostructured Metallic Thin Films , MO AHOUJJA, Physics Departrment, University of Dayton, Dayton, OH, PIYUSH SHAH, University of Dayton Research Institute, Dayton, OH, ANDREW SARAGAN, University of Dayton Electro-optics, Dayton, OH, SAID ELHAMRI, Physics Departrment, University of Dayton, Dayton, OH, ELENA GULIANTS, University of Dayton Research Institute, Dayton, OH — High surface area, porous, metallic (Ti, Cr) nanorod thin films with columnar microstructure can be deposited using conventional physical vapor deposition technique of E-beam evaporation. The technique relies on the physical vapor deposition onto a static substrate oriented in a position where flux from the source material (Ti, Cr) arrives at oblique angle. The adatoms provides geometrical shadowing which results in growth of nanorod columns in the direction of vapor source. Deposition conditions such as angle of the incoming vapor flux, substrate temperature, surface diffusion etc. have strong influence on the shape and arrangement of the columnar thin films. In this work, we demonstrate the growth and electrical characterization of these nanostructured thin films. Preliminary results on these films exhibit electrical resistivity anisotropy, when characterized by measuring their electrical resistivity using conventional van der pauw method. Origin and possible causes of this resistivity anisotropy is discussed.

S1.00106 An *Ab Initio* Study of SiC Double-Walled Nanotubes of Types 2 and 3[1] , KAPIL ADHIKARI, ASOK RAY, Department of Physics, University of Texas at Arlington — A hybrid density functional study of armchair SiC double walled nanotubes (DWNTs) of types 2 and 3 is presented. The geometries of individual DWNTs of types 2 and 3 have been spin optimized using the hybrid functional B3LYP (Becke's three-parameter exchange functional and the Lee-Yang-Parr exchange-correlation functional) and the basis set 3-21G* and the GAUSSIAN 09 software. A study of binding energies, Mulliken charge, density of states and HOMO-LUMO gaps has been performed for all nanotubes from (n,n)@(n+3,n+3) to (n,n)@(n+6, n+6) (n=3-6). Type 2 DWNTs do not conserve the coaxial geometry when the difference in chirality of outer and inner tube is 5 or less. For type 3, this occurs when the chirality difference of 4 or less. The gaps of types 2 and 3 DWNTs are less then the corresponding single-walled nanotubes and are significantly less than those of type 1 DWNTs.

[1]This work is supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525).

S1.00107 Effects of NO_2 physisorption and chemisorption on the conduction of graphene nanoribbons[1] , AHMED HASSAN, CORY KNICK , AMIR FARAJIAN, Mechanical and Materials Engineering, Wright State University — Graphene nanoribbons have the potential of being used as the functional part of nanoelectronic gas sensors. This study focuses on the changes induced in the conduction of graphene nanoribbons upon adsorption of NO_2. Both chemisorption and physisorption situations, i.e., NO_2 adsorption with and without chemical bond formation, are studied. We use ab initio electronic structure calculations with MP2 correlation energy in order to optimize the structures of graphene nanoribbons, with hydrogen-terminated edges, in presence of NO_2. Subsequently, quantum conductance calculations are performed using Green's function implementation of the Landauer's approach. We explain different conductance modulation patterns in terms of charge transfer and dipole interactions. The results clarify some of the basic functionality issues of nanoelectronic-based gas sensors.

[1]This project is supported by the National Science Foundation grant ECCS-0925939

S1.00108 An *Ab Initio* Study of Atomic Hydrogen and Oxygen Adsorptions on Armchair Si Nanotubes[1] , HAOLIANG CHEN, ASOK RAY, Physics Department, University of Texas at Arlington, Arlington, Texas 76019 — First principles calculations based on hybrid density functional theory have been used to study the electronic and geometric properties of armchair silicon nanotubes from (3, 3) to (12, 12). Full geometry and spin optimizations have been performed without any symmetry constraints with an all electron 3-21G* basis set and the B3LYP functional. The largest silicon nanotube studied has a cohesive energy of 3.47eV/atom. Atomic hydrogen and oxygen adsorptions on a (6, 6) tube have been studied by optimizing the distances of the adatoms from both inside and outside the tube. The on-top external site is the most preferred site for hydrogen with an adsorption energy of 5.97eV and an optimized distance of 1.50 A. For oxygen, the external bridge site is the most preferred site with an adsorption energy of 11.36eV, the optimized distance being 1.66A.

[1]Work partially supported by the Welch Foundation.

S1.00109 Structural, Electronic and Transport Properties of Gd/Eu Atomic Chains Encapsulated in Single-walled Carbon Nanotubes , JING ZHOU, XIN YAN, GUANGFU LUO, RUI QIN, HONG LI, JING LU, ZHENGXIANG GAO, State Key Laboratory for Mesoscopic Physics and Department of Physics, Peking University, Beijing 100871, P. R. China, WAI NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, Nebraska 68182-0266 — Structural, electronic, and transport properties of Gd/Eu atomic chains encapsulated in single-walled carbon nanotubes (SWCNTs) are studied by using first-principles density functional theory and nonequilibrium Green's function method. We find that the linear single-atom Gd and Eu chains occupy an off-centered position when encapsulated in the (8,0), (10,0), and (6,6) SWCNTs and considerable electrons are transferred from the Gd and Eu chains to the SWCNTs. The resulting composites are all ferromagnetic metals, with conductivity significantly larger than those of the pristine SWCNTs and the free-standing Gd/Eu linear single-atom atomic chains. The spin polarization of the finite Gd linear single-atom chain at the Fermi level is 67% when encapsulated in the (8,0) SWCNT from the quantum transport calculation.

S1.00110 Anisotropic Conductivities of Magnetic Carbon Nanotubes Embedded in Epoxy Matrices , IL TAE KIM, ALLEN TANNENBAUM, RINA TANNENBAUM, Georgia Institute of Technology — Maghemite (γ-Fe_2O_3)/carbon nanotubes (CNTs) hybrid-materials were synthesized and their anisotropic electrical conductivities resulting from their alignment in a polymer matrix under a magnetic field were investigated. The tethering of γ-Fe_2O_3 nanoparticles on the surface of CNT was achieved by a modified sol-gel reaction. These hybrid-materials, specifically, magnetized carbon nanotubes (m-CNTs) were readily aligned parallel to the direction of a magnetic field even when using a relatively weak magnetic field. The conductivity of the epoxy composites formed in this manner increased with increasing m-CNT mass fraction in the polymer matrix. Furthermore, the conductivities parallel to the direction of magnetic field were higher than those in the perpendicular direction, indicating that the alignment of the m-CNT contributed to the enhancement of the anisotropic electrical properties of the composites in the direction of alignment.

S1.00111 Double Layer Charging for Conductivity Enhancement of Pure Metallic and Semiconducting Single Wall Carbon Nanotubes[1]

, NATHANAEL MAYO, ALEXANDER KUZNETSOV, ANVAR ZAKHIDOV, Nanotech Institute - University of Texas at Dallas — Injecting high electronic charge densities can profoundly change the optical, electrical, and magnetic properties of materials. Evidence suggests a possibility of significantly improving conductivity of carbon nanotubes through double layer charge injection. Double layer charge injection can prove to be a powerful method when applied to carbon nanotubes because of theirs high surface area and chemical stability. Investigation has commenced on the effect of charging on various types of carbon nanotubes, specifically 99% purified single wall semiconducting and single wall metallic tubes. An electrical double layer is electrochemically introduced upon a sheet of carbon nanotubes via application of potential (up to $\pm$5 volts) to a sample immersed in ionic-liquid-based electrolyte. Resistance of carbon nanotube as a function of applied charging voltage is recorded to determine the effects of charge injection. Results show that the electrical double layer considerably reduces the resistance across both samples. ESR/LFMA studies combined with low temperature magnetic and transport measurements are conducted to search for charge injection induced superconductivity in carbon nanotubes.

[1]Supported by AFOSR grant FA 9550-09-1-0384

S1.00112 Synthesis, micro and electronic structure investigation of diamond nanorod spherules by High resolution NEXAFS coupled PEEM and field emission performance[1]

, SWATHI IYER, PAUL MAGUIRE, NIBEC, University of Ulster — We report the synthesis of Diamond nanorods/flake Spherules (DNRS) predominantly consisting of UNCD enveloped by graphite in the form of flake or a rod with nanodimension, projecting randomly outward in all directions. The diamond nanoflake with a diameter of $\sim$2 nm has a central diamond (111) core encapsulated by graphitic (0002) lacing. The structure composition by High Resolution Transmission Electron Microscopy (HRTEM) and X ray Photoemission Electron Microscopy (XPEEM) revealed that the nanoflakes predominant with core sp^3 laced with sp^2, is embedded in carbon matrix consisting of other nanocarbon, such as the nanotubes, nanoonion and nanowires/sheets. High resolution localized XPEEM combined with XAS complimented the Raman and the XPS with a weak π* peak, a prominent exitonic and a second band dip, which are the signature of diamond. The congregated nanorod spherules exhibits a low-threshold, high current-density of 10 mA/cm^2 at 2.9 V/m which appears to be exceptional when compared to many other electron emitting nanostructures. Bias enhanced DNRS were also characterized by XPEEM and their FE's compared.

[1]VCRS Scholarship

S1.00113 Heat transfer through a dual-walled carbon nanotube[1]

, KHOA BUI, The University of Oklahoma, CEDRIC COUSIN, Blaise Pascal University, Clemont-Ferrand, HUONG NGUYEN, The University of Oklahomoa, ALBERTO STRIOLO, DIMITRIOS PAPAVASSILIOU, The University of Oklahoma — Molecular Dynamics simulations are used to investigate the resistance to heat tranfer between the walls of dual-walled carbon nanotubes (DWCNTs). Recent computional results have indicated that the carbon nanotube to carbon nanotube thermal boundary resistance (TBR) can be as high or higher than the TBR between a nanotube and the surrounding matrix (e.g., epoxy or octane) in thee case of composites. This generates the question of whether heat transfer in multi-walled carbon nanotubes occures through the outer nanotube only or not. We discuss here results for a DWCNT composed of a (5,5) nanotube inside a (10,10) nanotube, as well as the differences between this case and the case of a (6,6) inside a (19,0).

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S1.00114 Aspect Ratio Dependant Buckling Mode Transition in Single-Walled Carbon Nanotubes under Compression[1]

, CHUN TANG, JEREMY FELICIANO, CHANGFENG CHEN, Department of Physics and Astronomy and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, NV 89154 — We have conducted molecular dynamics simulations on compressing behaviors of single-walled carbon nanotubes (SWCNTs) with a large variaty of aspect ratios. It is found that SWCNTs with large aspect ratios experience column buckling behavior at low strain levels, in contrast to commonly observed shell buckling of short SWCNTs. Further compression leads to a transition to a shell buckling mode, which is distinct from those of short SWCNTs under compression. It originates from the column buckling induced bending loadings. We extract the scaling law with respect to the aspect ratio of SWCNTs based on an analytical model of bending buckling.

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S1.00115 Intershell Interaction in a Double Wall Carbon Nanotube with Determined Chiral Indices under a Torsional Strain

, LETIAN LIN, Curriculum in Applied Sciences and Engineering, University of North Carolina at Chapel Hill, TAORAN CUI, SEAN WASHBURN, LU-CHANG QIN, Department of Physics and Astronomy, University of North Carolina at Chapel Hill — We have used a double wall carbon nanotube to build a torsional pendulum. The nanotube worked as a torsional bearing for a metal block. An external electric field was used to rotate the metal block to cause a fully elastic torsional deformation on the nanotube. Nano-beam electron diffraction patterns were taken before and while the nanotube was twisted. By analysis of the shift of the diffraction patterns, we were able to determine the nanotube chiral indices and measure the inner-shell torisonal responses to the torsional stress applied on the outer-shell. The inter-shell interactions and nanotube shear modulus were also calculated and discussed in connection to the theoretical estimations.

S1.00116 Large Band Gap in Graphene Induced by Inhomogeneous Mechanical Deformation

, IVAN NAUMOV, ALEXANDER BRATKOVSKY, Hewlett-Packard Laboratories, HEWLETT-PACKARD LABORATORIES COLLABORATION — Graphene is a prospective material for future electronics. However, in order to become useful and work in electronic chips, graphene should have a semiconducting energy gap. The seemingly simplest way to induce a gap is to subject the graphene to a strain. Recently, it was predicted within tight-binding approximation that by combining shear deformations and uniaxial strains one can open the gap up at moderate strains ($\sim$12%), well before the elastic limit of the material is reached. Here, we show with the help of ab-initio calculations that, in fact, the gap *cannot* be opened up by any kind of homogeneous deformations smaller that the graphene failure strain. The gap, however, can be opened up by *inhomogeneous* deformation, e.g. by the periodic out-of-plane atomic displacements with an "amplitude-to-wavelength" ratio on the order of 0.1, similar to Ref. [2], which translates roughly to only 10% elongation. The gap can be quickly pushed to values up to 1 eV by further increase of strain still far enough from the point of mechanical failure.

[1] G. Cocco, E. Cadelano, and L. Colombo, Phys. Rev. B **81**, 241412 (2010).
[2] I. Naumov, A. M. Bratkovsky, and V. Ranjan, Phys. Rev. Lett. **102**, 217601 (2009).

S1.00117 BIOLOGICAL PHYSICS —

S1.00118 Substrate Recognition of Histone H2B by DUBm , ELIZABETH HENDERSON, Hunter College, CHRISTOPHER BERNDSEN, CYNTHIA WOLBERGER, The Johns Hopkins University School of Medicine — The SAGA complex is a transcriptional coactivator that regulates gene expression in eukaryotes via histone acetylation and deubiquitination, which are crucial for transcription. Our lab is investigating the SAGA-dependent deubiquitination of histone H2B. The deubiquitinating module (DUBm) of SAGA is comprised of a ubiquitin-specific protease, Ubp8, and three other proteins. It is known that Ubp8 cleaves ubiquitin from histone H2B, however, the specific way in which the enzyme binds to the substrate remains elusive. In order to unravel this mechanism, we attempted to determine the crystal structure of the substrate binding complex. We obtained this substrate by exploiting the techniques of intein chemistry to artificially ubiquitinate a histone H2B peptide, which we then co-crystallized with DUBm. Additionally, we synthesized Ub-K63R-linked chains and Ub-K48-linked chains and co-crystallized them with DUBm.

S1.00119 pH Dependent Photoinduced Effects of Protoporphyrin IX to Human Serum Albumin , SARAH ROZINEK, JORGE PALOS-CHAVEZ, LORENZO BRANCALEON, University of Texas at San Antonio — Irradiation of the non-covalent complex between protoporphyrin IX (PPIX) and β-lactoglobulin (Blg), causes a modest unfolding of the protein localized to Trp19. That binding site is affected by pH of the solution. At physiological pH, PPIX is known to bind HSA in hydrophobic binding sites. However, no evidence is presented for the binding behavior of PPIX to HSA in non-physological pH confirmations, nor on the effects of irradiation on the bound system at any pH. The combination of spectroscopic data and molecular simulations suggests that distinct PPIX-compatible binding sites become available at each confirmation of HSA at pH 7.4, and 9 while the pH 3 conformation is unfavorable for binding. Photoinduced mechanisms produce changes in the ligand as well as the protein but they do not appear to be dependent on the presence of O_2 in solution. Therefore, the mechanism is not mediated by the formation of singlet oxygen and is likely the result of electron transfer between the porphyrin and amino acid residues.

S1.00120 Docking ellipticine to the V-VI transmembrane domain of the Kv11.1 potassium channel , DAWN LIPSCOMB, LORENZO BRANCALEON, Department of Physics and Astronomy, University of Texas at San Antonio, S. GENTILE, Department of Molecular Pharmacology and Therapeutics, Loyola University — Ellipticines such as 9-methoxy-N-2-methylellipticinium acetate (MMEA) and 9-hydroxy-N-2-methylellipticinium acetate (NMEA, Celiptium®) are antineoplastic drugs exerting their selective cytotoxicity against leukemia and endometrial carcinoma. Ellipticine's action is also related to severe physical side effects, but the link between undesired effects and pharmacological application is not well understood. We investigated the binding of Ellipticine derivatives with the Kv11.1 potassium ion channel using Autodock and revealed that hydroxyellipticinium derivatives provide binding configurations with Kv11.1, but the energy, location and estimated dissociation constant varied. The binding energy is as follows: Chloroceliptium (-6.60 kcal/mol) > Celiptium (- 6.37 kcal/mol) > Methoxyceliptium (- 6.20 kcal/mol) > Datelliptium (-6.08 kcal/mol). The data shows that some configurations enable these molecules to bridge among channel subunits, thus potentially inhibiting the flow of ions.

S1.00121 Effects of the range and strength of interparticle attraction on gelation , TONI PEREZ, JAMES GUNTON, Lehigh University, AMIT CHAKRABARTI, Kansas State University — Range and strength of interparticle attraction determine whether a complex assembly of particles will be ordered or disordered. For very short range interactions, the system seems to get trapped into a gel state as a result of arrested spinodal decomposition. On the other limit, for long range interactions, spinodal decomposition leads to phase separation. The nature of the gel transition at low volume fraction is still not well understood in between these two limits. Here, we study the dynamics of the gel transition at low volume fraction as a function of the range and strength of the attractive interparticle interaction. We perform Brownian dynamics simulations and study how gelation is affected as the range and strength of interparticle interaction are varied.

S1.00122 Explore the physical mechanism of Hofmeister series on protein structural dynamics , SANDIP KALEDHONKAR, LORAND KELEMEN, AIHUA XIE, Department of Physics, Oklahoma State University, Stillwater, OK 74078, XIE LAB TEAM — Hofmeister series, a classification of ions, are known to change the solubility and stability of proteins. We have found that Hofmeister series suppress functionally important structural dynamics of photoactive yellow protein (PYP). Here we investigate two possible mechanisms: (1) Hofmeister series increases the pK_a of Glu46, an active site proton donor to chromophore protonation of PYP, (2) Hofmeister series alter the energy landscape of surface exposed groups due to effective dehydration, making it difficult to change protein conformations. We will test these two hypotheses using strategic combination of protein engineering and time-resolved step-scan and rapid-scan FTIR difference spectroscopy. A variety of N-terminus tags are designed and employed to study the effect of effective dehydration of protein due to Hofmeister series. Time-resolved infrared structural biology will be used to capture light-triggered structural dynamic motions of PYP.

S1.00123 Time-resolved infrared structural biology: from active-site structural dynamics to proton transfer mechanism of photoactive yellow protein , SHUO DAI, LORAND KELEMEN, ZHOUYANG KANG, WOUTER HOFF, AIHUA XIE, Oklahoma State University, Stillwater, OK 74078 — Proton transfer is a fundamental process in biology. We employ photoactive yellow protein (PYP), a bacterial blue light receptor protein, as an ideal model system to study the physical mechanism of intra-molecular proton transfer in proteins. We employ time-resolved step-scan FTIR spectroscopy to detect functionally important structural changes in the active site of PYP before and after proton transfer from Glu46 to the negatively charged phenolic group of the p-coumaric acid chromophore in PYP, which occurs on a 250 microsecond time scale. In addition, we employ a combination of isotope editing and site-specific mutations to identify the vibrational modes and structural origins of infrared signals, and we develop and utilize vibrational structural markers to translate infrared signals to structural information. We will demonstrate the power of time-resolved infrared structural biology in structure-function studies of proteins and in proton transfer mechanism in photoactive yellow protein.

S1.00124 Exploring the effects of Hofmeister series ions on structural dynamics of water , NINGNING XU, THOMAS WRIGHT, SANDIP KALEDHONKAR, AIHUA XIE, Department of Physics, Oklahoma State University — Water is known as the lubricant of life. Most proteins lose their biological function upon dehydration. We found that in a variety of high concentration salt solutions, photoactive yellow protein, a blue light bacterial photoreceptor protein, loses its functionally important structural motions for receptor activation. We hypothesize that this effect is caused by reduced structural dynamics of water due to strong water-ion interactions. Here we report our experimental studies on the effects of salts on changes in structural dynamics of water at different time scales. The results are expected to provide deep insight regarding how Hofmeister series ions alter the structural dynamics of proteins.

S1.00125 Molecular Dynamics Simulations of Alpha-synuclein , MARIA SAMMALKORPI, CARL SCHRECK, ABHINAV NATH, DAVID DEWITT, ELIZABETH RHOADES, COREY O'HERN, Departments of Chemical Engineering, Physics, Mechanical Engineering and Materials Science, and Molecular Biophysics and Biochemistry, Yale University — We investigate the conformational dynamics of single alpha-synuclein proteins, which have been implicated in amyloid diseases such as Parkinson's and Alzheimer's disease, in solution using unconstrained and constrained all-atom, explicit solvent molecular dynamics simulations. The constraints on inter-residue separations are obtained from our single-molecule FRET measurements of eleven FRET pairs that span the protein. By comparing the simulation data satisfying different combinations of FRET constraints, we are able to identify those constraints that are most important in determining the radius of gyration and key features of the contact map of the protein.

S1.00126 InaD PDZs 4-5 Act as an Allosterically-Regulated Dynamic Scaffold , STEPHEN HELMS, UT Southwestern, PRASHANT MISHRA, Caltech, MICHAEL SOCOLICH, RAMA RANGANATHAN, UT Southwestern — The Drosophila scaffolding protein InaD is required for proper visual signaling. We previously identified that the fifth PDZ domain of InaD undergoes light-dependent PKC-mediated formation of a disulfide bond which disrupts the binding site. We investigated the interaction of this switch with the adjacent PDZ4 of InaD. We showed that PDZ4 destabilizes the disulfide bond and promotes binding of PDZ5 to its ligand, indicating a previously unidentified allosteric interaction between the two domains. We solved the structure of PDZ45 to 2.4Å, which revealed that PDZ4 forms an extensive interface with PDZ5 but does not alter its conformation. NMR HSQC spectra, however, indicated that nearly all of PDZ5 is in a different chemical environment in PDZ45. Finally, we identified that PDZ45 is phosphorylated by PKC in vitro at a site located near the domain interface. Intriguingly, the disulfide bond in PDZ5 is an evolutionary adaptation of just fast-flying flies, revealing the remarkable ability of evolution to rapidly build novel regulatory features into scaffolding proteins.

S1.00127 Tracking the Growth Transitions of A Solvent-Charged Model Globular Protein , JEREMIAH BABCOCK, JACOB FRIDAY, LORENZO BRANCALEON, University of Texas at San Antonio — Biophysical studies have shown that solutes like proteins undergo aggregation through specific pathways that often lead to long polymeric structures called fibrils. The knowledge of the size of early-stage protein aggregates (oligomers) has an important bearing on the elucidation of the dynamics of the process of protein unit combinations. In this study, bovine serum albumin, a well-characterized model protein known to polymerize in alkaline and acidic conditions in the normal (N) to basic (B) or (N) to (E) transition, was incubated at pH 9.0 and pH 3.1 for longer than eight days. Particle growth in solution was monitored by absorption, fluorescence and circular dichroism spectroscopy and concurrently measured by atomic force microscopy (AFM) methods to yield BSA oligomer size distributions. Results show that the BSA aggregation pathway is concentration-dependent and rapidly forms spherical aggregates, which preferentially come together to form flexible polymers.

S1.00128 Low frequency Raman study of the nucleosides , CRAIG KOONTZ, SCOTT LEE, University of Toledo — In both transcription and replication, the two helices of the DNA molecule move apart. Consequently, vibrations involving the relative motions of large portions of the molecule with respect to one another are of intrinsic interest. Such vibrations have relatively low frequencies because they involve weak bonds and large masses. Low frequency modes are difficult to observe in Raman spectroscopy because they are very close to the signal from the Rayleigh scattered light (which is very intense). In this poster, we will describe our results for the eight nucleosides: adenosine, deoxyadenosine, guanosine, deoxyguanosine, cytidine, deoxycytidine, uracil and deoxythymidine.

S1.00129 A temperature-dependent study of the low-frequency vibrational excitations in polynucleotides in solution , KRISTINA WOODS, Carnegie Mellon University, SCOTT LEE, Un. of Toledo — Far-infrared spectroscopy is a useful probe of low-frequency collective excitations of biomolecules, including DNA. These vibrational modes are believed to be related to conformational changes that occur in these molecules during their biological function and, therefore, are very important to study. In order to further our understanding of these modes, THz spectroscopy experiments were performed on solutions of polynucleotides between 20 to 100 cm^{-1} from room temperature to 90 $^{\circ}$C, covering the premelting and melting regimes. The samples studied include Poly(dA-dT), Poly(dA)-Poly(dT), Poly(dI-dC) and Poly(dI)-Poly(dC). Of particular interest, the intensity of a band at about 67 cm^{-1} is observed to increase as the melting proceeds.

S1.00130 Modification of DNA towards high conductance and transport measurements with mechanically controllable break junction electrodes , SHOUPENG LIU, Department of Physics, University of Konstanz, Germany, BENJAMIN BORNEMANN, SAMUEL WEISBROD, ZHUO TANG, ANDREAS MARX, Department of Chemistry, University of Konstanz, Germany, ARTUR ERBE, ELKE SCHEER, Department of Physics, University of Konstanz, Germany, DEPARTMENT OF PHYSICS, UNIVERSITY OF KONSTANZ, GERMANY TEAM, DEPARTMENT OF CHEMISTRY, UNIVERSITY OF KONSTANZ, GERMANY TEAM — The DNA molecule is proposed to be used as building block for molecular electronic devices by virtue of its unique recognition and self-assembling properties. However, electron transport properties of DNA are still not well established mainly because poor binding between DNA and gold electrodes. Here, we synthesized new DNA samples with terminal bases modified with a thiol group on its C5 atom and protected with Me3Si for better binding with gold electrodes and better conductivity because of better electron overlap. Its transport properties were measured with mechanically controlled break junction. Conductance with a current of 700 nA in 0.25V were obtained, which is higher than most of the former reports. We also measured conductance through DNA G-quadruple instead of double-stranded structure., which shows a more stable conductance when the distance between electrodes reversibly varied over a several nm.

S1.00131 QM/MM/3D-RISM study of solvation and electronic structure of DNA , NORIO YOSHIDA, FUMIO HIRATA, Institute for Molecular Science — It is well known that a DNA has high electronic conductivity in wet condition, while it doesn't in dry condition. Therefore, the solvent effects on the electronic properties of DNA got much attention in the field of biology, chemistry and physics. In the present study, we employ three-dimensional reference interaction site model method combined with quantum mechanics and molecular mechanics (QM/MM) method to treat the large DNA chain in solvent. By this theory, the electronic structure of DNA and solvent distribution around DNA can be determined simultaneously. The result shows the dramatic change of electronic structure of solute DNA molecule by solvation. The change strongly depends on the sequence of DNA.

S1.00132 The driving forces of membrane remodeling by non-intrinsically curved proteins , CHRISTOPHER J. RYAN, University of California, Berkeley, JEANNE C. STACHOWIAK, Sandia National Laboratories, EVA M. SCHMID, DANIEL A. FLETCHER, PHILLIP L. GEISSLER, University of California, Berkeley — Membranes are dynamically remodeled during numerous processes essential to cells. Among the most well-studied effectors of this remodeling are BAR family proteins, which are small and have a banana-like intrinsic curvature that senses, forms, and stabilizes curved membranes without expending energy as ATP or GTP. Recent experiments in reduced systems have shown, however, that small proteins that feature no such intrinsic curvature can similarly cluster at and dramatically remodel membranes. These proteins have no distinguishing features other than their size and their membrane-binding sites, and the dominant effect that is driving curvature is not well understood. Here, we present a coarse-grained simulation study that captures protein steric and binding effects as well as membrane fluctuations at large scales. We use this model to systematically test for the role that such attributes play in the resulting dynamics and equilibrium structures of remodeling processes that feature this motif.

S1.00133 Analysis of Striped Nanoparticle Complexation with Lipid Bilayers , REID VAN LEHN, ALFREDO ALEXANDER-KATZ, MIT — A recent study has shown that a new class of synthetic ligand-protected gold nanoparticles is able to penetrate the cell membrane without inducing poration or endocytosis. Furthermore, these nanoparticles fuse with pure lipid bilayers while retaining high solubility in biological conditions. This complexation behavior is related to the morphology of the ligand shell, which is composed of alternating ribbon-like domains of linear alkanes with either hydrophobic or charged end-groups. Spontaneous complexation is surprising given the large free energy barrier for moving charges through the hydrophobic bilayer core. In this work, we provide a thermodynamic analysis of bilayer complexation supported by multiscale simulations. We show that the key to bilayer complexation is the rearrangement of ligands by bending to maximize hydrophobic matching and minimize charge exposure. We believe this result will improve our understanding of transmembrane proteins and enable the design of nanoparticles for drug delivery and biosensing applications.

S1.00134 The Comparison of Lipid Compositional Uniformity of Giant Unilamellar Vesicles Synthesized From the Rapid Solvent Exchange liposomes with That From Dry Lipid Film , EDA BAYKAL-CAGLAR, JUYANG HUANG, Texas Tech University — Lipid bilayer, which is an important constituent of cell membranes, has been extensively studied. Cell membranes perform many vital cell functions such as signal transduction and transportation of materials needed for the functioning of the cell organelles. Understanding the dynamics of lipid bilayers is important for understanding the processes taking place in cell membranes. Giant Unilamellar Vesicles (GUVs) are cell-sized model systems that allow direct visualization of membrane-related phenomena using fluorescence microscopy. In this study, we synthesized DOPC/DSPC/cholesterol GUVs and diPhyPC/DPPC/cholesterol GUVs by the standard electroformation method using dry lipid film as well as by a modified method using liposomes made from Rapid Solvent Exchange (RSE) method. Second method has a potential of incorporating more varieties of membrane proteins to GUVs. We compare the uniformity of lipid composition of GUVs synthesized by the two methods by measuring the variation of phase transition temperature of individual GUVs through fluorescence microscopy; since a narrower distribution of transition temperature should correspond to a more uniform distribution in GUV lipid composition. We will present the results at several bulk lipid compositions and buffer ionic strengths.

S1.00135 Machanistic basis of rigidity sensing at biological interfaces , ALIREZA SARVESTANI, University of Maine — We have outlined a framework to investigate the thermodynamic equilibrium adhesion of a bio-membrane to a compliant substrate functionalized with immobilized bio-adhesive ligands. The membrane is modeled as a soft elastic shell, subjected to surface tension and reconstituted with mobile receptors and a repelling layer on the ventral side. The free energy function of the system is assumed to be comprised from the following contributions: the membrane–substrate non-specific interactions, stored elastic energy (in deformed membrane and substrate), binding enthalpy, and mixing entropy of mobile receptors. Assuming a van der Waals form for the interfacial non-specific potential, the equilibrium configuration of the system is studied in detail. We have shown that the equilibrium spread area of the adherent membrane is very sensitive to the rigidity of the underlying substrate and decreases as the surface compliance increases. This prediction is reminiscent of the experimental observations of spread area of cells attached to soft substrates. This is an interesting result considering the lack of contribution of intracellular signaling or actively regulated cytoskeleton in the proposed physical model for the adhesion. This suggests that the mechanistic pathways inherent to membrane–substrate thermodynamic interactions can be equally important as intracellular signaling pathways to mediate the process of rigidity sensing by cells.

S1.00136 Curved inclusions surf membrane waves , ROIE SHLOMOVITZ, UCLA Department of Chemistry, NIR GOV, Weizmann Institute of Science Dept. of Chemical Physics — There is mounting recent evidence for the existence and biological importance of a large family of curved membrane proteins (CMPs). In addition there is increasing interest in membrane waves, and the role they play in cell function. In this theoretical work, we examine the interaction between CMPs and membrane waves. We find that CMPs are advected on the cell surface by membrane waves. We calculate the relative drift velocity of the CMPs with respect to the wave velocity, for the case of sinusoidal waves. For relatively slow waves the CMPs move at the wave velocity, i.e. "surfing the wave." For fast waves the CMPs move back and forth with a Stokes drift that is inversely proportional to the quadrant of the wave velocity. For the more realistic case of decaying sinusoidal waves, we determine the equilibrium distribution of the CMPs, and find that such waves create a "hole" in the distribution of the CMPs on the cell membrane and calculate the size of that hole. Based on these calculations, we show how such proteins can be used in experiments to measure the properties of propagating membrane waves.

S1.00137 Chemotaxis and Autotaxis in Biofilm-Forming Systems , SHINJI STRAIN, SAMUEL BIENVENU, TRAVIS THATCHER, BENJAMIN COOLEY, VERNITA GORDON, University of Texas at Austin — Biofilms are multicellular, surface-bound communities of interacting unicellular organisms. In the initial stages of biofilm formation, discrete cells populate the surface and eventually form microcolonies (dense surface-bound clusters of cells). How much these microcolonies arise from clonal growth and how much they arise from attraction and active motility of non-clonal cells is not well-understood. One potentially important form of attraction is autotaxis, movement of cells toward like cells. Another is chemotaxis, movement of cells toward an attractive chemical, which could act to concentrate cells with no direct intercellular interaction. While both autotaxis and chemotaxis have been studied for three-dimensional, swimming, dense bacterial systems, they remain largely unstudied in sparse, surface-bound populations that initiate biofilms. Using microscopy and automated tracking and analysis algorithms, we will study how bacteria respond to each other and to chemoattractants, in a spatially-dependent manner. We will determine how variations in neighbor density and arrangement stimulate changes in the motility of E. coli and P. aeruginosa cells on a surface.

S1.00138 3D single molecule super-resolution imaging of cellular samples using MUM , ANDREA GROSSO, ANISH ABRAHAM, Department of Electrical Engineering, UT Dallas, JEFFREY KANG, JERRY CHAO, RAMRAJ VELMURUGAN, SRIPAD RAM, STEPHEN ANTHONY, ZHUO GAN, E. SALLY WARD, Dept. of Immunology, UT Southwestern Medical Center, Dallas, TX, RAIMUND J. OBER, Department of Electrical Engineering, UT Dallas — Localization based super-resolution imaging techniques (e.g., PALM, fPALM, STORM, etc.) represent a powerful tool to image single molecules at nanoscale resolution in two dimensions. However, the extension of these techniques to three dimensions poses several technical challenges, foremost being the poor depth discrimination inherent to conventional microscopes which is typically used by these techniques. Previously, we developed an imaging modality, multifocal plane microscopy (MUM), which overcomes the poor depth discrimination capability of conventional microscopes. We also introduced a 3D localization algorithm MUMLA and demonstrated experimentally that it provides the best possible accuracy with which the 3D position of single molecules can be determined. Here, we extend the application of MUM and MUMLA for super-resolution imaging and demonstrate 3D imaging of single molecules at nanometer scale resolution in a cellular sample.

S1.00139 Accuracy of single molecule localization using electron-multiplying charge-coupled device cameras , JERRY CHAO, Department of Electrical Engineering, University of Texas at Dallas, Richardson, Texas, E. SALLY WARD, Department of Immunology, University of Texas Southwestern Medical Center, Dallas, Texas, RAIMUND J. OBER, Department of Electrical Engineering, University of Texas at Dallas, Richardson, Texas — The electron-multiplying charge-coupled device (EMCCD) is an important technology for imaging under extremely low light conditions. Whereas a weak signal acquired under low light conditions can be overwhelmed by the readout noise of a conventional charge-coupled device (CCD), it is amplified in the case of an EMCCD such that the readout noise becomes insignificant. The EMCCD is therefore a commonly used image detector in applications such as single molecule microscopy. However, despite its wide use, there has been a lack of rigorous analyses to determine how accurately parameters of interest (e.g., location of a single molecule) can be estimated from an image it produces. Here, we model the EMCCD's stochastic multiplication of electrons as a geometrically multiplied branching process, and develop the theory for calculating the Fisher information for estimating parameters from an EMCCD image. A "noise coefficient" is also introduced which enables the comparison of a CCD and an EMCCD in terms of the best accuracy with which parameters can be estimated from the images they produce.

S1.00140 Simultaneous AFM force spectroscopy and FRET measurements on single biological molecules , HUI LI, CHI-FU YAN, SANJEEVI SIVASANKAR, Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, DEPARTMENT OF PHYSICS AND ASTRONOMY, IOWA STATE UNIVERSITY, AMES, IOWA 50011 TEAM — Single Molecule Fluorescence Resonance Energy Transfer (FRET) and single molecule force measurements with the Atomic Force Microscope (AFM) are two powerful techniques that have facilitated much progress in the biological sciences. However each of these techniques suffers from limitations that can be overcome by the use of a combined single molecule AFM-FRET approach. Here, we describe an instrument that successfully combines single molecule AFM with FRET to apply forces on individual biological molecules and simultaneously monitor their conformational dynamics. To validate this technique, we measured the force induced shearing of dye-labeled, double stranded DNA. Single DNA molecules were sheared and mechanical transitions corresponding to DNA rupture were correlated with changes in FRET.

S1.00141 The Heterogeneity of Mutational Tolerance in a Protein is Dependent on the Strength of Selective Pressure Correlating with Sectors of Co-evolving Residues , MICHAEL STIFFLER, RAMA RANGANATHAN, UT Southwestern Medical Center — Proteins are capable of tolerating mutations at many positions while still maintaining fold and function. Previous studies have failed to consider how tolerance to random mutagenesis might depend on the strength of selective pressure. To examine this, we measured the fitness of every single point mutation of TEM-1 beta-lactamase across a range of ampicillin concentrations utilizing a novel application of deep-sequencing. We found that the relative mutational robustness between positions varied considerably with respect to ampicillin concentration: at a low ampicillin concentration only a few positions are intolerant of mutations, while at a higher ampicillin concentration many additional positions are as equally intolerant of mutations. Using an analytic method termed statistical coupling analysis (SCA) to measure the co-variation between all positions in a sequence alignment of beta-lactamases revealed sectors of co-evolving positions associated with groups of residues having increased sensitivity to mutagenesis at either low or high ampicillin concentrations. Our findings suggest that nature has "designed" proteins to be robust to random mutagenesis by loading the constraints for fitness on discrete networks of co-evolving positions depending on the strength of selective pressure.

S1.00142 The Evolutionary Design of Proteins , FRANK J. POELWIJK, Green Center for Systems Biology, UT Southwestern Medical Center, Dallas. Laboratory of Living Matter, Rockefeller University, New York, ARJUN S. RAMAN, Green Center for Systems Biology, UT Southwestern Medical Center, Dallas, STANISLAS LEIBLER, Laboratory of Living Matter, Rockefeller University, New York, RAMA RANGANATHAN, Green Center for Systems Biology, UT Southwestern Medical Center, Dallas — Proteins fold spontaneously into precise, well-packed 3D structures, and execute complex functions such as specificity in molecular recognition, and efficient catalysis. Despite this, many studies show that proteins are robust to random mutagenesis. Additionally, proteins are evolvable. What principles underlying the design of natural proteins explain these properties? Recent work examining correlated evolution of amino acid positions shows that many positions in proteins are nearly statistically independent while 10-20% are organized into groups of co-evolving positions – termed "protein sectors" – that underlie conserved, independently varying biological activities. These findings suggest that the basic design of natural proteins is fundamentally tied to the nature of fluctuations in the selection pressures during evolution. We propose to test this hypothesis using a system for high-speed laboratory evolution and determine how variation in selection pressures influences the architecture of amino acid interactions within a protein.

S1.00143 Laser-Neuron Interaction with Femtosecond Beat-Modulated 800-1200 nm Photon Beams, as the Treatment of Brain Cancer Tissue. Laser Neurophysics[1] , V. ALEXANDER STEFAN, Stefan University — I propose a novel mechanism for the brain cancer tissue treatment: nonlinear interaction of ultrashort pulses of beat-photon, $(\omega_1 - \omega_2)$, or double-photon, $(\omega_1 + \omega_2)$, [2] beams with the cancer tissue. The multiphoton scattering is described via photon diffusion equation. The open-scull cerebral tissue can be irradiated with the beat-modulated photon pulses with the laser irradiances in the range of a few mW/cm^2, and repetition rate of a few 100s Hz generated in the beat-wave driven free electron laser.[3] This highly accurate cancer tissue ablation removal may prove to be an efficient method for the treatment of brain cancer.

[1]Work supported in part by Nikola Tesla Laboratories (Stefan University), La Jolla, CA.

[2] Maria Goeppert-Mayer, **Über Elementarakte mit zwei Quantensprüngen**, *Ann Phys* **9**, 273, 95. (1931).

[3]V. Alexander Stefan, **Laser Neurophysics.** 2010 **APS March Meeting**, V. Alexander Stefan, 2009 **APS March Meeting**; V. Stefan, B. I. Cohen, and C. Joshi, **Nonlinear Mixing of Electromagnetic Waves in Plasmas***Science* 27 January 1989: V. Alexander Stefan, **Genomic Medical Physics: A New Physics in the Making**, (S-U-Press, 2008).

S1.00144 The effect of Ag nanoparticles on PC3 cells ultraweak bioluminescence , MARIUS HOSSU, XIAOJU ZOU, Univ Texas at Arlington, LUN MA, WEI CHEN, Univ Texas at Arlington — Ultraweak intrinsic bioluminescence of cancer cell is a noninvasive method of assessing bioenergetic status of the investigated cells. This weak emission generated by PC3 cell line was measured during various stages of growth with or without the presence of Ag nanoparticles. The comparison between nanoparticles concentration, bioluminescence and cell survival showed that even though Ag nanoparticles doesn't significantly affect cell survival at used concentration it affects cell metabolism, possibly making them more susceptible to other form of therapies.

S1.00145 Steinberg "AUDIOMAPS" Music Appreciation-Via-Understanding: Special-Relativity + Expectations "Quantum-Theory": a Quantum-ACOUSTO/MUSICO-Dynamics (QA/MD) , LEE FENDER, RUSSELL STEINBERG, FUZZYICS=CATEGORYICS(SON OF TRIZ)/CATEGORY-SEMANTICS, EDWARD CARL-LUDWIG SIEGEL, FUZZYICS=CATEGORYICS(SON OF TRIZ) — Steinberg wildly popular "AUDIOMAPS" music enjoyment/appreciation-via-understanding methodology, versus art, music-dynamics evolves, telling a story in (3+1)-dimensions: trails, frames, timbres, + dynamics amplitude vs. music-score time-series (formal-inverse power-spectrum) surprisingly closely parallels (3+1)-dimensional Einstein(1905) special-relativity "+" (with its enjoyment-expectations) a manifestation of quantum-theory expectation-values, together a music quantum-ACOUSTO/MUSICO-dynamics(QA/MD). Analysis via Derrida deconstruction enabled Siegel-Baez "Category-Semantics" "FUZZYICS"="CATEGORYICS ('TRIZ") Aristotle SoO DEduction , irrespective of Boon-Klimontovich vs. Voss-Clark[PRL(77)] music power-spectrum analysis sampling-time/duration controversy: part versus whole, shows QA/MD reigns supreme as THE music appreciation-via-analysis tool for the listener in musicology!!! Connection to Deutsch-Hartmann-Levitin[This is Your Brain on Music, (06)] brain/mind-barrier brain/mind-music connection is subtle/compelling/immediate!!!

S1.00146 CuS Nanoparticles for Photothermal Ablation of Tumor Cells , WEI CHEN, Department of Physics, University of Texas at Arlington, Arlington, TX 760190059, YUEBIN LI, Department of Physics, University of Texas at Arlington, TX, CHUN LI, WEI LU, QIAN HUANG, MIAO HUANG, The University of Texas M. D. Anderson Cancer Center, Houston, Texas 77030, UNIVERSITY OF TEXAS AT ARLINGTON, ARLINGTON, TX 76019-0059 TEAM, THE UNIVERSITY OF TEXAS M. D. ANDERSON CANCER CENTER, HOUSTON, TEXAS 77030 TEAM — Here, we report the photothermal ablation effects of 3-nm CuS nanoparticles. CuS nanoparticles exhibited strong absorption in the near infrared (NIR) region. Irradiation by a laser beam at 808 nm elevated the temperature of aqueous solutions of CuS nanoparticles as a function of exposure time and nanoparticle concentration. CuS nanoparticles mediated photothermal destruction of HeLa cells in a laser dose- and nanoparticle concentration-dependent manner, and displayed minimal cytotoxic effects with a profile similar to that of gold nanoparticles. Owing to their unique optical property, small size, low cost of production, and low cytotoxicity, CuS nanoparticles are promising new nanomaterials for cancer photothermal ablation therapy.

S1.00147 Characterization of Blood Flow in Capillaries by Numerical Simulation , TONG WANG, Department of Mathematics, Nanjing University of Aeronautics and Astronautics, Nanjing, Jiangsu, 210016, China, ZHONGWEN XING, Department of Materials Science and Engineering, Nanjing University, Nanjing, Jiangsu, 210093, China — We presents a numerical investigation of the axisymmetric, pressure driven motion of single file erythrocyte (i.e., red blood cell) suspensions flowing in capillaries of diameter 8-11μm. The governing Navier-Stokes equations are discretized using the operator splitting technique and solved by the finite element method. The study takes consideration the particulate nature of the blood. The red blood cell (RBC) is modeled as a closed membrane filled with a Newtonian fluid which has the same viscosity as the surrounding plasma. The cell membrane is described by a spring model so that the deformability of the cells can be considered. An immersed boundary method is also developed for dealing with the cell/fluid interaction in the flow. Our study successfully recreates several important in vivo hemodynamic and hemorheological properties of microscopic blood flow, such as parachute shape of the cells, blunt velocity profile, and the Fahraeus effect, and they have been shown to have strong dependence on cell deformability, hematocrit and vessel size.

S1.00148 Sensing Labeled and Immunocomplexed DNA with solid-state nanopores[1] , BRIAN THOMAS, DANIEL FOLOGEA, DAVID S. MCNABB, Department of Biological Sciences, University of Arkansas, Fayetteville, AR 72701, JIALI LI, Department of Physics, University of Arkansas, Fayetteville, AR 72701 — We report the detection of labeled and immunocomplexed DNA molecules using silicon nitride nanopores. We compared the characteristics of the current blockade signal measured from double-stranded DNA, biotinylated DNA, and immunocomplexed DNA samples. Single biotin-binding site Fab fragments as well as multiple-binding sites Monoclonal Biotin Antibodies were used to bind biotinylated DNA molecules. The electrical current blockage signature measured from the nanopores show that the current drop amplitude, time duration, and the integrated area of events can be used to discriminate DNA with and without labels, and the species of the labels. Our studies show that the single molecule nanopore measurement is more sensitive than bulk electrophoresis in detecting labeled DNA molecules.

[1]We acknowledge the funding support provided by NHGRI/NIH R21HG003290, NHGRI /NIH R21HG00477, NSF/MRSEC 080054, and ABI-111/710.

S1.00149 The translocation time of DNA and protein molecules in solid-state nanopores[1] , BRADLEY LEDDEN, RYAN ROLLINGS, DAVID TALAGA, Department of Chemistry and Biochemistry, Montclair State University, Montclair, NJ 07043, JIALI LI, Department of Physics, University of Arkansas. Fayetteville, AR 72701 — The time that a biopolymer takes to translocate through a nanopore contains the properties of the polymer including its size, conformation, electrical charge and charge distribution. We measured the dependence of the translocation times on the size, charge and charge distribution, voltage, and conformation states of DNA and protein molecules. To quantitatively fit the time distributions measured, 1-D Langevin and 1-D Fokker-Planck equations were used for DNA and native state proteins. Kramers reaction rate theory was used to fit the time distribution of unfolded proteins. It was observed that native-state protein and DNA translocation approximately follows simple one-dimensional biased diffusion of charged particles. Due to the heterogeneous charge sequence of polypeptides, unfolded proteins obey a coupled electrophoretic and thermally activated process that is sequence specific. Deviations between models and experimental results as well as future challenges for single molecule DNA and protein characterization using solid-state nanopores will be discussed.

[1]Funding support provided by NHGRI/NIH R21HG003290, NHGRI /NIH R21HG00477, and NIH R01GM071684 to DST.

S1.00150 Emission line shape of B850 band of light-harvesting complex II[1] , PRAVEEN KUMAR, SEOGJOO JANG, Department of Chemistry & Biochemistry, Queens College of the City University of New York, 65-30 Kissena Boulevard, Flushing, New York 11367 — A theoretical framework is developed for the emission line shape of the single complex spectroscopy (SCS). The quantum mechanical characteristics of the single complex emission line shapes for the model B850 band of the light harvesting complex 2 of purple bacteria are studied including both static and quasi-static disorders within the exciton Hamiltonian. The bath is modeled as an infinite sum of harmonic oscillators. For the Gaussian type of disorder, we examined the dependencies of the spectral line shapes on the temperature, polarization of the radiation, and on the type of exciton-bath coupling. Theoretically obtained emission profile is also compared with the absorption profile in the frequency domain. It is observed that emission profile contains an extra inhomogeneous term coming from the entanglement of the system and bath degrees of freedom in the initial equilibrium density operator. Contribution of this term to the overall emission line shape is studied in detail.

[1]This research was supported by the Department of Energy, Office of Basic Energy Sciences.

S1.00151 Quantum Mechanisms of Electronic Signal Propagation Along a Microtubule[1] , TRAVIS CRADDOCK, DOUGLAS FRIESEN, JACK TUSZYNSKI, University of Alberta — Evidence has been accumulating for the involvement of quantum coherence and entanglement in light harvesting photosynthetic complexes. This tests the adage that biological systems are too "warm and wet" to support quantum phenomena. Recent advancements in experiment and theory have allowed investigators to probe other warm systems for coherent phenomena including polymer chains, bacteriorhodopsin and ion channels. A debate has raged for over a decade regarding hypothetical quantum coherence/ entanglement in microtubules. Here we theoretically investigate coherent energy transfer in microtubules via dipole excitations coupled to the environment in networks of chromophoric amino acids. We present the spatial structure and Hamiltonian, containing localized site energies and couplings between aromatic amino acids, for the microtubule constituent protein tubulin. Energy transfer is discussed in terms of quantum walk formalism and energy transfer efficiency. Plausibility arguments are presented for the conditions favoring a quantum mechanism of electronic signal propagation along a microtubule.

[1]Funding provided by NSERC.

S1.00152 An exactly solvable model for decoherence-assisted transport , ADRIANA MARAIS, ILYA SINAYSKIY, FRANCESCO PETRUCCIONE, Quantum Research Group, School of Physics and National Institute for Theoretical Physics, University of KwaZulu-Natal, Durban, 4001, SA, ARTUR EKERT, Centre for Quantum Technology, National University of Singapore, 2 Science Drive 3, 117542, Singapore, QUANTUM RESEARCH GROUP, SCHOOL OF PHYSICS AND NATIONAL INSTITUTE FOR THEORETICAL PHYSICS, UNIVERSITY TEAM, CENTRE FOR QUANTUM TECHNOLOGY, NATIONAL UNIVERSITY OF SINGAPORE, 2 SCIENCE DRIVE 3, 117542, SINGAPOR TEAM — The processes of energy and information transfer in quantum networks play an important role for quantum communication and quantum computation. Unavoidable interaction of the quantum system with the environment leads to decoherence and dissipation, processes typically associated with a destruction of quantum coherence in the system. However, recently the signature of long-lasting quantum coherence has been identified in conjugate polymers and in photosynthetic light harvesting complexes. Here we present an exactly solvable model where interaction with a decoherent environment plays a crucial role in assisting the transport in a quantum subsystem. Based on exact solution, we study different regimes of the parameters of the system, and identify the role of the correlations between the environments for assisting of the transitions in the quantum subsystem.

S1.00153 Circularly Polarized Light and Growth of Plants , PAVEL SHIBAYEV, ROBERT PERGOLIZZI, Bergen Academies, Hackensack, New Jersey — The influence of linearly polarized light on the direction of plants growth has been recently demonstrated. The state of circularly polarized (CP) light can also change when it is reflected from the surface of leaves and stems. However, the role of light handedness in the development of plants and CP light interaction with the complexes of chlorophyll molecules have still not been studied enough. In this work, the role of left CP light in the accelerated growth of lentil and pea plants is revealed and studied. The mechanism of such an enhancement is discussed in terms of the model considering transmission, absorption, and scattering of CP light on micro and macro levels of leaf organization. Theoretical modeling of light interaction with the interior of the leaf was conducted for a number of recently proposed models of organization of chlorophyll molecules and chloroplasts. All the calculations were performed by employing a 4x4 matrix method in solving Maxwell equations. It is shown that left-handed chiral organization of chlorophyll molecules can greatly enhance the absorption of light and therefore lead to the enhanced growth of the whole plant under CP light.

S1.00154 Design of Targeted Inhibitors of Polo-like Kinase 1 (Plk1) , D.S. DALAFAVE, The College of New Jersey — Computational design of small molecule inhibitors of Polo-like Kinase 1 (Plk1) is presented. Plk1, which regulates cell cycle, is often overexpressed in cancers. Its downregulation was shown to inhibit cancer progression. Most inhibitors of kinases' interact with the highly conserved ATP binding site. This makes the development of Plk1-specific inhibitors challenging, since different kinases have similar ATP sites. However, Plk1 also contains the polo-box domain (PBD), which is absent from other kinases. In this study, the PBD site was used as a target for designed Plk1 inhibitors. Common structural features of experimentally known Plk1 ligands were first identified. The information was used to design putative small molecules that specifically bonded Plk1. Druglikeness and possible toxicities of the designed molecules were determined. Molecules with no implied toxicities and optimal druglikeness were used for docking studies. The docking studies identified several molecules that made stable complexes with the Plk1 PBD site. Possible utilization of the designed molecules in drugs against cancers with overexpressed Plk1 is discussed.

S1.00155 DelPhi webserver: Comprehensive suite for electrostatic calculations of biological macromolecules and their complexes , SHAWN WITHAM, BRETT BOYLEN, BARR OWESEN, Clemson University, WALTER ROCCHIA, Italian Institute of Technology, EMIL ALEXOV, Clemson University — Electrostatic forces and energies are two of the major components that contribute to the stability, function and interaction of biological macromolecules. The calculations of the electrostatic potential distribution in such systems, which are comprised of irregularly shaped objects immersed in a water phase, is not a trivial task. In addition, an accurate model requires any missing hydrogen atoms of the corresponding structural files (Protein Data Bank, or, PDB files) to be generated in silico and, if necessary, missing atoms or residues to be predicted as well. Here we report a comprehensive suite, an academic DelPhi webserver, which allows the users to upload their structural file, calculate the components of the electrostatic energy, generate the corresponding potential (and/or concentration/dielectric constant) distribution map, and choose the appropriate force field. The webserver utilizes modern technology to take user input and construct an algorithm that suits the users specific needs. The webserver uses Clemson University's Palmetto Supercomputer Cluster to handle the DelPhi calculations, which can range anywhere from small and short computation times, to extensive and computationally demanding runtimes. The work was supported by a grant from NIGMS, NIH, grant number 1R01GM093937-01.

S1.00156 Using DelPhi capabilities to mimic conformational reorganization with amino acid specific dielectric constants[1] , LIN WANG, Clemson University, SUBHRA SARHAR, Clemson, WALTER ROCCHIA, Italian Institute of Technology, EMIL ALEXOV, Clemson University — Many molecular events are associated with small or large conformational changes occurring in the corresponding proteins. Modeling such changes is a challenge and requires significant amount of computing time. From point of view of electrostatics, these changes can be viewed as a reorganization of local charges and dipoles in response to the changes of the electrostatic field, if the cause is insertion or deletion of a charged amino acid. Here we report a large scale investigation of modeling the changes of the folding energy due to single mutations involving charge group. This allows the changes of the folding energy to be considered mostly electrostatic in origin and to be calculated with DelPhi assigning residue-specific value of the internal dielectric constant of protein in the range from 2 to 20. The predicted energy changes are benchmarked against experimentally measured changes of the folding energy on a set of 300 single mutations. The best fit between experimental values and predicted changes is used to find out the effective value of the internal dielectric constant for each type of amino acid.

[1]The work was supported by a grant from NIGMS, NIH, grant number 1R01GM093937-01.

S1.00157 Normal mode analysis with reduced Hessians for multi-scale modeling techniques , AN GHYSELS, University of California - Berkeley, BENJAMIN T. MILLER, National Institues of Health, MICHEL WAROQUIER, Center for Molecular Modeling, BERNARD R. BROOKS, National Institutes of Health — Normal mode analysis is a straight-forward technique to gain insight into the principal motions of molecular systems. Diagonalizing the mass-weighted second derivative matrix (Hessian) results in eigenfrequencies and eigenmodes which indicate the time scale and spatial shape of the vibrations. For large systems, it is often necessary to use Hessians of reduced size in order to limit the required computational resources as well as the amount of information. Methods such as coarse-grained multi-scale models, the Mobile Block Hessian approach, the Vibrational Subsystem Analysis, or the Partial Hessian Vibrational Analysis, focus on specific parts of the spectrum: localized and/or global modes with varying degrees of coupling with the environment. In this presentation, the link between the different approaches will be studied with size-independent metrics and overlap techniques.

S1.00158 Raman Spectroscopy Studies of Normal and Burned Biological Tissue , FARANAK ZARNANI, Department of Physics, University of Texas at Dallas, Richardson, TX 75080, DAVID MAASS, AHAMED IDRIS, Department of Surgery, University of Texas Southwestern Medical Center, Dallas, TX 75390, ROBERT GLOSSER, Department of Physics, University of Texas at Dallas, Richardson, TX 75080 — Burn injuries are a significant medical problem, and need to be treated quickly and precisely. Burned skin needs to be removed early, within hours (less than 24 hrs) of injury, when the margins of the burn are still hard to define. Studies show that treating and excising burn wounds soon after the injury prevents the wound from becoming deeper, reduces the release of proinflammatory mediators, and reduces or prevents the systemic inflammatory reaction syndrome. Also, removing burned skin prepares the affected region for skin grafting. Raman spectroscopy could be used as an objective diagnostic method that will assist burn surgeons in removing burned skin precisely. As a first step in developing a diagnostic tool, we present Raman spectroscopy information from normal and burned ex vivo rat skin, and a comparison of our findings. Raman spectroscopy is explored for its specificity and sensitivity.

S1.00159 Time-resolved infrared structural biology: Identification of Signature Vibrational Signals from the Active Site Tyrosine of Photoactive Yellow Protein , ZHOUYANG KANG, BEINING NIE, LORAND KELEMEN, Departments of Physics, Oklahoma State University, Stillwater, OK, 74078, RACHANA RATHOD, WOUTER D. HOFF, Department of Microbiology & Molecular Genetics, Oklahoma State University, Stillwater, OK, 74078, AIHUA XIE, Departments of Physics, Oklahoma State University, Stillwater, OK, 74078 — Hydrogen bond interactions are indispensable for protein structure and function. We are developing techniques for time-resolved infrared structural biology that offers high sensitivity to hydrogen bonding interactions, excellent time resolution, and a broad time window. Here we report the identification of signature vibrational signals from the active site Tyr42 of photoactive yellow protein for quantifying hydrogen bond interactions using a strategic combination of site-directed mutagenesis (Y76F, Y94F, Y98F, Y118F), specific Tyr isotope labeling, and time-resolved FTIR spectroscopy. These PYP mutants preserve functional activity, thus optimal for probing functionally important structural changes at the active site. This experimental approach is broadly applicable to other proteins, paving the way to transform time-resolved infrared spectroscopy to time-resolved infrared structural biology.

S1.00160 Fluorescence Measurement of Burned Skin Tissues , HECTOR MICHAEL DE PEDRO, CHUAN-I. CHANG, HUE NGUYEN, ANTON MALKO, FARANAK ZARNANI, ROBERT GLOSSER, Physics Department, University of Texas at Dallas, D. MAAS, A. IDRIS, Department of Surgery, University of Texas Southwestern Medical Center — Early removal of affected tissues from burn patients can significantly increase the success of their recovery, since burns continue to spread and damage surrounding tissues after hours of injury. The rationale behind this procedure is that burns trigger the body's immune system to overreact, causing additional damage. Therefore it is important to locate and identify the burn (area and thickness) so that it can be removed as quickly as possible. Our project explores the use of autofluorescence as a tool to identify the burned tissues from healthy ones. Here we present that our fluorescence results show differences between burned and normal skin in both its spectra and lifetime.

S1.00161 Point Spread Diffraction Patterns and Super-Resolution Particle Localization , STEPHEN ANTHONY, SRIPAD RAM, ANISH ABRAHAM, JERRY CHAO, E. SALLY WARD, Dept. of Immunology, UT Southwestern, RAIMUND OBER, Dept. of Electrical Eng., UT Dallas — Sub-diffraction limit localization of fluorophores depends upon fitting the observed photon distribution to the point spread function (PSF). As such, accurate knowledge of the PSF is important to super-resolution microscopy and critical to determining the trajectories and dynamics of molecules within cells. While simple geometrical optics serves well to represent light propagation on the macroscopic level, more elaborate wave representations are necessary to describe light propagation within a few wavelengths of focal points, such as single fluorophores imaged by microscope objectives. As a result, numerous theoretical approximations to experimental PSFs exist as the exact theoretical PSF is unknown. Further consideration must be given that for realistic experiments, frequently events of interest will not entirely match the design conditions of the microscope; most events of interest will not be perfectly in focus, nor can the index of refraction of a living cell be controlled. Additionally, a number of imaging modes explicitly rely upon out-of-focus images. Through serial sectioning microscopy, we explore the experimental PSF in comparison with various models, determining which models are robust and provide accurate sub-diffraction limit localization for realistic data.

S1.00162 Sensing calcium ions at high hydrostatic pressure using the dual-wavelength calcium-sensitive dye indo-1[1] , JORDAN RYAN, PAUL URAYAMA, Miami University — Because calcium often serves as a signaling ion in biological systems, accurate sensing of calcium-ion concentration under pressure is important in understanding cellular piezophysiologic effects. Indo-1 is a dual-wavelength fluorophore routinely used for calcium-ion sensing at ambient pressure, with an emission spectrum that changes upon calcium-ion binding. When subject to physiological pressures of up to 50 MPa, we observe piezochromic behavior in the excited-state emission which depends more on solvent polarity than on solvent viscosity. A two-state model is used to determine the thermodynamic volume change upon calcium dissociation from indo-1, which we find to be consistent with the value for other metal-ion chelators. Since, despite its piezochromicity, indo-1 continues to follow two-state binding-unbinding behavior, indo-1 remains useful under pressure as a probe for quantitative calcium-ion sensing.

[1]Supported by an award from Research Corporation. JR was supported by Miami University's Undergraduate Summer Scholars program.

S1.00163 DLS microrheology at the onset of weak elasticity during thermal denaturation of BSA , ULF NOBBMANN, CARLOS A. REGA, HANNA JANKEVICS, SAMIUL AMIN, Malvern Instruments, Grovewood Rd, Malvern, WR14 1XZ, UK — The ability to precisely detect the onset of protein aggregation to draw insights into microstructural characteristics plays a critical role in a variety of biotechnological applications such as therapeutic protein stability.[1] Rheological techniques are very sensitive to evolution of an aggregating network but have been limited in biotechnology, due to large sample volume and moderately high viscosity requirements in traditional mechanical rheometry. Dynamic Light Scattering (DLS) overcomes these limitations as experiments can be carried out on very dilute samples and small volumes. We present a method based on optical microrheology[2] to study the onset of bovine serum albumin (BSA) aggregation to develop an understanding of the evolving network structure. The exponent of the tracer mean squared displacement power law fit and the elastic modulus G' emerge as two key parameters. The impact of probe chemistry and probe size on the extracted microrheological response is discussed.

[1]A Saluja et al., "Ultrasonic rheology of a monoclonal antibody (IgG_2) solution: implication for physical stability of proteins in high concentration formulations" J. of Pharm. Sci. (2007) 96, 3181-3195.
[2]D Weihs et al., "Bio-microrheology: a frontier in microrheology" Biophys. J. (2006) 91, 4296-4305.

S1.00164 Bacteria turn on surfaces by oversteering with Type IV pili , FAN JIN, University of California, Los Angeles, JACINTA C. CONRAD, University of Houston, MAXSIM L. GIBIANSKY, GERARD C.L. WONG, University of California, Los Angeles — Type-IV pili (TFP) are linear nano-actuators that enable bacteria to crawl on surfaces. Analysis of TFP-mediated crawling in *P. aeruginosa* reveals that it always alternates between two types of distinct movements: a linear translation of constant velocity is followed by a combined translation-rotation that is ∼10x faster in instantaneous velocity. The latter process can turn the cell body by over-steering so that the rear of the cell loses traction with the surface. Orientational distributions of these movements suggest that the former is due to pulling by multiple TFP, whereas the latter is mostly due to release by single TFP.

S1.00165 Automated detection and analysis of key transitions in biofilm formation , TRAVIS THATCHER, BENJAMIN COOLEY, VERNITA GORDON, Center for Nonlinear Dynamics and Department of Physics, University of Texas at Austin — Biofilms are cooperative, dynamic, multicellular systems made of interacting, surface-bound bacteria and/or yeast. The growth of biofilms is an inherently developmental process, characterized by changes in gene expression in response to cues from the environment and other cells. These changes in gene expression are associated with transitions in the behavior of bacteria in the developing biofilm. There are other transitions in behavior that may result from nongenetic influences, such as the conditioning of the surface with bacteria-produced extracellular materials. The early development of biofilms show several key transitions as bacteria move from discrete, swimming cells into surface-bound, dense microcolonies. Each of these transitions is associated with a loss of entropy and, therefore, must result from biological activity that compensates for this loss of entropy. We present a set of approaches for automatically identifying each of these transitions and localizing them in space and time.

S1.00166 Noise Induced Biological Adaptation Differs between Analogous Differentiation Circuits , MARK KITTISOPIKUL, Green Ctr. for Sys. Biology and Dept. of Pharm., UT Southwestern, Dallas, TX USA75390, ANDREW MUGLER, FOM Institute for Atomic and Molecular Physics (AMOLF), Science Park 104, Amsterdam, The Netherlands, ALEKSANDRA M. WALCZAK, Laboratoire Physique Theorique, Ecole Normale Supérieure & CNRS, 24 rue Lhomond, 75231 Paris Cedex 05, France, TOLGA ÇAGATAY[1], CHRIS H. WIGGINS, Dept. of Applied Physics and Applied Math., Ctr. for Comp. Biology and Bioinformatics, Columbia University, New York, NY 10027, GÜROL SÜEL[2] — Analogous genetic regulatory networks with alternate orders of activation and repression can have comparable functions and generate similar average dynamics but differ in terms of stochastic variability (noise). Here we examine if noise affects biological adaptation to stress by comparing the induction dynamics of the native *B. subtilis* competence differentiation network to a synthetic network implemented *in vivo* by Çagatay et al. that recapitulates mean dynamics but differs in noise. We use fluorescence microscopy to study the networks in live cells and stochastic models solved via the spectral method. The adaptability of the organism is affected by the circuit's ability to access different dynamic regimes as a function of stress.

[1]affiliation same as first author
[2]affiliation same as first author

S1.00167 CHEMICAL PHYSICS –

S1.00168 ABSTRACT WITHDRAWN –

S1.00169 Where the Periodic Table of Elements Ends? Additional Explanations

, ALBERT KHAZAN, IMET — Already 40 years ago, physicists claimed that the elements with number higher than 110 cannot exist. However at this day, Period 7 has been complete. Experiementalists syntesed 10 new syperheavy elements during only the last because. The method of synthesis is so finely developed that the experimentalists of Dubna tell about element No.150 as the higher limit of theTable of Elements (they do not provide a ground to the calculation). In contrast, our calculation are based neither on calculation of the stability of the electronic shells of the atoms, nor synthesis of the superheavy elements. Our caculation is based on study of the chemical processes, which give a new law of the Periodic Table (Albert Khazan. Upper Limit in Mendeleev's Periodic Table—Element No. 155. Svenska fysikarkivet, Stockholm, 2009). The core of the delusion of numerous scientists was that they, in their calculationsbased on Quantum Mechanics, initially set up the number of the elements (number of the protons) then calculated the atomic mass proceeding from the data. According to our theory, the atomic mass of the last element (411.66) should be calculated first, only then its number (155)!

S1.00170 Scaling of Nonclassical Nucleation Rates of Methanol

, GERALD WILEMSKI, FAWAZ HRAHSHEH, Missouri University of Science and Technology, Rolla MO, ABDALLA OBEIDAT, Jordan University of Science & Technology, Irbid, Jordan — Nonclassical gradient theory (GT) calculations of nucleation rates are presented for methanol, an associating vapor system. The calculations use the SAFT-0 equation of state (EOS) that accounts for the effects of molecular association based on the statistical association fluid theory (SAFT). Calculated rates were compared to the experimental rates of Strey, et al. [*J. Chem. Phys.* **1986**, 84, 2325]. The GT nucleation rates showed improved T and Sdependence compared to classical nucleation theory (CNT). The GT rates were also improved by factors of 100-1000 compared to CNT. Despite these improvements, GT does not describe the reported T and S dependence of the nucleation rates. To explore this further, the GT and experimental rates were analyzed using Hale's scaled model [*J. Chem. Phys.* **2005**, 122, 204509]. This analysis reveals an inconsistency between the predictions of GT, which scale relatively well, and the experimental data, which do not scale. It also shows that the measured rate data have an anomalous T and S dependence. A likely source of this anomaly is the inadequate thermodynamic data base for small cluster properties that was used originally to correct the raw rate data for the effects of association.

S1.00171 Hybrid Monte Carlo Method In Path Space

, PATRICK MALSOM, FRANK PINSKI, University of Cincinnati — We are interested in understanding the ways a collection of atoms are able to undergo conformational change, or change of state. In particular, we are studying atoms as they move under Brownian (over-damped Langevin) dynamics. In many cases, such transitions are blocked by an energy barrier and conformational changes become rare events when the thermal energy is small compared to the barrier height. Our technique attempts to sample these transition paths efficiently while preserving the sample's thermodynamic significance. Our approach is based on a Hybrid Monte Carlo scheme (Beskos *et al.*) that incorporates auxiliary variables. The relative probability of paths is computed using the Onsager-Machlup functional. This method correctly handles the fractal nature of the Brownian paths. We illustrate this method by investigating one of the low energy transitions in the 14-atom Lennard-Jones cluster. In addition, we will show preliminary results for the gas-to-liquid transition in a 2-dimensional Lennard-Jones system.

S1.00172 Small methanol cluster growth/decay rate constant ratios and application to nucleation data analysis

, BARBARA HALE, GERALD WILEMSKI, Missouri University of Science & Technology — The Bennett Monte Carlo technique is used to calculate growth/decay rate constant ratios for small methanol clusters using the model potential of van Leeuwen and Smit [J. Chem. Phys. **99**, 1831 (1995)] at temperatures of 220K, 240K and 260K. The resulting data are used to examine temperature scaling properties of the rate constant ratios and to illustrate how heat release from subcritical cluster formation affects the results of adiabatic nucleation rate measurements.

S1.00173 A Look at a Seires of Alkyl and Perfluoroalkyl Bromides

, BRITTANY LONG, GARRY GRUBBS, STEPHEN COOKE[1], University of North Texas, RADIO SPECTROSCOPY GROUP TEAM — The pure rotational spectrum of bromoperfluoroethane between 9.0-13.0 GHz has been measured on a chirped pulse Fourier transform microwave spectrometer. A total of 839 transitions were observed for the six isotopolouges. Only the $trans$ conformer was observed for which the rotational constants are reported. Nuclear electric quadrapole coupling constants have been determined and reported. Also, two dipole forbidden/quadrapole allowed $\Delta J = 2$ transitions were observed in the spectra.

[1]Research Advisor

S1.00174 Water-like Anomalous Properties and Polyamorphism in a Liquid with Smooth (Differentiable) Pair Interactions[1]

, JOEL ABRAHAM, NICOLAS GIOVAMBATTISTA, Department of Physics, Brooklyn College-CUNY, Brooklyn, NY 11210, USA — We perform molecular dynamics simulations of a system of particles interacting via a spherically symmetric, core- softened pair potential, which is a smooth version of the (non- differentiable) Jagla pair potential. Although liquid properties are extremely sensitive to the details of the pair interactions, we show that the smooth version of the Jagla potential preserves the main properties of the original model. Specifically, both pair potentials result in liquids that show (i) water-like thermodynamic and dynamical anomalous properties, as well as (ii) liquid and (iii) glass polymorphism (i.e., the presence of more than one liquid and glass form, respectively). The pressure-temperature phase diagram of our smooth potential shows, as observed in computer simulations using the Jagla model, a liquid-liquid first order transition line separating two liquid phases and ending in a critical point; such a critical point being accessible in equilibrium simulations.

[1]We thank the Research Foundation of CUNY for support (PSC-CUNY 40)

S1.00175 Modeling Adsorption on fcc(nnm) Surfaces[1]

, ALAIN PHARES, Villanova University, DAVID GRUMBINE, JR., St. Vincent College, FRANCIS WUNDERLICH, Villanova University — In general, fcc(*nnm*) surfaces consist of very long armchair (111) terraces separated by steps. The number M of atomic sites in the width of the terraces depends on the Miller indices (*nnm*). The model considers values of $M \leq 6$, with adsorbate-substrate interaction energy on step-sites different from those on bulk sites, takes into account first- and second-neighbor adsorbate-adsorbate interactions, and specializes to the case of attractive first-neighbors. We obtain the complete low temperature, 3-dimensional, energy phase diagrams. The occupational configurations of the phases exhibit features similar to those of the phases obtained in the infinite-width limit, or flat fcc(111) surfaces. This yields a classification of the phases into types, and, within each type, the phases are grouped into families. This suggests a number of generalizations for any value of M beyond 6, leading to a better understanding of the competing interaction energies and of the evolution of the phase diagrams with increasing width M of the terraces. The relevance of these results to experiments is discussed within the context of preferential adsorption on step sites, and applied to the adsorption of water on Pt(335).

[1]Work supported in part by NSF through TG-resources by PSC and NICS, grant # TG-CHE050014N.

S1.00176 Tethering Peptides to Functionalized Self-Assembled Monolayers on Gold Through Two Chemical Linkers Using the Huisgen Cycloaddition[1]

, IGNACIO GALLARDO, The University of Texas at Austin, LAUREN WEBB — A biocompatible platform has been made by tethering a helical peptide to a surface at two points. The presence of the peptide should be an ideal interface between inorganic substrates and proteins. The artificially synthetized alpha-helical peptide composed of alternating leucine and lysine residues, with two residues replaced with cyanophenylalanine to react with two neighboring surface-bound azide groups is linked to the azide-terminated self-assembled monolayer through a tetrazole made by a Husigen Cycloaddition. Surface analysis is done with ellipsometry, infrared spectroscopy and x-ray photoelectron spectroscopy. The cycloaddition and reaction conditions are supported by similar reactions of other smaller molecules like Methoxybenzonitrile and controls show no physisorption under our reaction conditions. Reaction yields from 80 to 98 percent are reported from the optimized reactions. The helical structure of the peptide in solution has been confirmed under our reaction conditions with circular dichroism and the peptide amide I and II modes studied by infrared spectroscopy and their comparison with a computational model of the peptide showed that the peptide is probably randomly oriented on the surface.

[1]Army Research Office (Grant No. W911NF-10-1-0280).

S1.00177 Size effect of silicon nanowires on their pH response

, SEONGJAE LEE, IN-BOK BAEK, XIANHONG LI, Hanyang University — The silicon nanowire is a promising material for the bio-chemical electronic sensors because the local change in the surface charge density can be easily transduced to the conductivity change of the nanowire due to its high surface-to-volume ratio. We investigated the pH-dependent electronic transport characteristics of FETs comprised of silicon nanowire channels of different sizes. Starting from the p-type SOI wafer with the top silicon layer of 40 nm thickness, we employed the conventional 'top-down' process to fabricate the FET devices with various silicon nanowires: 100, 135, 180, 220, 300 nm in width and 2, 5, 10, 20 μm in length. The devices were electrochemically characterized by I_D-V_G measurements with a reference electrode as a gate in the phosphate buffer solutions of a pH value ranging from 2 to11. The threshold voltages of all devices were extracted from the I_D-V_G curves and their relations to pH were compared with simulation results based on the Gouy-Chapman-Stern-Graham model. A good linear relation between the threshold voltage and pH was observed for all devices in the range of 4 $<$ pH $<$11 with a high sensitivity of 56 mV/pH which is much higher than the bulk devices and very close to the Nernst limit. However, the systematic increase of a threshold voltage shift as decreasing nanowire's dimension (width and length) was also observed and possible origins are discussed within the scope of the Gouy-Chapman-Stern-Graham model.

S1.00178 Role of Surfactant Molecular Structure on Self Assembly: Aqueous SDBS on Carbon Nanotubes[1]

, MANASWEE SUTTIPONG, Chulalongkorn University, JOHN R. THOMPSON, NAGA RAJESH TUMMALA, The University of Oklahoma, BOONYARACH KITIYANAN, Chulalongkorn University, ALBERTO STRIOLO, The University of Oklahoma — Stabilizing aqueous dispersions of carbon nanotubes mono-dispersed in diameter and chirality remains elusive. Surfactants have proven useful in deploying ultra-centrifugation techniques, but the molecular mechanism responsible for their effectiveness remains not fully understood. Based on a number of recent molecular simulation results, including those from our group, it appears that the morphology of the self-assembled surfactant aggregates on the carbon nanotubes strongly affects the effective potential of mean force between pairs of interacting carbon nanotubes. In this work we explore the effect of surfactant molecular structure on the properties of aqueous surfactant self-assembled aggregates. We employ equilibrium all-atom molecular dynamics simulations. We consider the surfactant SDBS (sodium dodecyl benzene sulfonate) with benzene ring located on the fifth or on the twelfth carbon atom in the tail, and the surfactant AOT [sodium bis(2-ethylhexyl) sulfosuccinate]. The simulations are conducted at room conditions for different surface coverages on (6,6), (12,12), and (20,20) single walled carbon nanotubes. These new results will help us identify the surfactant properties that allow us to manipulate nanotube-nanotube effective interactions.

[1]Research supported by the Department of Energy via CANTEC.

S1.00179 Properties of Aqueous Electrolytes within Narrow Slit-Shaped Pores[1]

, TUAN A. HO, DIMITRIOS ARGYRIS, ALBERTO STRIOLO, The University of Oklahoma, School of Chemical, Biological and Materials Engineering — We report equilibrium molecular dynamics simulation results for structural and dynamic properties of aqueous electrolyte solutions confined within narrow pores. The slit-shaped pores are carved from cristobalite silica, corundum alumina, magnesium oxide, and other materials. The pore width is in the range 0.8 – 2.0 nm. The aqueous solutions contain NaCl, CsCl, $CaCl_2$, and $SrCl_2$ electrolytes at 1M concentration or larger. Equilibrium simulations are performed at ambient conditions within the NVT ensemble. The data suggest the formation of layered structures, which are consistent with results obtained for thin films of solution supported on free-standing surfaces. However, confinement enhances the differences in transport properties observed between those ions that are near the solid and those at the pore center. Because the self-diffusion coefficient is faster as the distance from the solid increases, the ions that are at the pore center diffuse more quickly through the pore than those adsorbed closer to the wall. Thus our results could be used to design membranes to separate, e.g., aqueous NaCl from CsCl solutions.

[1]Research supported by the Department of Energy and, in part, by the National Science Foundation.

S1.00180 Chemisorption of Guanine on Cu(110)

, JERONIMO MATOS, ABDELKADER KARA, University of Central Florida — We use density functional theory (PBE) to calculate the adsorption of a guanine molecule on Cu(110). At saturation coverage, guanine adsorbs tilted with the oxygen atom strongly bound to one of the surface atoms at a height of 2.12 Å above this surface atom with a binding energy of 430 meV/molecule. The substrate top layer atoms show a buckling of 0.22 Å , while the molecule experiences a twist from the flat configuration in the gas phase. The dz^2 state of the copper atom -that is bound to the oxygen atom- presents an enhancement in its density near the Fermi level. We calculated a drop in the work function of 0.34 eV upon adsorption of guanine on Cu(110). These effects classify this system as chemisorption.

S1.00181 Proton transfer induced by receding water in Glycine—$(Water)_2$ Complex

, RAJEEV PATHAK, Department of Physics, University of Pune, India — We investigate molecular co-operativity in the zwitterionic configuration of Glycine (Gly) with two proximal water molecules, Gly—$(Water)_2$, by deliberately making one of the water molecules recede from the remaining complex. The consequent intra-molecular proton transfer that renders the zwitterionic configuration into a neutral one is viewed under two scalar field descriptors: Molecular Electrostatic Potential (MESP), reflecting the modifications in the environment and the HOMO (highest occupied molecular orbital) electron density. We quantify the process further by energetics, through a many-body analysis of the interaction energy as well as salient IR spectral signatures associated with the proton-transfer. While we employ the decent MP2/aug-cc-pvDZ level of theory to seek optimal structures, it is gratifying that a prescription within density functional theory (DFT) also provides a reliable description of this process.

S1.00182 Compositional-Dependent Structural Analysis of Cu_xPt_{38-x} Nanoparticles

, JOSAFAT GUERRERO-JORDAN, Posgrado en Ciencias (Fisica), Universidad de Sonora, ROY L. JOHNSTON, School of Chemistry, University of Birmingham, ALVARO POSADA-AMARILLAS, Dept. Inv. en Fisica, Universidad de Sonora — We present an exhaustive study of the lowest energy Cu_xPt_{38-x} clusters structures obtained through a genetic algorithm, which incorporates the Gupta potential to mimic interatomic bonding. A symmetric parameterization of the Gupta potential was used including a weighting factor (w) in order to search for different potential energy surfaces describing 38-atom Cu-Pt nanoparticles. This weighting factor was varied from 0 to 1 in steps of 0.1 to obtain a structure map which provides information on the structural distribution in terms of the composition. According to this structure map, the most abundant structural motif corresponds to the truncated octahedron. Atomic segregation was maximum for w = 1.0. We also present the plot of excess energy as a function of the weighting factor values for the complete compositional range. The most stable structures were found for w = 0.0. The most relevant structures were chosen to be reoptimized by using the DFT method. We found that the interatomic distances changed compared to those obtained with the genetic algorithm.

S1.00183 Evidences of Homogenous Nucleation in Nano Confined Secondary Alcohol[1] , SAMUEL AMANUEL, AMER KHRAISAT, JARGALSAIKHAN DULMAA, Department of Physics and Astronomy, Union College, Schenectady, NY 12308 — We have made comparative measurements to study the phase transition of physically confined 2-decanol in nano porous silica in the presences of excess bulk 2-decanol. We have systematically controlled the amount of excess bulk and studied how its existence influences freezing and melting temperatures. It appears that there is a lower limit in size, where freezing of the confined is not influenced by the presences or absence of the bulk. In our case this lower limit occurred with the average pore diameter of 100 nm. For 2-decanol confined in pore sizes larger than 100 nm, however, its freezing occurred at T = -23 $^\circ$C, which was triggered by the freezing of the excess bulk. In absence of the bulk, freezing occurred at a lower temperature depending on size. Melting of the confined 2-decanol, on the other hand, was not influenced by the presences or absence of the bulk. Generally, the melting of the confined 2-decanol preceded the melting of the bulk. These suggest that the nucleation of 2-decanol confined to pore sizes less than 100 nm is homogenous and controlled by its extent of supercooling.

[1]This work has been supported by Faculty Research Fund, Union College.

S1.00184 Universal Patterns of Cluster Growth in Aqueous Sugars Observed by Dynamic Light Scattering[1] , TRI TRAN, DAVID SIDEBOTTOM, Creighton University — Dynamic light scattering was performed on aqueous sugar solutions to monitor the growth of sugar clusters as a function of sugar concentration and temperature. Three sugars (glucose, maltose and sucrose) were investigated. Analysis of the hydrodynamic radius of the diffusing clusters suggests a two-stage process of cluster growth. At low volume fractions of sugar, a cluster phase consisting of nearly monodisperse clusters forms with a mean cluster mass that increases in proportion to the volume fraction. A second stage of growth develops when clusters reach a size where they begin to overlap. In this later stage, cluster-cluster aggregation occurs and the cluster size grows in a common, but temperature dependent, power law fashion in advance of a percolation threshold near 83 wt% sugar.

[1]This work is supported by a grant from National Institute of Biomedical Imaging and Bioengineering (R01EB009644)

S1.00185 Quantification of molecular topology using small angle scattering. , RAMNATH RAMACHANDRAN, DURGESH RAI, GREGORY BEAUCAGE, University of Cincinnati — A recent method to quantify molecular topology of various materials using small angle scattering will be presented. Small angle x-ray and neutron scattering has been used to characterize ceramic aggregates and polymer structures systems respectively. The structural differences in various systems arise from the competition between thermal and spacial constraints. The details in ceramic aggregates like branch fraction, number of segments in an aggregate and the short circuit path, coordination number, the number end groups *etc* are extracted. Amongst the polymer systems, details of topological quantification of polymer systems such as stars, cyclics and branched polymers like polyolefins will be presented. In polyolefins, the method provides a unique measure of the average long-chain branch length and the hyperbranched (branch-on-branch) characteristics. The quantification using scaling models are important in order to understand the structure-property relationship amongst materials.

S1.00186 Effects of Iridium interfacial nanolayers on stability and barrier hights of TCO/Si nano-holes Solar cell structures , BED SHARMA, MOHEMAD BOUANANI, University of North Texas — There is still a significant gap between currently achieved efficiencies and theoretical one. A fundamental understanding of physico-chemical and electronic properties as well as tuning and control of transparent conducting oxides (TCOs) and nano-structured semiconductor absorber material interfaces is critical. One of the many issues is the suspected formation of silicon oxides due to transport of oxygen from TCO to silicon that degrades the effectiveness of light generated charge transfer which eventually degrades final efficiency of solar cell. The fabrication of 3-D nano-holes in Si was obtained by electrochemical etching through anodic nano-porous alumina. The nano-porous alumina was prepared by depositing thick 1micrometer aluminum layer on RCA cleaned Si samples, annealing in Ar and using hard anodization process. One to few mono-layers of Ir were inserted at the TCO/Si interfaces to block the depletion of oxygen to stabilize the interface and tune its barrier height. Both ITO and ZnO were used as TCOs. The effect of Ir on the band alignment at these interfaces is evaluated by Ultraviolet Photoelectron Spectroscopy (UPS). The interface stability and chemical nature is evaluated by X-ray Photoelecton Spectroscopy (XPS).

S1.00187 Charge transfer energies of tetraphenyl-porphyrin-fullerene dyads[1] , RAJENDRA ZOPE, University of Texas at El Paso, MARCO OLGUIN, University of Texast at El Paso, TUNNA BARUAH, University of Texas at El Paso — Porphyrin-fullerene dyads are extensively studied for their photoinduced charge transfer properties. They form a donor-acceptor pair where the fullerene is the acceptor. Accurate theoretical estimate of the charge transfer energies in such systems has proven to be a challenge. In this study we examine the charge transfer energetics for such dyads using our recently developed density functional based excited state method which can yield reliable estimates of charge transfer energetics. In this study the effect of varying both the donor and acceptor components are studied by changing the tetra-phenyl-porphyrin (TPP) to Zn-TPP. Similarly the acceptor component is changed from C60 to C70. The structures were optimized using DFT-D3 theory at the all-electron level. Among the donor-acceptor pairs studied, we find that the ZnTPP-C60 has the lowest charge transfer energy (1.69 eV) and the TPP-C70 (2.13 eV) has the highest charge transfer energy.

[1]Supported by the Division of Chemical Sciences, Geosciences and Biosciences, Office of Basic Energy Sciences of the US Department of Energy through grant DE-SC0002168.

S1.00188 Strong field DC slice imaging , LU YAN, Department of Chemistry, Wayne State University, Detroit, MI, 48202, MICHAEL DOYLE, YUNFEI LIN, WEN LI, ARTHUR SUITS — A new, "universal" variation of the DC slice ion imaging method is reported. This approach allows the central slice of the photofragment ion cloud to be recorded and the relevant speed and angular distributions for a molecular photodissociation to be obtained without any inversion methods, but does so using femtosecond non-resonant strong-field ionization. The probe laser is also implemented in a "raster imaging" approach that records only the central section of an expanded photofragment distribution and avoids interaction with the molecular beam itself. This is achieved by using the probe laser displaced off-axis from the molecular beam with application a narrow time gate to a multichannel plate detector. To avoid high background level and space charge effect, the detection region is in ultrahigh vacuum and we utilize a second differential stage to the molecular beam. Several examples will be presented illustrating the method.

S1.00189 FLUIDS AND SOFT MATTER –

S1.00190 Molecular Dynamics of Colloidal binary mixtures in an electric field , MANUEL VALERA, ATHULA HERAT, ETHAN CORLE, Slippery Rock University — We have studied a system of colloidal binary mixtures in an external electric field. The simulations were performed in the string fluid regime, low packing fraction, and high density regime under the influence of a strong electric field. In the dilute regime we studied the system structure for different concentrations and size ratios. For the high density regime we studied a 50:50 concentration with a size ratio or 1.2/1.0. We show the pair correlation function and diffusion coefficient. A partial phase diagram for the 50:50 concentration and 1.2/1.0 size ration is also presented.

S1.00191 Capillary Condensation: Novel Method for Patchy Particle Fabrication[1]

, NINA IVANOVA, NICOLE ZACHARIA[2], Texas A&M University — Patchy particles are patterned particles with at least one patch for anisotropic interaction. A novel route for their synthesis involves capillary condensation of a chemical species into the voids of an ordered colloidal sphere array. Polystyrene and silica particles ranging in diameter from 20 nanometers to 1 micron are assembled into crystalline arrays via evaporation induced self-assembly. The chemical condensed into the voids is then reacted with metal nanoparticles to produce novel patchy particles. The particles are characterized using FTIR, EDX and SEM. The size of these patches is quantitatively shown to reduce in size in proportion with increased particle radius. Surface Enhanced Raman Spectroscopy is explored as one of the possible applications for these novel particles.

[1]Special thanks for financial support is extended to Texas Engineering Experiment Station (TEES) and Texas A&M University, Department of Mechanical Engineering.
[2]Professor

S1.00192 Phase Equilibrium Model for Nanoparticle-Filled Nematic Liquid Crystals

, EZEQUIEL SOULE, Dept. of Chemical Engineering, McGill University,Montreal, Canada - Nanomaterials Group, Institute of Materials Science, Mar del Plata, Argentina, JONATHAN MILETTE, LINDA REVEN, Dept. of Chemistry, McGill University, 801 Sherbrooke St. W, Montreal, H3A2K6, Qc, Canada, ALEJANDRO REY, Dept. of Chemical Engineering, McGill University,3610 University St, Montreal, H3A2B2, Qc, Canada — This work presents an integrated characterization of phase transitions and structure formation in mixtures of nanoparticles (NP) and liquid crystals (LC), by means of a model for phase equilibrium and an experimental study on the system composed by 5CB and gold NPs. The model takes into account mixing, nematic ordering of the LC, crystalline ordering (self-assembly) of NPs, and LC-NP interactions. Generic features of phase diagrams for NP-LC mixtures are discussed. The model can explain some experimental observations, like the formation of NP aggregates and distinctive nematic textures, as a function of experimental parameters like NP concentration and the nature of the NP surface are changed. The parameters that produce these changes in phase behaviours can be directly correlated with experimental variables.

S1.00193 Observation of nematic/smectic liquid crystal configurations in a prolate spheroidal confinement

, JOONWOO JEONG, MAHN WON KIM, KAIST — Polymer-dispersed liquid crystal (PDLC) is a composite of dispersed LC droplets in a polymer matrix. The electro-optic properties of PDLCs, such as reorientation field strength and response time, are strongly related to the director configuration. Various factors including the intrinsic properties of LC/polymer and the size/shape of droplets affect the liquid crystal configuration. A balance between the bulk elastic energy and the surface anchoring energy determines the configuration. To study systematically the effect of size/shape of droplets on the configuration, we have prepared thin PDLC films with 4-Cyano-4'-pentylbiphenyl (5CB)/ 4-Cyano-4'-octylbiphenyl (8CB) and Polydimethylsiloxane (PDMS) elastomer. Using polarized optical microscopy, we have observed the change in the director configuration of LC droplets as a function of the aspect ratio up to 6 by stretching the film unidirectionally. We have also observed the effect of surface anchoring on the configuration.

S1.00194 Automation of Dielectric Characterization of Liquid Crystals

, SHANE DRYE[1], JOSAPHAT UVAH[2], CHANDRA PRAYAGA[3], University of West Florida — This report describes the complete automation of a setup for the dielectric characterization of liquid crystals (LC). A capacitor cell filled with the LC 8CB is housed in a temperature controlled environment. The temperature of the sample is varied between 25°C and 45°C with a stability and precision of 0.001K, with a PTC10 PID controller. The range covers the phase transitions of the LC. The purpose is to measure the dielectric properties of the liquid crystal near the phase transitions. The capacitance is measured with a SR830 lock-in amplifier and a Fluke4360 LCR meter upto 100kHz. An Agilent 4395A Network Analyzer is used to extend the frequency into the MHz range. In this work, the entire process is automated. All the instruments are connected to a computer through a GPIB (IEEE-488) interface. The program is designed using LabVIEW to control the instruments, send commands and inputs including temperature range and frequencies, receive data, calculate the capacitance, and plot the data automatically. Results of measurements will be presented.

[1]Undergraduate Student
[2]Department of Mathematics
[3]Department of Physics

S1.00195 Carbon nanotubes effects on the order parameter and crystal structure of 5CB liquid crystal

, GEORGI GEORGIEV, ERIN GOMBOS, MICHAEL MCINTYRE, Assumption College, PEGGY CEBE, Tufts University, ASSUMPTION / TUFTS TEAM — Carbon nanotubes (CNTs) are elongated anisotropic molecular size cylinders that can form a liquid crystal (LC) phase in lyotropic solutions. When dispersed in LCs their nematic directors couple. We have observed a large downshift in transition voltage during Freedericksz transition in LC/CNT nanocomposites. We are interested in the effect that CNTs have on the order parameter of LCs and their phase diagram and crystal structure. We measured using polarized UV/Vis absorption spectra a systematic increase of the order parameter of LC/CNT cells with increase of the CNTs content. The order parameter vs temperature slope decreases with increased CNTs content, which shows that CNTs support an increased order of the LCs to higher temperatures. This makes the Nematic-to-Isotropic transition sharper increasing its first order phase transition characteristics. The main mechanism for the strong nematic coupling is pi-pi stacking between the aromatic rings of the CNTs and LCs which we measure using FTIR and Raman difference spectroscopy. Through Polarized Microscopy, Ellipsometry and DSC we observed a change in crystalline order and an increase in nematic to crystal phase transition temperature with increasing CNTs concentration due to their crystal nucleation activity.

S1.00196 Brownian motion of particles in nematic fluids

, XUXIA YAO, KARTHIK NAYANI, JUNG PARK, MOHAN SRINIVASARAO, Georgia Institute of Technology — We studied the brownian motion of both charged and neutral polystyrene particles in two nematic fluids, a thermotropic liquid crystal, E7, and a lyotropic chromonic liquid crystal, Sunset Yellow FCF (SSY). Homogeneous planar alignment of E7 was easliy achieved by using rubbed polyimide film coated on the glass. For SSY planar mondomain, we used the capillary method recently developed in our lab. By tracking a single particle, the direction dependent diffussion coefficients and Stokes drag were measured in the nematic phase and isotropic phase for both systems.

S1.00197 Fluorescence of CdSe nanoparticles in the Liquid Crystal 8CB near the Phase Transitions

, JODIE GRAY, SHANE DRYE, DARREN NORTH, SAMUEL BECK, Undergraduate Physics Research, TIM ROYAPPA, Department of Chemistry, LASZLO UJJ, CHANDRA PRAYAGA, Department of Physics — The liquid crystal 4'octyl—4-cyanobiphenyl (8CB) doped with cadmium selenide nanoparticles was injected into a commercially available liquid crystal cell (INSTEC, Inc). The cell was housed in a temperature controlled environment constructed in the lab and exposed to light from a frequency doubled Nd: YAG laser. Fluorescence from the sample was filtered from the incident light and detected using a photodiode and measured with a lock-in amplifier. Measurements have been made over the temperature range 25° to 45°C. The sample was stabilized at each temperature, and the fluorescence intensity was measured at several temperatures. The results show a significant change in fluorescence near the nematic-isotropic phase transition. The temperature control and precision allowed more than 1000 data points to be taken between 25-50°C, with most of these clustered in the transition region between 38.5– 39.5°C, where the change in intensity was observed.

S1.00198 Spectral Measurements of Fluorescence of CdSe nanoparticles in Liquid Crystals near Phase Transitions

, SAMUEL BECK, JODIE GRAY, SHANE DRYE, DARREN NORTH, Undergraduate-Physics Research, TIM ROYAPPA, Department of Chemistry, CHANDRA PRAYAGA, LASZLO UJJ, Department of Physics — The liquid crystal 4'octyl-4-cyanobiphenyl (8CB) doped with cadmium selenide nanoparticles was injected into a commercially available liquid crystal cell (INSTEC, Inc). The cell was housed in a temperature controlled environment constructed in the lab and exposed to light from a frequency doubled Nd: YAG laser. The spectrum of fluorescence from the sample was measured at several temperatures over the range 250 to 450C, covering the smectic-nematic and nematic-isotropic phase transitions. The sample was held at each temperature with a precision and resolution of 1mK before taking the spectrum. It was therefore possible to approach very close to the phase transitions. The results show a significant change in the fluorescence spectrum near the nematic-isotropic phase transition.

S1.00199 Electro-optical properties of polymer-dispersed liquid crystals containing gold nanoparticles[1]

, ALFONSO HINOJOSA, SURESH SHARMA, UT Arlington — It is known that additions of relatively small concentrations of gold nanoparticles (Au NPs) can significantly change electro-optical properties of a polymer-dispersed liquid crystal (PDLC). For example, it has been shown that the addition of Au NPs to a PDLC microstructure lowers the operating voltage and increases transmission in a manner that depends on the concentration of the NPs and applied electric field.[2] We have extended these measurements to PDLCs synthesized with a different liquid crystalline material and doped with varying concentrations of the Au NPs. We discuss the electro-optical data on two different PDLCs as functions of the concentration of the Au NPs, as well as the polarization and intensity of the incident laser beam. We also present ideas to assess the role of the surface plasmon excitations in modifying the electro-optical properties of Au NPs containing PDLCs.

[1]Supported, in part, by US Department of Education GAANN grant P200A090284-10

[2]A. Hinojosa and S. C. Sharma, Applied Physics Letters, **97**, 081114 (2010)

S1.00200 Fluorescence decay of CdSe nanoparticles in Liquid Crystals near Phase Transitions

, DARREN NORTH, SAMUEL BECK, JODIE GRAY, SHANE DRYE, Undergraduate Physics Research, CHANDRA PRAYAGA, LASZLO UJJ, Department of Physics, TIM ROYAPPA, Department of Chemistry — The liquid crystal 4'octyl-4-cyanobiphenyl (8CB) doped with cadmium selenide nanoparticles (Sigma-Aldrich) was injected into a commercially available liquid crystal cell (INSTEC, Inc). The cell was housed in a temperature controlled environment constructed in the lab and exposed to light from a frequency doubled pulsed Nd: YAG laser. The decay of fluorescence from the sample was measured at several temperatures over the range 25° to 45°C, covering the smectic-nematic and nematic-isotropic phase transitions. The sample was held at each temperature with a stability and resolution of 1mK before taking the measurement. The fluorescence was detected using a high-speed detector and the decay was measured using a boxcar averager. With the temperature control available, it was possible to approach very close to the phase transitions, with milliKelvin resolution. The results show a significant change in the decay of fluorescence near the nematic-isotropic phase transition.

S1.00201 Deformable viscoelastic cholesteric films with nanoparticles

, PETR SHIBAEV, CRISTINA SCHLESIER, Department of Physics, Fordham University, New York — Large spectral shifts of the selective reflection band and color changes are achieved in highly viscous mixture of cholesteric polymers and low molar mass liquid crystals filled with nanoparticles and subject to mechanical deformations. The color of the material changes instantaneously during deformation; the time for the color to be completely restored increased with the viscosity of the polymer mixture. The viscosity increases with increasing concentration of polymer or nanoparticles. This composite material was used to build highly sensitive mechanical sensor that was used to visualize both stress and deformation. The model describing the relation between the color and deformation is suggested. This model takes into account non-linear response to deformation and structural rearrangements inside the liquid crystalline matrix.

P.V. Shibaev, R. Uhrlass, S.Woodward, C. Schlesier, and Eckhard Hanelt, Liquid Crystals, v.37, pp. 587-592, 2010

S1.00202 Specific heat at the micellization and phase transitions in a triblock copolymer-water system[1]

, LORENZO DUMANCAS, DAVID SIMPSON, D.T. JACOBS, The College of Wooster — The triblock copolymer ("unimer") of PPO-PEO-PPO (commercially known as 17R4) has hydrophobic ends and a hydrophilic center. When placed in water, a network of unimers can self-assemble at higher concentrations or temperatures to form micelles of different geometries. We have measured the micellization line marking the transition from only unimers in solution to some micelles. There is also a one- to two-phase transition at higher temperatures that is an Ising-like, LCST critical point. Specific heat measurements from our adiabatic calorimeter provide the enthalpy, entropy and free energy of micellization along the micellization line at different prepared compositions.

[1]We acknowledge the support from Research Corporation, NSF-REU grant DMR 0649112, and The College of Wooster.

S1.00203 Vesicle membrane fluctuations at nm resolution

, KEJIA CHEN, SUNG CHUL BAE, CHANG-KI MIN, STEVE GRANICK, University of Illinois at Urbana-Champaign, GRANICK GROUP TEAM — We measure membrane thermal fluctuations with nanometer spatial resolution and microsecond time resolution, extending a scattering technique used at the Curie Institute to study red blood cell dynamics (Timo Betz et al., Proc. Nat. Acad. Sci. USA 106, 15320, 2009). A laser beam is focused at the leading edge of a phospholipid vesicle membrane and the forward scattered light is detected by a quadrant photodiode. The measurements over 4 orders of magnitude of frequency allow quantification of more complete fluctuation spectra than competing methods, and therefore fuller understanding of the vesicle membrane mechanics. As a proof of concept, we quantify how adsorbed nanoparticles stiffen giant unilamellar vesicles (GUVs).

S1.00204 Interactions of End-Functionalized Nanotubes with Lipid Vesicles: Spontaneous Insertion and Nanotube Self-organization

, MEENAKSHI DUTT, OLGA KUKSENOK, University of Pittsburgh, MICHAEL NAYHOUSE, University of California at Los Angeles, STEVEN R. LITTLE, ANNA C. BALAZS, University of Pittsburgh — Via Dissipative Particle Dynamics (DPD) approach, we study the self-assembly of amphiphilic nanotubes into a lipid vesicle, which is immersed in a hydrophilic solvent. Individual lipids are composed of a hydrophilic head group and two hydrophobic tails. Each nanotube encompasses an ABA architecture, with a hydrophobic shaft (B) and two hydrophilic ends (A). To allow controlled transport through the nanotube, we also introduce hydrophilic tethers at one end of the tube. We show that nanotubes initially located in the outer solvent spontaneously penetrate the vesicle's membrane and assume a trans-membrane position, with the hydrophilic tethers extending from the surface of the vesicle. We add nanotubes one at a time after the previous nanotube has been inserted. We characterize the interactions among the nanotubes that have self-assembled into the vesicles' membrane and focus on their clustering within the membrane. We also show that the nanotube insertion and clustering within the vesicle strongly affects the vesicle shape in cases of a sufficiently large number of tubes. Ultimately, these nanotube-lipid systems can be used for making hybrid controlled release vesicles.

S1.00205 Electrospray fabrication and osmotic response of fluid core-viscoelastic shell microcapsules , ZHIYONG MENG, CHINEDUM OSUJI, Yale University — Microcapsules with fluid-core in viscoelastic shell is interesting partially because of their unusual elasticity/rigidity. Electrospray technique, more flexible and scalable than traditional bulk and microfluidic emulsification, was used to generate spherical microcapsules. In particular, sodium alginate fine droplets generated by electrospray was surface cross-linked by either Ca(II) or chitosan to form polyelectrolyte microcapsules. By adjusting the needle inner diameter, concentration of sodium alginate, and applied voltage, we can control the droplet size to the designated range. Furthermore, we can tune the thickness and thereby rigidity/elasticity of the viscoelastic shell by adjusting the residence time of microcapsules in gelation solution to control the rigidity/elasticity of microcapsules. These polyelectrolyte microcapsules were subject to the osmotic pressure of synthetic water-soluble polymers, such as poly(ethylene glycol), with progressively lower concentration to observe their osmotic swelling behavior.

S1.00206 Crossover Between 2D and 3D Fluid Dynamics in the Diffusion of Islands in Ultra-Thin Freely Suspended Smectic Films[1] , ZOOM NGUYEN, MARKUS ATKINSON, CHEOL PARK, JOSEPH MACLENNAN, MATTHEW GLASER, NOEL CLARK, University of Colorado-Boulder — fluid requires no force, leads, via the Einstein relation, to an infinite diffusion coefficient D for the disc. Saffman and Delbrück proposed that if the 2D fluid is a thin film immersed in a 3D viscous medium, then the film should behave as if it were of finite size, and $D \sim -\ln(a\eta')$, where a is the inclusion radius and η' is the viscosity of the 3D medium. By studying the Brownian motion of islands in freely suspended smectic films a few molecular layer thick, we verify this dependence using no free parameters, and confirm the subsequent prediction by Hughes, Pailthorpe and White of a crossover to 3D Stokes-like behavior when the diffusing island is sufficiently large.

[1]This work was supported by NASA Grant NAG-NNX07AE48G, NSF MRSEC DMR 0820579, and NSF DMR 0606528

S1.00207 Decoupling of ionic conductivity from the structural relaxation in ionic liquids , PHILIP GRIFFIN, Dept. of Physics and Astronomy, Univ. of Tennessee, ALEXANDER AGAPOV, Dept. of Polymer Science, Univ. of Akron, ALEXANDER KISLIUK, ALEXEI SOKOLOV, Dept. of Chemistry, Univ. of Tennessee and Chemical Sciences Division, ORNL — In numerous technological applications, notably battery technology, the need for a highly conductive ionic material is critical. Ionic liquids are well suited for these applications, but the fundamentals of their physical properties are still not well understood. To investigate the temperature dependence of the conductivity and structural relaxation in these systems, a combination of light scattering techniques as well as dielectric spectroscopy measurements were performed on the ionic liquid [C4mim][NTf2]. Combining these measurement techniques enables us to characterize the dynamics in a time window that spans more than twelve decades. Detailed analysis of our results shows that the temperature dependence of the conductivity decouples from that of the structural relaxation. Furthermore, the structural relaxation exhibits a dynamical crossover similar to that observed in many glass forming liquids, while the conductivity exhibits no sign of the crossover. Contrary to the traditional theory, these observations suggest that the mechanism controlling ionic conductivity in this system is different from the mechanism controlling structural relaxation.

S1.00208 Bistable Shear-Induced Alignment and Isotropy in Nematic Cylindrical Micelles , LOUIS MADSEN, KYLE G. WILMSMEYER, XIAOLIN ZHANG, Department of Chemistry and Macromolecules and Interfaces Institute, Virginia Tech, Blacksburg, VA 24061 — Wormlike micelles (WLMs), such as cetyltrimethylammonium bromide in water, are long flexible cylinders of surfactant molecules that self-assemble as a function of concentration and temperature. By placing a driven rheological cell into an NMR instrument, we use "rheo-NMR" to correlate molecular-scale to micron-scale details available by NMR with macroscopic behaviors, with precise control over the sample shear rate. We directly observe alignment of WLMs induced by shear and magnetic field, as well as anisotropic diffusion, providing us with a nematic phase diagram that is modulated by shear. Here we focus on conditions where WLMs do not spontaneously field align (at 9.4 T), but rapidly and stably field align after application of shear. This "bistable" fluid persists in either the isotropic state or the field aligned state (after shearing) for $>$ 12 hrs. We will further describe measurements of the nonlinear dynamics of director reorientation, with which we quantify anisotropic elastic constants and viscosities.

S1.00210 Measuring the Nonergodicity in Glasses by Ensemble-Averaged Photon Correlation Spectroscopy[1] , ERIC SVINGEN, DAVID SIDEBOTTOM, Creighton University — Although dynamic light scattering is used to monitor the dynamics of glass-forming liquids above the glass transition temperature, in the glass phase the absence of ergodicity results in a partial arrest of these dynamics and traditional time-averaged measures fail to monitor the remaining dynamics. Instead, scattering data must be processed in an ensemble-averaged manner by integrating the scattering from multiple regions by slowly translating the sample. We report studies of glass-forming 2Ca(NO3)2:3KNO3 (CKN) obtained below the glass transition temperature using a motorized translation system. Our findings will be used to assess the temperature dependence of the so-called nonergodic level that is predicted by certain mode-coupling theories to exhibit "cusp" near the mode coupling critical temperature.

[1]This work is supported by a grant from NSF (DMR-0906640).

S1.00211 Direct imaging of spatially and temporally heterogeneous two-state dynamics on metallic glass and amorphous silicon surfaces well below T_g[1] , SUMIT ASHTEKAR, GREGORY SCOTT, JOSEPH LYDING, MARTIN GRUEBELE, University of Illinois Urbana Champaign — Probing glassy dynamics of atomic glass formers with atomic resolution far below the glass transition has remained elusive due to the long waiting times and the small length scales involved. Here we report atomic resolution movies acquired using time-lapse scanning tunneling microscopy on metallic glass and amorphous silicon (a-Si) surfaces at room temperature well below their respective glass transition temperatures (Tg of glasses studied lie between 600-1000K). We find the clusters on metallic glass surfaces with size 2-8 atomic spacings exhibit dynamics which are almost exclusively two-state ($P_{3-state} \sim 0.06$) [1]. The two-state dynamics was found to be both spatially and temporally heterogeneous. We attribute the two-state dynamics to the secondary β relaxations which remains active well below the glass transition. Similar dynamics were found on amorphous silicon surfaces providing the first evidence for the existence of glass-like dynamics on pure a-Si surfaces at non-cryogenic temperature.

[1] S. Ashtekar et.al. J. Phys. Chem. Lett., 2010, 1 (13), pp 1941–1945

[1] This work was funded by support from the Eiszner family (James R. Eiszner Chair), and NSF grant CHE 0948382

S1.00212 Frequency Dependence of Aging Dynamics in a Colloidal Glass , AJAY NEGI, CHINEDUM OSUJI, Yale University — The aging response of glassy particulate systems originates due to slow structural rearrangements of its constituent matter. It is reasonable to speculate that structural rearrangements on different length scales should manifest themselves in dynamical response on different timescales. Here we consider the frequency dependence of aging in a colloidal glassy system using parallel superposition bulk rheology. The aging behavior of the system is characterized by time evolution of the complex modulus in response to a sinusoidally varying probe stress of different frequencies superimposed on a steady background stress. Strikingly, the system displays more rapid aging when observed at smaller frequencies. This suggests that, by comparison, it is more arrested on shorter length scales (higher frequencies) than on the longer length scales where many-particle correlated motions are in effect. Such correlated motions are believed to be responsible for relaxation in glassy materials. The variation in the aging dynamics at different frequencies is more prominent at higher background stresses where the system is more fluidized.

S1.00213 Scaling, clustering and avalanches for steel beads in an external magnetic field[1] , ALYSE MARQUINEZ, INGRID THVEDT, S.Y. LEHMAN, D.T. JACOBS, The College of Wooster — We investigated avalanches using uniform 3mm steel spheres ("beads") dropped onto a conical bead pile within a uniform magnetic field. The bead pile is built by pouring beads onto a circular base where the bottom layer of beads had been glued randomly. Beads are then individually dropped from a fixed height after which the pile is massed. This process is repeated for thousands of bead drops. By measuring the number of avalanches of a given size that occurred during the experiment, the resulting avalanche size distribution was compared to a power law description as predicted by self-organized criticality. As the magnetic field intensity increased, the beads clustered to give a larger angle of repose and we measured the change in the avalanche size distribution. The moments of the distribution give a sensitive test of mean-field theory as the universality class for these bead piles.

[1]We acknowledge support from Research Corporation and NSF-REU grant DMR 0649112.

S1.00214 Particle trajectories in 2D granular avalanches with imposed vibrations , NORA SWISHER, BRIAN UTTER, James Madison University — We study particle trajectories of photoelastic grains in a 2D circular rotating drum subjected to imposed vertical vibrations in order to characterize the jamming behavior of granular materials. Jamming appears in many systems (grain silos & chutes, landslides, mixing industrial materials, etc.) and vibration (granular temperature) is a primary factor in the jamming/unjamming transition. Images are taken and each particle's position is found for every frame then compared between frames to find the velocities. Particle tracking allows us to quantitatively measure the flow and mixing properties in our experiment. We present data on avalanching statistics, mean flow, the width of the shear band, and properties related to mixing (fluctuations and trajectories of neighboring grains). We find that vibrations induce more rearrangements of the grains and cause the pile of grains to become more compact over time. At constant peak acceleration we find that low frequency/high amplitude caused more grain movement than high frequency/low amplitude in both the stationary and rotating case.

S1.00215 Submerged granular flow of hydrophobic and hydrophilic sand , BEN FOLTZ, BRIAN UTTER, James Madison University — We experimentally investigate submerged granular flows of hydrophobic and hydrophilic grains in a rotating drum. While slurry and suspension flows are common in nature and industry, effects of surface chemistry on flow behavior have received little attention. The experiment consists of a cylindrical drum containing various concentrations of hydrophobic and hydrophilic grains of sand submerged in water and rotated at a constant angular velocity. Images of the resulting avalanches are taken and analyzed. While it is known that at slow speeds, submerged avalanches appear qualitatively similar to dry flows, our results suggest that the surface properties of the grains affect underwater flow significantly. High concentrations of hydrophobic grains result in the formation of aggregates. At concentrations larger than 75% hydrophobic sand, the avalanches do not behave in a manner which is typical for sand, but as the concentration decreases, the aggregates are smaller, the angle of repose decreases, and the grains start showing properties similar to those in regular sand. We present data on the size of the aggregates, slope, and avalanche statistics with changes in concentration.

S1.00216 Phase transition of colloidal particles on curved surfaces , GUANGNAN MENG, JAYSON PAULOSE, DAVID NELSON, Department of Physics, Harvard University, VINOTHAN MANOHARAN, Department of Physics and School of Engineering and Applied Sciences, Harvard University — Defects and disclinations have to appear in crystalline domains on a curved surface with non-zero Gaussian curvature. These geometrical frustrations can qualitatively change the physics of phase transition. We encapsulate micron sized polystyrene (PS) colloidal particles within emulsion droplets and use nanometer sized polyNIPAM hydrogel particles to introduce depletion attraction between PS particle and interface, as well as between PS particles. We use this experimental model system and confocal microscopy to study phase transitions on curved surfaces. We will present both experimental phenomena and theoretical analysis.

S1.00217 Self and Directed Assembly of Thin Metallic Films exposed to Pulsed Laser Irradiation , YUEYING WU, U. Tennessee, JASON FOWLKES, ORNL, PHILIP RACK, U. Tennessee, LOU KONDIC, NJIT, JAVIER DIEZ, UNCPBA — The synthesis and assembly of functional metallic nanomaterials is critical for realizing many important applications of nanoscience and nanotechnology. In this study, we investigate dewetting of metal films via pulsed nanosecond laser melting. We study film instabilities that result from the interplay of capillary forces and liquid-solid interaction, which can lead to thin film break-up and subsequent nanoparticle formation. We have also explored the dewetting and nanopattern formation of other liquid metal geometries, such as rings and lines. We will discuss how nano-lithographically defined features can be used to direct the assembly of nanoparticles with desired properties, concentrating in particular on the role of stochastic fluctuations.

S1.00219 Fabrication and Characterization of High Aspect Ratio Membranes and Microporous Filters made from PMMA , ALEX BURANT, Dept. of Physics and Astronomy, James Madison University, Harrisonburg, VA, BRIAN AUGUSTINE, Dept. of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA, CHRIS HUGHES, Dept. of Physics and Astronomy, James Madison University, Harrisonburg, VA — This experiment shows a new way to create high aspect ratio membranes and microporous filters by curing a liquid monomer, methyl methacrylate (MMA), into poly(methyl methacrylate) (PMMA) structures. Holes were cut in 200 μm PMMA sheets by laser cutting. Membranes were made by filling these holes with wax and cooling until the wax solidified. The liquid monomer solution was flowed over the wax-filled holes and photopolymerized to make a thin membrane. The membrane thickness could be controlled by adding 3-10 μm, 30-50 μm, or 50-100 μm silica beads to the monomer solution. Filters were made by filling the holes with curing solution containing 3-10 μm beads, photopolymerizing, and etching the silica with hydrofluoric acid. The filter porosity could be controlled by varying the weight percentage of silica beads added to the monomer solution. Scanning electron microscopy was used as a method for characterizing both membrane thickness and filter porosity.

S1.00220 Enhanced shear separation for chiral magnetic colloidal aggregates[1] , CARLOS MENDOZA, Materials Research Institute, UNAM, CARLOS MARQUES, FABRICE THALMANN, Institute Charles Sadron — We study the designing principles of the simplest colloidal propeller, an architecture built from four identical spheres that can couple translation with rotation to produce controlled drift motion. By considering superparamagnetic beads, we show that the simultaneous action of a magnetic field and a shear flow leads to the migration of the cluster in the vorticity direction. We investigate the dependence of the migration velocity on the geometrical parameters of the cluster, and find that significant cluster separation can be achieved under the typical operation conditions of microfluidic devices. Reference: C.I. Mendoza, C.M. Marques, and F. Thalmann, "Enhanced shear separation for chiral magnetic colloidal aggregates" arXiv:1011.1488

[1]Partial financial support: Chemistry Department of the Centre National de la Recherche Scientifique and DGAPA-PAPIIT Grant No. IN-115010.

S1.00221 Numerical Analysis of Micromixers for Optimization of Mixing Action[1]

, YOGENDRA PANTA, PARAM ADHIKARI, Department of Mechanical Engineering, Youngstown State University — Micro-bio/chemical applications often require rapid and uniform mixing of a number of fluid streams that carries bio/chemical species in the solution. At microscale, fluid flow is highly laminar with low Reynolds number, fluids mixing mechanism is primarily by diffusion and free from any turbulence. Demand for highly efficient micromixers for microfluidic networks is due to slower mixing process for larger bio-molecules such as peptides, proteins, and nucleic acids compared to micro-scale molecules. Passive and active mixers are two basic mixers that are currently in use for these applications. Passive mixers often require very long mixing channels where are most active mixers require bulky moving parts to stir the fluids. In this study, electroosmotic effects orthogonally aligned with the fluid flowstream are utilized for optimum mixing effect in various micromixers. Cross-dependencies among several geometrical, electrical, and fluid parameters and their significance are studied in order to achieve an optimum mixing effect. It has been planned to optimize the mixer by non-moving stirring actions provided by an external magnetic field.

[1]Acknowledgements to School of Graduate Studies and Research at YSU for URC Grant and RP Award 2009-2010.

S1.00222 A multiscale model for nanoparticle binding dynamics under shear flow

, YALING LIU, JIFU TAN, Lehigh University, KYTAI NGUYEN, University of Texas at Arlington — Nanomedicine poses a new frontier in medical technology with the advantages of targeted delivery and patient specific design. In applications of nanoparticle targeted drug delivery, the delivery efficiency is controlled by the physical properties of the nanoparticle such as its size, shape, ligand density, as well as external environmental conditions such as blood flow rate, blood vessel diameter. Proper drug dosage choice relies on determination of the attachment and detachment rates of the nanoparticles at the active region and the understanding of the complex process of targeted drug delivery. A few particulate models have been proposed to study the adhesion probability of individual spherical or non-spherical nanoparticles. Meanwhile, continuum convection-diffusion-reaction models have been widely used to calculate the drug concentration, which usually assumes specific binding and de-binding constants. However, there has not been any study that links the particulate level nanoparticle size and shape information to the system level bounded particle concentration. A hybrid particle binding dynamics and continuum convection-diffusion-reaction model is presented to study the effect of shear flow rate and particle size on binding efficiency. The simulated concentration of bounded nanoparticles agrees well with experimental results in flow chamber studies.

S1.00223 Modeling spreading of nematic droplets[1]

, TE-SHENG LIN, LINDA CUMMINGS, LOU KONDIC, New Jersey Institute of Technology — Experiments by Poulard & Cazabat[2] on spreading droplets of nematic liquid crystal reveal a surprisingly rich variety of behavior, including at least two different emerging lengthscales resulting from a contact line instability. In earlier work[3] we modified a lubrication model for nematic liquid crystals due to Ben Amar and Cummings[4], and showed that, in a qualitative sense, it can account for much of the observed behavior. In the present work we propose a new approach, that allows us to explore the effect of anchoring variations on the substrate. This in turn gives a simple way to model the presence of defects, which are always present during such liquid crystal flows. The new model leads to additional terms in the governing equation. We first explore the influence of these additional terms for some simple flow scenarios, to gain a basic understanding of their influence, before extending our simulations to the experimental geometry and comparing our results to the experiments.

[1]This work was partially supported by NSF Grant No. DMS-0908158
[2]C. Poulard, A. M. Cazabat, Langmuir, 6270, vol. 21 (2005)
[3]L. J. Cummings, T.-S. Lin, L. Kondic, sumitted (2010)
[4]M. Ben Amar, L. J. Cummings, Phys. Fluids, 1160, vol. 13 (2001)

S1.00224 Drop evaporation and triple line dynamics

, BENJAMIN SOBAC, DAVID BRUTIN, Université de Provence, JEROME GAVILLET, CEA LITEN, UNIVERSITÉ DE PROVENCE TEAM, CEA LITEN TEAM — Sessile drop evaporation is a phenomenon commonly came across in nature or in industry with cooling, paintings or DNA mapping. However, the evaporation of a drop deposited on a substrate is not completely understood due to the complexity of the problem. Here we investigate, with several nano-coating of the substrate (PTFE, SiOx, SiOc and CF), the influence of the dynamic of the triple line on the evaporation process. The experiment consists in analyzing simultaneously the motion of the triple line, the kinetics of evaporation, the internal thermal motion and the heat and mass transfer. Measurements of temperature, heat-flux and visualizations with visible and infrared cameras are performed. The dynamics of the evaporative heat flux appears clearly different depending of the motion of the triple line

S1.00225 Nanoscale heterogeneity in alkyl-methylimidazolium bromide ionic liquids

, DAVID PRICE, BACHIR AOUN, MARIE-LOUISE SABOUNGI, ANDREAS GOLDBACH, MIGUEL A. GONZÁLEZ, SHINJI KOHARA — High-energy x-ray diffraction measurements on 1-alkyl-3-methylimidazolium bromide ionic liquids with ethyl, butyl and hexyl alkyl chains reveal a peak at low scattering vector Q that rises and moves to lower Q with increasing chain length. Atomic molecular dynamics simulations, which give results in excellent agreement with the x-ray data, show that this behavior is most pronounced in the partial structure factor for the tails of the alkyl chains but is also seen in those for the imidazolium ring centers and anions. The heterogeneity with a length scale of 1.9 nm established for the liquid with the hexyl chain is quantified by a density heterogeneity order parameter that shows a clustering of the tails. Our results are consistent with explanations in the literature of the increase in viscosity with alkyl chain length in terms of nanoscale segregation.

S1.00226 On segregation of noble gases in water-based Single Bubble Sonoluminescence

, MOGENS LEVINSEN, Niels Bohr Institute, Univ. of Copenhagen — A long-standing issue in the field of long time stable water based single bubble sonoluminescence has been the close similarity of the spectra to that of blackbody radiation. Looking for the effects of possible segregation of noble gases has been suggested as a means to investigate whether the similarity is just a weird coincidence with the bubbles being on the whole transparent to their own radiation. We have investigated spectra from bubbles seeded with various mixtures of helium and neon with xenon and argon using a novel transformation that allows for a single parameter characterization of the spectra, with the surprising result that although no trace of segregation is found, the radiation seems to be highly thermalized in all cases.

S1.00227 Generating a Pulsatile Pulmonary Flow after Fontan Operation by Means of Computational Fluid Dynamics (CFD)

, MOSTAFA GHOREYSHI, Sharif University of Technology — This study considers blood flow in total cavopulmonary connection (TCPC) morphology, which is created in Fontan surgical procedure in patients with single ventricle heart disease. Ordinary process of TCPC operation reduces pulmonary blood flow pulsatility; because of right ventricle being bypassed. This phenomenon causes a lot of side effects for patients. A cardiac surgeon has suggested that keeping main pulmonary artery (MPA) partially open, would increase pulmonary flow pulsations. MPA gets closed in ordinary TCPC operation. The purpose of current study is to verify the effects of keeping MPA partially open on pulmonary flow pulsations, by means of computational fluid dynamics (CFD). 3D geometry is reconstructed from CT Angiography (CTA) scan of a patient who has undergone an ordinary TCPC procedure. The stenosed MPA or pulmonary stenosis (PS) is virtually added to the original geometry. Flow field is studied in six different models in which average antegrade flow (AF) -coming through PS- increases gradually. Results show that adding AF increases flow pulsations in both pulmonary arteries. Moreover, power loss increases with respect to average AF. We conclude that adding AF is an impressive way to increase pulsations of pulmonary flow, but energy losses should be considered too.

S1.00228 Designing self-oscillating cilia using active polymer gels , PRATYUSH DAYAL, AMITABH BHATTACHARYA, OLGA KUKSENOK, ANNA C. BALAZS, University of Pittsburgh — Using theory and simulations, we model the dynamic behavior of synthetic cilia made from soft, active materials. In designing this system, we harness the properties of polymer gels that undergo photosensitive Belousov-Zhabotinsky (BZ) reaction. Driven by the periodic reduction and oxidation of a ruthenium catalyst that is grafted onto the polymer backbone, these BZ gels undergo rhythmic swelling and de-swelling by chemo-mechanical transduction. When these BZ gels are tethered to a substrate, they form cilia that can pulsate autonomously in response to the BZ reaction. To simulate the behavior of the BZ cilia, we developed a nonlinear 3D model that captures the effect of the diffusive exchange of BZ reagents between the gel and the fluid. Using this approach, we determine the factors that govern the bending and beating of individual cilium. We then turn our attention to multiple cilia and show that their collective dynamics strongly depends on the spacing between them. We also establish criteria to regulate the collective behavior of multiple cilia using light as the external stimuli. Our findings provide guidelines for designing ciliated surfaces that can exhibit biomimetic functionality.

S1.00229 APPLICATIONS —

S1.00230 Terahertz microbolometers based on disordered GaAs and GaN heterostructures , KAI WANG, University at Buffalo, SUNY, R. RAMASWAMY, A. MURAVIEV, A. SERGEEV, V. MITIN, R. GASKA, Sensor Electronic Technology, Inc. — We present our results on design, fabrication, and characterization of hot-electron bolometers based on low-mobility two-dimensional electron gas (2DEG) heterostructures for THz heterodyne detection. Microbolometers based on GaAs/AlGaAs and GaN/AlGaN heterostructures have been fabricated and tested. Low contact resistances (0.2 ohm-mm for GaN and 0.7 ohm-mm for GaAs) were achieved. We determined the carrier concentration from the Hall measurements and the electron relaxation time from the mobility measurements. We also investigated kinetic parameters: temperature derivate of the resistivity and the electron cooling time. Optical characterization includes the transitivity measurements. The results show that the coupling to the THz radiation is mainly due to the Drude absorption, which increases in disordered structures. Temperature-dependent resistivity and electron cooling are determined by inelastic electron scattering on optical phonons. Finally, we compare GaAs and GaN microbolometers and analyze their parameters for various applications in THz sensing.

S1.00231 Quantum cascade lasers as LO for THz mixers , RAHUL RAMASWAMY, Uni at Buffalo , ANDREY MURAVIEV, KAI WANG, CHRISTOPH DEUTSCH, JAEKYU CHOI, DAVID EASON, GOTTFRIED STRASSER, MICHAEL SHUR, ANDREI SERGEEV, VLADIMIR MITIN — In this research we fabricate and characterized a number of Fabry-Perot type, multi mode terahertz quantum cascade lasers operating in the range 2 – 3 THz. AlGaAs/GaAs heterostructures for terahertz QCLs have been grown using molecular beam epitaxy (MBE) on a SI-GaAs substrate. The active region design is based on a vertical transition in which a combination of resonant tunneling and LO-phonon scattering is used to selectively depopulate the lower radiative state. Double-sided metal waveguide is employed for QCL mode confinement. Spectral properties of the QCLs have been investigated by means of Fourier transform spectroscopy. All QCLs show the gain spectral band tunability by varying the applied bias voltage. Single mode laser operation is observed in a certain range of applied bias voltages. Our QCLs have an inherently narrow line-width, which is limited in our measurements by the spectrometer resolution of 0.1cm^{-1}.

S1.00232 Voltage Tunable Multicolor GaAs/AlGaAs Coupled Quantum Well Infrared Photodetector , JAE KYU CHOI, DAVID EASON, GOTTFRIED STRASSER, NIZAMI VAGIDOV, VLADIMIR MITIN, University at Buffalo, SUNY — Tunable quantum well infrared photodetectors (QWIP) has attracted attention because of the mature growth technique of GaAs/AlGaAs quantum wells and their diverse applications such as remote temperature sensing, chemical analysis, military applications, and so on. We have designed, grown, and characterized a voltage tunable multicolor QWIP for the long wavelength infrared detection (7.5 – 12.4 μm). The QWIP structure was grown by MBE, and the device is designed to have bound to bound and bound to quasi-continuum transitions in an asymmetrically doped double quantum well. At zero bias we observed several distinctive spectral lines in photoresponse. The device demonstrates strong dependence on a magnitude and a polarity of the bias that is confirmed by the shift of energy levels in the electric field calculated by nextnano^{3}software. In particular, switching bias from +3V to -5V we change the photoresponse of our detector from 8.39 μm to 10.21 μm.

S1.00233 Localized and Synchronous Measurement of Second and Third Order Nonlinearity in Superconductive Transmission Line Resonators[1] , ANNELLE EBEN, Calvin College, STEPHEN REMILLARD, Hope College — A method to locally observe the generation of nonlinearity of multiple orders inside the passband of $Tl_2Ba_2CaCu_2O_8$ and $YBa_2Cu_3O_7$ superconducting resonators has been developed. Nonlinear emission is stimulated locally in the vicinity of the probe by off-resonance, low frequency signals. By mixing of two very low frequency local currents and of one current in the passband, 2^{nd} and 3^{rd} order intermodulation distortion (IMD) occurs around resonance, permitting the determination of the currents associated with each order of nonlinearity. Synchronous measurement of different orders eliminates the ambiguity of emissions occurring on different time scales and at different skin depths. Comparison of synchronous 2^{nd} and 3^{rd} order IMD characterizes the extent of time reversal symmetry breaking (TRSB) in the superconductor. This technique is being used to perform spatially resolved TRSB studies, to examine the effect of doping on nonlinearity in $Tl_2Ba_2CaCu_2O_8$, and to search for a correlation between lithographic edge quality and 2^{nd} and 3^{rd} order nonlinearity.

[1]Supported by NSF REU Grant PHY/DMR-1004811, by a Cottrell College Science Award from Research Corp., and by Mesaplexx, pty ltd of Eight Mile Plains, Au.

S1.00234 ABSTRACT WITHDRAWN —

S1.00235 Analysis and Simulation of Generating Terahertz Surface Waves in Laser-Assisted Field Emission , MARK HAGMANN, NewPath Research L.L.C., GAGAN KUMAR, SHASHANK PANDEY, AJAY NAHATA, University of Utah — When the radiation from two lasers is focused on a field emission diode the electric field from the radiation is superimposed on the applied DC field, and the nonlinear dependence of the emitted current on the electric field causes the current to oscillate at the difference frequency for the two lasers. Finite Difference-Time Domain simulations and analytical solutions for a paraboloidal model of the field emission tip show that the current oscillations create a transverse-magnetic (TM) surface wave on the tip. The analytical solution for the TM fields in paraboloidal coordinates consists of products of regular and irregular Coulomb wave functions. The width of the tip is much smaller than the skin depth so interior and exterior solutions are required and a summation of the products is required to satisfy the boundary conditions at the surface of the tip. The simulations are consistent with the analytical solution and show that there is a quasi-stationary region near the apex, a transition region where the surface waves are formed, and the far-field where the waves propagate outward on the tip.

S1.00236 Antireflective Coatings using Layer by Layer Self Assembly of Silica and Titania Nanoparticles

, ANITESH LAL, RAISA VELASCO CASTEDO, DAN MAZILU — Antireflective coatings have a wide range of applications and its usefulness can be found in devices such as cameras, binoculars, microscope lenses, solar panels etc. The major expectation for this research is to add an antireflective coating to a glass substrate which will reduce the reflectance and increase the transmittance of light of the substrate. From theory it is known that uncoated glass substrates transmit approximately 92% of light and reflect approximately 8% of it. However, if an antireflective coating is introduced on the surface of the substrate, there will be some light reflected from the first interface and some from the second interface. If these two reflected rays are made to interfere destructively, reflection can be minimized thus maximizing transmittance. We conducted various experiments with silica particles only in which we tried to change the properties of this antireflective coating such that maximum destructive interference could be achieved. Currently, we are working with a combination of silica and titania nanoparticles with varying thicknesses whereby layers have thickness of a quarter of the desired wave length. So far a number of different factor-level combinations have exhibited transmittance in excess of 96%, well above that of an untreated slide and comparable to commercial coatings.

S1.00237 Light Instability in Pulsed Quantum Cascade Lasers[1]

, YUTING HUANG, Princeton University, YU YAO, Princeton University and MIRTHE, KAIS AL-NAIMEE, National Institute of Applied Optics, University of Florence, Florence, Italy, CLAIRE GMACHL, Princeton University and MIRTHE, MIRTHE TEAM — The instability observed in the light output of high power, pulsed Quantum Cascade (QC) lasers is investigated for potential periodic behavior. We built a set-up to monitor the real-time pulse shape of up to 5,000 sequential light pulses at a fixed pulsed current. In analyzing the data, we use the Fast Fourier Transform to find their frequency components. We found likely quasi-periodic behavior, as well as a broader range of frequencies around the fundamental pulse frequency. To also research a potential spatial component in the laser instability, i.e. beam steering, we modified the set-up to split the beam spatially into two parts, each monitored in real-time over 5,000 pulses. A correlation between the two pulse trains on the two detectors separates the spatial and pure power components of the instability. Subsequently eliminating this instability will help to achieve QC lasers with optimal performance.

[1]This work is supported in part by MIRTHE (NSF-ERC).

S1.00238 Modeling Laser-Tissue Interactions: Implementing the Heat Diffusion Equation and Wave Equation to Simulate Thermal Interactions of Absorber Distributions in Biological Tissues[1]

, FREDERICK BARRERA, ELHARITH AHMED, PATRICK NASH, DHIRAJ SARDAR — The tracking of photons through turbid media (e.g. tissues) has been studied extensively from an experimental vantage point. These turbid media are difficult to characterize- since their components are exceedingly variegated- and thus present many challenges to clinicians who require models which precisely predict the location and time evolution of energy deposition. Furthermore, the interaction of the turbid media sample with the source of radiation typically involves many dynamic mechanisms (e.g. photothermal etc.) Using diffuse light transport, and an electromagnetic wave approach (e.g. Maxwell's equations), an analysis of thermal energy distribution in tissues is performed. Assuming a highly absorbing chromophore model of melanocytes in tissues, a comparison of the variation of thermal energy is determined for different collections of melanocyte spatial distributions.

[1]This work was funded by NIH/NIGMS MBRS-RISE GM60655.

S1.00239 Tunable TiO2 Nanotubes as Nanotemplate for Solar Cells[1]

, JIA LU, DONGDONG LI, USC, NAMI TEAM — Titanium oxide (TiO2) is an n-type semiconductor with a bandgap energy of 3.0-3.2 eV. It has broad applications, because of the versatile functionalities. Synthesis of anodic titanium oxide (ATO) nanotube templates has gained significant progress in fluoride-ion-contained electrolytes. The one-dimensional (1D) structure provides a large specific surface area as well as a direct pathway for charge transport, thus rendering superior capabilities in lightharvesting, electrochromic switching, environmental sensing, energy storage, etc. In this work, highly ordered ATO nanotubes film has been synthesized by two-step anodization method. After using a reductive doping approach, the metal materials (Cu and Ni) can be electrodeposited into the nanotubes. The versatile process yields reproducible tubular structures in ATO nanotubes due to the conductive nature of crystallized TiO2, indicating great potential for nanotemplate application. A dye-sensitized solar cell is also demonstrated by employing the ATO films. It is observed that bottom treatment greatly enhances short current density and filling factor resulting in improved energy conversion efficiency.

[1]DOE EFRC

S1.00240 Theoretical Investigation on Cysteine Interactions with Gold Nanoparticles

, JESSICA CARR, HONG WANG, JAMES LEWIS, Physics Department, West Virginia University, Morgantown, WV 26506-6315 — Gold nanoparticles have been intensely investigated due to wide applications in colloidal chemistry, catalysis, medical science, etc. Lately, experiments have shown that ligand-stabilized gold nanoparticles provide a platform for precisely probing the structural and electronic properties of isolated gold nanoparticles, allowing us to further understand the interaction between gold nanoparticles and attaching ligand molecules. Using density functional theory approach, we investigate a series of gold nanoparticles with a size scale of 0.5 to 2 nm that are passivated by a monolayer of cysteine molecules [R-SH, with R=$CH_2CH(COOH)(NH_2)$]. There is a controversy about the attaching pattern of the cysteine monolayer around the gold nanoparticles. We speculate that there is hydrogen bonding between the cysteine molecules, leading to stabilized gold nanoparticles. This research shows potential hydrogen bonding forming with the gold nanoparticle surface, as well as hydrogen bonding between cysteine molecules.

S1.00241 Photocurrent enhancement of an individual gallium nitride nanowire decorated with gold nanoparticles[1]

, JENCY PRICILLA SUNDARARAJAN, MEREDITH SARGENT, DAVID N. MCILROY, Department of Physics, University of Idaho, Moscow, ID 83844 — Variation in electron transport properties of individual n-type gallium nitride (GaN) nanowire and gold decorated gallium nitride (Au-GaN) nanowire were studied with respect to laser exposure of different wavelength and intensity. Single nanowire devices were manufactured by photolithography process in nanotechnology cleanroom, were characterized by scanning electron microscope (SEM) and transmission electron microscope (TEM). A drop in electrical conductivity of Au-GaN nanowire was observed relative to bare GaN nanowire. Under laser illumination, we noticed an enhancement in photocurrent in Au-GaN nanowire, which increased with increase in excitation power at ambient conditions. We present a comparative study of the opto-electrical behavior of bare GaN nanowire vs Au-GaN nanowire and explain the IV characteristics and FET characteristics with respect to the length and diameter of nanowire.

[1]USDA, UI-BANTech

S1.00242 Pulsed Laser Synthesized Magnetic Cobalt Oxide Nanoparticles for Biomedical Applications , HARI BHATTA, Missouri State University, RAM GUPTA, KARTIK GHOSH, PAWAN KAHOL, ROBERT DELONG, ADAM WANEKAWA — Nanomaterials research has become a major attraction in the field of advanced materials research in the area of Physics, Chemistry, and Materials Science. Biocompatible and chemically stable magnetic metal oxide nanoparticles have biomedical applications that includes drug delivery, cell and DNA separation, gene cloning, magnetic resonance imaging (MRI). This research is aimed at the fabrication of magnetic cobalt oxide nanoparticles using a safe, cost effective, and easy to handle technique that is capable of producing nanoparticles free of any contamination. Cobalt oxide nanoparticles have been synthesized at room temperature using cobalt foil by pulsed laser ablation technique. These cobalt oxide nanoparticles were characterized using UV-Visible (UV-Vis) spectroscopy, transmission electron microscopy (TEM), and dynamic laser light scattering (DLLS). The magnetic cobalt oxides nanoparticles were stabilized in glucose solutions of various concentrations in deionized water. The presence of UV-Vis absorption peak at 270 nm validates the nature of cobalt oxide nanoparticles. The DLLS size distributions of nanoparticles are in the range of 110 to 300 nm, which further confirms the presence nanoparticles. This work is partially supported by National Science Foundation (DMR- 0907037).

S1.00243 Diffusion Through Tubular Nanotubes , DIVYA NARAYAN ELUMALAI, Louisiana Tech University, HERVIN MONLOUIS, Grambling State University, PEDRO DEROSA, Louisiana Tech University and Grambling State University — Nanotubes exhibit exceptional properties that make them promising candidates for many applications that require the transport, storage and/or delivery of fluids, through nanotubes. In order to efficiently plan potential applications, transport properties and interactions such as adsorption, diffusion, and solvent interactions must be understood. Our study focuses on the mechanisms that inhibit or encourage diffusion through these nanostructures and the nature of the interactions responsible for movement of any sort in these regimes. As a specific case we study diffusion through tubular nanotubes. This work treats each interaction individually and aims at successfully modeling the diffusion of particles through the nanotubes as a function of the interaction between the diffusing particles and the nanotube walls. To conduct this research we have employed Monte Carlo calculations, implementing a specific forced random walk algorithm. Preliminary results suggest that any delay in diffusion occurs due to a strong molecule-wall interaction. We believe this is due to the columbic attraction between the diffusing particles and the wall.

S1.00244 Role of CNTs in inorganic electroluminescence , JIN-YOUNG KIM, Sungkyunkwan Univ., SEGI YU, Hankuk Univ. Foreign Studies — Inorganic electroluminescence (EL) has been considered to be utilized in flat panel displays in the future. However, the progress of the display device utilizing EL phosphor is rather mild due primary to its low brightness, high voltage operation, and poor expectation lifetime. Carbon nanotubes (CNTs) has been focused in many areas since this material has a number of useful characteristics such as good chemical inertness, high aspect ratio, good thermal conductivity, and etc after the first observation by Dr. Iijima. By adopting (CNTs) in inorganic EL devices of ZnS-based powder phosphor, the performance of devices has improved substantially, i.e., high brightness but with reduced current density. The main reason for this improvement is considered to be caused by the strong local field near the end tips of CNTs. Further efforts have been poured to use the enhanced local field around CNTs but with an intention to maintain the low current density. The details will be posted in this poster and underlying mechanism for this phenomenon will be explained. Email: segiyu@hufs.ac.kr

S1.00245 Graphene Transistor fabricated by Helium Ion Milling , KAIWEN ZHANG, XIANGMING ZHAO, XIANGFAN XU, VISWANATHAN VIGNESH, BAOWEN LI, DANIEL PICKARD, BARBAROS ÖZYILMAZ, National University of Singapore, DEPARTMENT OF PHYSICS, NATIONAL UNIVERSITY OF SINGAPORE TEAM, DEPARTMENT OF ELECTRICAL & COMPUTER ENGINEERING, NATIONAL UNIVERSITY OF SINGAPORE TEAM, ENANOCORE, NATIONAL UNIVERSITY OF SINGAPORE TEAM — We report the direct patterning of graphene for various nano-device applications. The Helium Ion Microscope (HIM), able to resolve nano-scale features on solid samples with an edge resolution of a mere 0.25 nm, has a number of attributes which make it attractive for the imaging of graphene structures. Even more compelling is the ability to directly modify graphene, through surface sputtering, enabling direct pattern transfer for the fabrication of graphene devices. The integration of the HIM with a vector pattern generator (Nano Pattern Generation System, NPGS), provides the capability to directly pattern graphene into nano-ribbons. We have successfully fabricated sub-100nm graphene nano-ribbon devices on Si/SiO2 substrate. Resistance measurement has been made as a function of temperature.

S1.00246 Novel nanostructured high efficiency light-harvesting device structure for a solar cell application , KYUNG-MIN LEE, POOJA SINGH, ARUP NEOGI, SANG-KWON LEE, TAE-YOUL CHOI — In this study, we present a novel photoconductive device structure for a solar cell application. β-Silicon Carbide (β-SiC) nanowire(NW) was placed in between silver (Ag) nanodot(ND) array. With much shorter size than an incoming photon wavelength, Ag ND created plasmonic oscillation, mainly attributed to dipole oscillating term, according to Mie scattering theory. Because of more optical modes in the higher refractive index, the radiation pattern from the dipole oscillation was mostly expanded onto the β-SiC NW rather than free space. We found that Ag ND array played role as collecting and concentrating light to create denser optical paths into the semiconducting β-SiC NW, which in turn provided higher quantum yield for photoconductivity. Since the structure was nanoscaled (i.e. NW and ND), this novel device structure can be a miniaturized building block for high demanding solar cell applications as one of the energy solutions.

S1.00247 Ultrafast Optical Measurements of Thermal Conductivity and Sound Velocity of Amorphous SiC[1] , DONALD HONDONGWA, LAUREN OLASOV, BRIAN DALY, Vassar College, SEAN KING, JEFF BIELEFELD, Intel Corporation — We present ultrafast optical measurements of longitudinal sound velocity and thermal transport in hydrogenated amorphous carbon (a-SiC:H) films. The films were grown on Si wafers by PECVD using combinations of methylsilanes and H_2 and He diluent gases. The films were well characterized and found to have densities (1.0 – 2.5 g cm^{-3}) and dielectric constants (2.8 – 7.2) that spanned a wide range of values. Prior to their measurement, the a-SiC:H films were coated with 40-70 nm of polycrystalline Al. The pump-probe measurements were performed at room temperature using a modelocked Ti:sapphire laser. Transient reflectivity changes that are associated with very high frequency sound waves (picosecond ultrasonics) and the cooling rate of the SiC sample (Time Domain Thermorerflectance (TDTR)) were measured. We extract values for the thermal conductivity and sound velocity of the SiC films, and analyze the results in terms of rigidity percolation effects within the SiC layers.

[1]This work was supported by NSF award DMR-0906753.

S1.00248 Ultrafast optical measurements of ultrasound attenuation in amorphous silicon at 50 and 100 GHz[1] , BRIAN DALY, DONALD HONDONGWA, Vassar College, THEODORE NORRIS, University of Michigan, BAOJIE YAN, JEFF YANG, SUBHENDU GUHA, Uni-Solar Ovonic LLC — We present ultrafast optical measurements of the attenuation of 50 – 100 GHz ultrasound in hydrogenated amorphous silicon (a-Si:H) thin films. The films were grown using a modified very high frequency glow discharge method on steel substrates. The deposition conditions were similar to those used for high efficiency solar cells. The measurements were performed at 300 K using the picosecond ultrasonics technique. Films of varying thickness were measured so that the effect of intrinsic acoustic loss within the a-Si:H could be determined. We find that the ultrasonic attenuation in a-Si:H at 100 GHz is more than an order of magnitude lower than is found in other amorphous materials. Our results may impact theoretical models of thermal transport in amorphous materials, and could provide a new avenue for studying voids in a-Si:H and nanocrystalline Si films.

[1]This work was supported by NSF award DMR-0906753.

S1.00249 Charge Carrier Mobility in Conjugated Organic Polymers–A Multi-Step Computational Approach[1]

, YAPING LI, JOLANTA B. LAGOWSKI, Memorial University of Newfoundland — In this work, we investigate charge transport characteristics of conjugated organic polymers (mostly fluorene and carbazole based) used in the construction of the organic solar cells using computational means. In particular we employ a multi-step approach that involves the use of the density functional theory (DFT), semiempirical (ZINDO), and Monte Carlo (MC) theoretical methods to determine their transfer integrals, reorganization energies, transfer rates and mobilities. We find that, in organic conjugated polymers, one dimensional (1D) approach to estimating trends in mobilities gives reasonable results, i.e. is in good agreement with experiment trends, provided their relative intermolecular distances can be obtained with some accuracy. However, greater understanding of the mobilities must take into account the three dimensional (3D) structure and/or the inherent disorder that is present in the organic thin films. We illustrate this requirement with some case studies. Another case study involving orientational disorder will also be presented. The proposed approach illustrates that theoretical computations/simulations based on chemical structure and known morphology of organic semiconductors is an important and reliable approach to studying charge mobility in organic materials used in devices such as solar cells.

[1]This work was, in part, funded by Natural Sciences and Engineering Research Council of Canada.

S1.00250 High Thermoelectric Performance from Solution-Processed Conducting Polymer/Inorganic Composite Films

, NELSON COATES, SHANNON YEE, University of California, Berkeley, KEVIN SEE, JEFFREY URBAN, Lawrence Berkeley, National Laboratory, RACHEL SEGALMAN, University of California, Berkeley — Conducting polymer/inorganic composite films have great potential for use as thermoelectrics due to the possibility of combining the high electrical conductivity of inorganic materials with the low thermal conductivities of polymer materials. Additionally, the possibility of engineering nanoscale interfaces in these hybrid systems provides a unique means of optimizing thermoelectric figures of merit. We have fabricated films from this new class of materials, and examined their thermoelectric properties. Our solution-processed films, which consist of an inorganic nanostructure matrix linked with conducting polymer ligands, exhibit an electrical conductivity that is greater than either of its components and a thermopower that varies as a function of inorganic nanocrystal-conducting polymer ratio.

S1.00251 Probing the Fluid-Graphene Interface for Electrochemical Storage by *in-situ* Synchrotron X-ray Scattering

, HUA ZHOU, PAUL FENTER, Argonne National Laboratory, JAKE MCDONOUGH, VOLKER PRESSER, YURI GOGOTSI, Drexel University, PASQUALE FULVIO, SHENG DAI, Oak Ridge National Laboratory — The interactions of electrolyte fluids with solids control many complex interfacial processes encountered in electrochemical energy storage systems. In this talk, we will demonstrate how to develop a fundamental atomic-scale understanding of interfacial structures and processes at the electrolyte-graphene interface. We have performed systematic measurements of high resolution X-ray reflectivity from epitaxial graphene films in contact with electrolytes including aqueous solutions and room temperature ionic liquids. The electron density profiles and structural models from the fully analyzed data reveal the intrinsic interfacial structures of these systems. Moreover, we have developed successfully a customized electrochemical sample cell that allows the solvent reorientation and ion adsorption measurements to be done in-situ with control of the surface potential. Specular Bragg rod and resonant anomalous X-ray reflectivity measurements were performed in combination with electrochemical characterizations. The combination of in-situ structural measurements with electrochemical controls will lead to fundamentally new insights and provide unique tests of atomistic fluid-solid interface models for energy storage systems.

S1.00252 *ab initio* Thermodynamic Approach to Identify Good Solid Sorbents for CO_2 Capture Applications

, YUHUA DUAN, National Energy Technology Lab. — By combining thermodynamic database searching with first principles density functional theory and phonon lattice dynamics calculations, a theoretical screening methodology to identify most promising candidates for CO_2 sorbents has been proposed (Duan & Sorescu, PRB(2009), JCP(2010)). For given solids, first we can search their thermodynamic properties from thermodynamic databases and literatures. If their thermodynamic properties are unknown, we perform *ab initio* thermodynamic approach to calculate them out. These properties are used for computing the thermodynamic reaction equilibrium properties of CO_2 absorption/desorption cycle based on the chemical potential and heat of reaction analysis. According to the pre- and post- combustion technologies and conditions in power-plants, based on our calculated thermodynamic properties of reactions for each solid capturing CO_2 varying with temperatures and pressures, only those solid materials, which result lower energy cost in the capture and regeneration process and could work at desired conditions of CO_2 pressure and temperature, will be selected as promised candidates of CO_2 sorbents and further be considered for experimental validations.

S1.00253 ABSTRACT WITHDRAWN –

S1.00254 Development of semi-rigid coaxial cables for application to low temperature experiments

, AKIHIRO KUSHINO, Asahikawa National College of Technology, SOICHI KASAI, COAX CO., LTD. — Fast signal readout with low noise is essential for spectrometric research. Superconducting spectrometers operating below ∼1K are promising with their high spectral resolution, detection efficiency and counting rate. Cables connecting these spectrometers and electronics at high temperature must be coaxial and have low thermal conductance in order to reduce heat into low temperature. We have developed thin semi-rigid coaxial cables using low thermal conductivity alloys, CuNi, SUS and NbTi, for both center and outer conductors. The outer conductor is seamless and separated from the center conductor by a PTFE electrical insulator. We have assembled an adiabatic demagnetization refrigerator (ADR) at the 2nd stage of a GM cryocooler, which enables to cool the coaxial cables below 1K, and have measured low thermal conductance and performance of the cables at high frequencies up to ∼5 GHz.

S1.00255 HIGH PRESSURE PHYSICS –

S1.00256 High-Pressure Structural Studies of AuX_2 (X = Al, Ga, In)[1]

, JASON BAKER, RAVHI KUMAR, ANDREW CORNELIUS, HiPSEC and Dep. Physics, University of Nevada, Las Vegas — High-pressure x-ray diffraction experiments were performed on the group of intermetallic compounds, AuX2 (X = Al, Ga, and In), which at ambient conditions crystallize in the CaF2 [Space group Fm3m] structure. The previously reported retention of the CaF2 phase until 24 GPa in AuIn2 was not observed in these experiments, and instead was observed to undergo a pressure-induced phase transition at 13 GPa. Both AuAl2 and AuGa2 undergo pressure-induced phase transitions at 15 GPa and 9 GPa, respectively. The structural details and the phase transition sequence in these compounds will be presented.

[1]Work at UNLV is supported by DOE [DE-FC52-06NA27684] and NNSA.

S1.00257 High Pressure XRD Structural Study of Intermetallic Hydrogen Storage Material $ZrFe_2$[1] , DANIEL ANTONIO, RAVHI KUMAR, ANDREW CORNELIUS, HiPSEC, Physics Dep. University of Nevada, Las Vegas — Intermetallic compounds show high hydrogen sorption capacities when pressurized with hydrogen. Further, they are also used in hydride compressors [1]. The structure of intermetallic $ZrFe_2$, which can contain about 1.7 wt/GPa, was studied using XRD at high pressures up to 47 GPa using a diamond anvil cell and synchrotron x-rays. The cubic Fd3m Laves phase is found to be stable and the bulk modulus was found to be 163.5 GPa which compares well with other intermetallics. The variation of unit structural parameters and the equation of state are discussed.

[1]Work at UNLV is supported by DOE [DE-FC52- 06NA27684]

S1.00258 Towards a phase diagram for accreting neutron star crusts: total energy calculations of close packed lattices , TYLER ENGSTROM, VINCENT CRESPI, BENJAMIN OWEN, Penn State University — Neutron star crusts are somewhat less exotic than their cores, but may still play an important role in observable astrophysical phenomena, such as pulsar glitches and cooling rates. Recent nucleosynthesis calculations of accreting material being burned and buried on a neutron star crust indicate the possible presence of many species, ranging from around Z=8 to Z=34. In the outer crust regime where these species are completely pressure ionized and have screened-Coulomb interactions due to the relativistic Fermi electron gas, we expect some close-packed lattices may have a lower free energy than the bcc structure that is usually assumed to exist. Our poster shows the results of ground state energy calculations for several candidate binary and ternary close-packed lattices. We compare these ground state energies to those for pure phase separated bcc and fcc structures.

S1.00259 Structure stability of multiferroic compound Bi2NiTiO6 under high pressure and temperature , JINLONG ZHU, Los Alamos National Laboratory, CHANGQING JIN, Institute of Physics, CAS, YANCHUN LI, XIAODONG LI, JING LIU, Institute of High Energy Physics — Structural of multiferroics Bi2NiTiO6 under high pressure was studied in diamond-anvil cell (DAC) combined with synchrotron radiation X-ray diffraction. Crystal structure refinement shows that there are two isostructural phase transitions at $\sim$2 GPa and in the range of 15.5$\sim$18.5 GPa, respectively. The bulk modulus was derived from Birch-Murnaghan equation of state (EOS). Bi iron discontinuous movement is thought to be the source of all the isostructural phase transitions. Temperature dependence of X-ray diffractions were collected from room temperature up to 550 $^{\circ}$C. Structure refinement shows that an isostructural phase transition at temperature higher than 550 $^{\circ}$C can be compare with the isostructural phase transition in the range of 15.5$\sim$18.5 GPa.

S1.00260 GENERAL PHYSICS II —

S1.00261 Proposal to reduce the carcinogenic character of electromagnetic radiation (EMR) , MARJORIE LUNDQUIST, The Bioelectromagnetic Hygiene Institute — Non-ionizing electromagnetic radiation (NIEMR) interacts with matter in 3 ways:[1] it can transfer energy, linear momentum, and angular momentum to matter. At high frequencies (*e.g.*, microwaves), evidence exists of a carcinogenic effect on living creatures irradiated with NIEMR.[2] Which effect is carcinogenic? NIEMR heats matter by transfer of energy; this effect is used to **kill** established cancers. Transfer of linear momentum to matter merely alters the local pressure; cancer has never been associated with pressure changes. So the transfer of non-zero angular momentum to matter is the interaction most likely to be carcinogenic. EMR polarization can be circular, elliptical, or plane. Only plane-polarized EMR possesses **zero** angular momentum and therefore **cannot** transfer any angular momentum to matter. Everything that is true of NIEMR is also true of ionizing EMR, so it seems likely that the carcinogenic potential of **all** EMR (whether ionizing or non-ionizing) will be minimized by filtering it or taking other steps to make it plane-polarized before using it to irradiate a person or animal. Obvious applications are medical/dental X-rays and the full body scanners used on travelers at airports.

[1]M. Lundquist, **BAPS 51**(1):518 (2006).
[2]M. Lundquist, **BAPS 49**(1):1296 (2004).

S1.00262 Good science, deceptive science, and fraud, plus a brief discussion of peer review , MARJORIE LUNDQUIST, The Bioelectromagnetic Hygiene Institute — What makes scientific publication different from other types of publication? Traditionally, it was that scientists published not only their conclusions, but also their data (which enabled others wanting to re-evaluate the data to do so). Publishing their data helped keep scientists honest. In the mid-20^{th} century the policies of scientific journals changed, partly because very large data sets were being evaluated via computer. Many (but not all) scientific journals paid homage to scientific tradition by establishing archives for data serving as the basis for published scientific papers, while only a description of the study and the conclusions were published in the peer-reviewed scientific journals. This set the stage for scientific deception and scientific fraud, which became widespread in certain fields of study during the latter part of the 20^{th} century. Indeed, some organizations were established that appeared to be legitimate scientific societies, but in fact existed for the purpose of promoting the **incorrect** evaluation of scientific data and publishing deceptive studies masquerading as sound scientific studies. The field of medicine has also become more science than art, with its current emphasis on "evidence-based medicine." The different types of scientific deceit/fraud are identified, and a lifetime of experience with the correction of scientific error, plus encounters with scientific deception and scientific fraud, is summarized.

S1.00263 Both Perelmans Thrown Down Gauntlets Versus Would-Be "Science" But Alas Sadly Mere "SEANCES" Put Jargonial-Obfuscation Sociological-Dysfunctionality(S-D) Ridden/Dominated Would-Be "Sciences" But Alas Sadly Mere SEANCES in "Peril, Man"!!! , J. CARLSON, F. YOUNG, LONDON CLAY, EDWARD CARL-LUDWIG (PHYSICAL-MATHEMATICIST/MATHSICIST) SIEGEL, EMET/TRUTH-in-the-"SEANCES" — Both Perelman (Grigory[Poincare-conjecture: partial(with Richard Hamilton!!!)-"sole"-prover: by turning down first the Fields Medal at International Congress of [S-D right there: not mathematICS, but mathematicIANS!!!] Mathematicians (2007: Madrid); then the million-dollar Clay-Institute of Mathemat"ICS" (but really mathematicIANS POLITICIANS: Carlson, Yau,...et. al.) millennium-problem prize, revealing that it and its INSIDER POLITICS/POLITICIANS has/have "Feet of Clay"!!!], as sumarized by Naser-Gruber[Manfold-Destiny, The New Yorker, (August, 2007)] and separately Carlos Castro[with Corredoira: Against the Tid (2008)] put, by revealing the Jargonial-Obfuscation(J.-O.) (Bradshaw[Healing the SHAME that BINDS You, Hazelden(1980s)]-Martin[Brian, Wollongong University]-...ad INFINITUM (i.e. most if not all scientists), ad NAUSEUM!!! (disgusted with "games people play!!!)) S-D ridden/ dominated "games people play" would-be "sciences" (maths, physics,...: ad infinitum; ad NAUSEUM!!!) but alas sadly only mere Bradshaw-Martin S-D DOMINATED "SEANCES"!!!, in "peril, man"!!!

S1.00264 Jargonial-Obfuscation(J-O) DISambiguation Elimination via Siegel-Baez Cognition Category-Semantics(C-S) in Siegel FUZZYICS=CATEGORYICS (Son of TRIZ)/(F=C) Tabular List-Format Dichotomy Truth-Table Matrix Analytics , CARL LUDWIG SIEGEL, EDWARD CARL-LUDWIG SIEGEL, FUZZYICS=CATEGORYICS(SON OF TRIZ)/CATEGORY-SEMANTICS — NOT "philosophy" per se but raising serious salient Arnol'd [Huygens and Barrow, Newton and Hooke(96)] questions begged is Rota empiricism Husserl VS. Frege maths-objects Dichotomy controversy: Hill-Haddock[Husserl or Frege?(00)]as manifestly-demonstrated by Hintikka[B.U.]-Critchey[Derrida Deconstruction Ethics(78)] deconstruction; Altshuler TRIZ; Siegel F=C/C-S; Siegel-Baez(UCR) Cognition C-S = "Category-theory "+" Cognitive-Semantics[Wierzbica-Langacker-Lakoff-Nunez[Where Maths Comes From(00)]-Fauconnier-Turner[Blending(98)]-Coulson[Semantic-Leaps (00)]]-Hofstadter[Fluid-Analogies For Creative-Thinking(94)]]-Holyoak[Analogy/ Metaphor] -Hademard[Maths-Mind(45)]-Graeser[Text-*comprehension* VIA (7-dimensional orthogonal-QUERY-space: WHAT?, WHERE?, (+) WHEN?, WHY?; (DYS-functional)WHO?) VS. TRADITIONAL/BY-ROTE: How?; How Much?]-Belew [Finding Out About(00)]-Hubbard[World According to Wavelets(96)]. Detailed are Siegel PHYSICS discoveries/approaches to ostensibly "pure"-maths Benford-law and Millennium-Problems proofs: FLT (CCNY;1964) <<< Wiles(1994); P=/NP; BSD-Conjecture; Riemann-hypothesis.

S1.00265 POST-DEADLINE —

S1.00266 Structural and Dielectric Study of (Dy,Er,Ho)CrO_3 Biferroic Compounds[1] , CESAR MEZA, JESUS SIQUEIROS, ALEJANDRO DURAN, CNYN-UNAM — Technological progress, especially in electronic applications, demands increasingly advanced substances, capable of performing a variety of tasks while simultaneously occupying less space than their predecessors. An answer to this demand lies within the realm of multiferroics. Multiferroic materials are defined as those single phase compounds where more than one ferroic order coexists; they generally belong to the perovskite group. One manifestation of multiferroicity, magnetoelectricity, requires the coexistence of spontaneous electric polarization and magnetic ordering. It is for this reason that rare-earth chromites have been selected as suitable candidates. This work is concerned with synthesis, characterization and dielectric response of the $DyCrO_3$, $ErCrO_3$ and $HoCrO_3$ ceramic compounds. The samples were synthesized by both the traditional solid state ceramic method, and the self-propagating combustion method. The resultant chromites were characterized by TG, DTA and XRD, which confirms the Pbnm space group. Additionally, conductivity analysis was performed and the associated activation energy determined for each system using experimental values and Arrhenius law.

[1]Thanks are due to DGAPA-UNAM for financial support through projects no. IN112909 and IN105711.

S1.00267 Simulation of infrared photodetectors from single-electron models[1] , NELSON STUDART, Dept. de Fisica - UFSCar, MARCOS H. DEGANI, MARCELO Z. MAIALLE, FCA - UNICAMP, PAULO F. FARINAS, Dept. de Fisica - UFSCar — We present results from simulations of potential structures with the method of the split operator. The method is applied to solve for electrons in potential profiles that are typical in the description of quantum dot infrared photodetectors. Various quantities of interest are calculated without the necessity of having the energy spectrum, simulating quantities like the photocurrent directly from a model hamiltonian. By using realistic band offset and mass parameters taken from devices, we are able to explain recent exeperimental results by referring to multiple-photon absorptions. In particular, strong resonance peaks observed in the $\sim 10\mu$m wavelength range in recently fabricated InAs quantum dot infrared photodetectors are obtained from the direct use of intrinsic band and mass parameters. Multiphoton scattering of electrons localized in the quantum dots are not only in accordance with the observed patterns, but are also necessary to explain the photocurrent spectrum obtained in the single-electron calculations.

[1]The authors aknowledge support from CNPq

S1.00268 Extremely nondegenerate two-photon absorption in semiconductors , DAVID HAGAN, CREOL, University of Central Florida, CLAUDIU CIRLOGANU, Georgia Institute of Technology, SCOTT WEBSTER, DMITRY FISHMAN, ERIC VAN STRYLAND, CREOL, University of Central Florida — Degenerate two-photon absorption, 2PA, in direct-gap semiconductors has long been known to scale with the inverse third power of the band gap, resulting in very large 2PA coefficients for narrow-gap semiconductors. We show that for any given pair of photon energies, (sum $=\hbar\omega_1 + \hbar\omega_2$), the 2PA is smallest for the degenerate case, $\omega_1 = \omega_2$, and is enhanced by orders of magnitude in the extremely nondegenerate case ($\omega_1/\omega_2 >> 1$ *or* $\omega_1/\omega_2 << 1$). We experimentally demonstrate that 2PA in direct-gap semiconductors (e.g. GaAs, CdTe, ZnSe, ZnO, GaN) is enhanced over the degenerate value by up to 3 orders of magnitude using extremely nondegenerate pairs of photons (energy ratios $\sim$10/1). These extremely nondegenerate 2PA coefficients are similar in magnitude to coefficients obtained in narrow-gap semiconductors such as InSb and make 2PA feasible for applications such as subfemtosecond gated detection, all-optical switching etc. We demonstrate gated detection in a GaN LED used in a reverse-biased detection mode with fs 5.6μm and 400nm pulses. We see nearly 4 orders of magnitude enhancement over the degenerate case and can also easily detect sub-nW of IR light using modulation methods.

S1.00269 Transport properties of superconducting La and Ce-based ferropnictides , S.J. SINGH, School of Physical Sciences, Jawaharlal Nehru University New Delhi-110067 India, J. PRAKASH, A.K. GANGULI, Department of Chemistry, Indian Institute of Technology New Delhi-110016 India, S. PATNAIK, School of Physical Sciences, Jawaharlal Nehru University New Delhi-110067 India — To understand the role of chemical pressure, we have synthesized a variety of La and Ce-based ferropnicides (La/Ce)OFeAs with substitution of Y, F, Co and Sb in place of La/Ce, O, Fe and As respectively. A broad spectrum of characterizations involving XRD, SEM, magnetoresistance, magnetization, penetration depth, Hall effect and thermoelectric power have been undertaken on these phase pure superconducting compounds. The transition temperature and upper critical field reached maximum of 48.6 K & 146 T in Ce-based sample whereas 35 K and 122 T in La-based superconductor. The magnetization measurements of all samples showed negligible hysteresis reflecting weak link behaviour or an imperfectly connected superconducting state. The thermoelectric power and Hall measurement confirmed the dominant role played by electrons in these multiband superconductors. The rf penetration depth analysis indicated s-wave pairing symmetry with multiple gap values.

S1.00270 Pulsed versus d.c. I-V characteristics of charge-ordered $LuFe_2O_4$, BERTINA FISHER, JAN GENOSSAR, LARISA PATLAGAN, GEORGE MICHAEL REISNER, Physics Department, Technion, Haifa — We report on electronic transport measurements in a polycrystalline sample of $LuFe_2O_4$, over a wide range of electric fields and at temperatures above 230 K , - the range of temperatures was limited by the high resistivity of the sample . This work was motivated by reports about striking non-linear conductivity in polycrystals and single crystals of this multiferroic, in relatively moderate electric fields. Using short ($\sim$msec) single current pulses four probe measurements detected no deviations from linearity in the I-V characteristics, in fields up to E $\approx$ 500 V/cm. However, strong non-linearity and hysteresis were found in d.c. measurements at fields that decreased with increasing temperatures, suggesting self-heating. We include a set of oscillograms showing the time dependence of the voltages between the various probes at fixed current and temperature, which emphasize the importance of time domain studies of non-linear conductivity effects. We gratefully acknowledge Prof. Young Sun from the Institute of Physics, Chinese Academy of Sciences, Beijing, P.R. China, for providing us with the $LuFe_2O_4$ sample.

S1.00271 A Ferroelectric Photovoltaic Capacitor Capable of Direct Solar Energy Conversion and Storage

, CHI-WEI LO, Materials Science Program, University of Wisconsin Madison, CHENSHA LI, HONGRUI JIANG, Department of Elecrical and Computer Engineering, University of Wisconsin Madison — Current solid state photovoltaics and conventional photoelectrochemical cells are not capable of directly storing the converted energy which has to be facilitated by connecting to external storing devices, thus increasing the system complexity. It would thus be highly desirable to create photovoltaic devices that can store solar energy directly. We here report a photo-rechargeable photoelectrochemical capacitor with direct conversion and storage capability by utilizing ferroelectric polyvinylidene fluoride (PVDF) gel with energy storing capability between anode and cathode. With the aid of ferroelectric effect, the device is able to maintain equilibrium between electric field and diffusion force. Results have shown that the device can be charged photovoltaically under 1 sun equivalent of irradiance to an open-circuit voltage of 0.47V, and with capacity of 40.63mC/cm^2. The storage lasts more than 24 hours. Electrochemical impedance analysis and ferroelectric hysteresis are also carried out to show its energy storing capability.

S1.00272 Chiral noncoplanar magnetic ordering driven by itinerant electrons on the pyrochlore lattice[1]

, GIA-WEI CHERN, Department of Physics, University of Wisconsin - Madison — In magnets with strong geometric frustration, the inability of spins to simultaneously satisfy the preferred local correlations leads to an extensive ground-state degeneracy at the classical level. The macroscopic degeneracy is lifted when other perturbations are taken into account. In general, collinear or coplanar magnetic orders are selected by perturbations which preserve the spin-rotational symmetry. Here we show that a complex *noncoplanar* magnetic order with a quadrupled unit cell is stabilized by itinerant electrons on the pyrochlore lattice [1]. Specifically we consider a Kondo-lattice model in which itinerant electrons interact with localized spins via on-site exchange coupling. The electron Fermi 'surface' at quarter filling is topologically equivalent to three intersecting Fermi circles. The noncoplanar magnetic order stems from a weak-coupling instability caused by perfect nesting of the Fermi circles. The magnetic structure characterized by a definite handedness also breaks the chiral symmetry. The chiral order might persist without magnetic order in a chiral spin liquid at finite temperatures.

[1] Gia-Wei Chern, Phys. Rev. Lett. **105**, 226403 (2010).

[1]The author acknowledges the support of ICAM and NSF Grant DMR-0844115.

S1.00273 Including many-body screening into self-consistent calculations–tight-binding model studies with Gutzwiller approximation[1]

, YONGXIN YAO, Iowa State University, J. SCHMALIAN TEAM, C. Z. WANG TEAM, K. M. HO TEAM — We introduce a scheme to include many-body screening process explicitly into self-consistent equations for electronic structure calculations by employing Gutzwiller approximation. The method is illustrated by applying to a tight-binding model of the strongly correlated γ-Ce. The critical Coulomb repulsion U^c_{ff} between the $4f$ electrons for electronic phase transition can be greatly raised over the usual screened value by including the main onsite many-body screening $5d$ channels. The method provides a promising way towards parameter-free *ab initio* Gutzwiller density functional theory.

[1]Work at the Ames laboratory was supported by the U.S. Department of Energy, Office of Basic Energy Science, including a grant of computer time at the National Energy Research Supercomputing Center (NERSC) under Contract No. DE-AC02-07CH11358.

S1.00274 Predicting Sommerfeld coefficients for heavy-fermion materials

, MUNEHISA MATSUMOTO, SERGEY SAVRASOV, UC Davis, JUNYA OTSUKI, Tohoku University, Japan — From electronic-structure calculation standpoint we predict the appearance of heavy-fermion behavior for Cerium and Plutonium-based materials. Local-density approximation (LDA) combined with dynamical-mean field theory (DMFT) formulated for localized f-electrons gives an efficient realistic Kondo-lattice description [1] for the target materials, yielding a quasiparticle renormalization factor z_c for conduction electrons. We invert the data to get the quasiparticle renormalization factor z_f for f-electrons, and restore the effective total density of states to predict the Sommerfeld coefficient γ. Summarizing our data on an analogous "Doniach phase diagram" plotted for z_c, z_f, and γ, γ is found to have a peak around the magnetic quantum critical point and Ce-115's are found to have the largest γ's among target materials.

[1] PRL **103**, 096403 (2009).

S1.00275 Atomic Green's function calculations using GPU

, REI SAKUMA, Chiba University — GPU computing or GPGPU has been successfully applied to many scientific computations, such as Monte-Carlo and molecular dynamics. In this presentation we present the application of GPU computing to the calculations of non-relativistic and relativistic atomic Green's functions including the Coulomb interaction.

S1.00276 Production of Short-Lived ^{37}K[1]

, HEATHER STEPHENS, Rose-Hulman Institute of Technology, DAN MELCONIAN[2], PRAVEEN SHIDLING[3], Texas A&M University — The purpose of our work during the summer months of 2010 was to produce a beam of ^{37}K with $\geq$ 99% purity and characterize in detail the remaining contaminants. A projectile beam of ^{38}Ar at 25 and 29 MeV/nucleon from the K500 cyclotron generated the ^{37}K by reacting with an H_2 gas target. The *MARS* spectrometer was then used to separate the reaction products of interest from the primary beam and other unwanted reaction products. From analysis of our production experiment, we were able to successfully produce 807 counts/nC of ^{37}K with 99.19% purity at 25MeV/u and 1756 counts/nC with 98.93% purity at 29MeV/u. The purity of this beam and rate of production is more than adequate for use in determining the half-life of ^{37}K, the next step to be done by the team in August 2010. This measurement will be accomplished by implanting the activity into a Mylar tape, placing it between two high-efficiency gas counters and counting the amount of beta decays as a function of time. It is expected the half-life will be measured using the ^{37}K produced from ^{38}Ar at 29MeV/u.

[1]Funded by DOE and NSF-REU Program.
[2]Cyclotron Institute
[3]Cyclotron Institute

S1.00277 Self-Assembled Double-Quarter Antireflective Coatings using Silica and Titania Nanoparticles

, ANITESH LAL, RAISA CASTEDO VELASCO, DAN MAZILU, Washington and Lee University — Antireflective coatings have a wide range of applications, from eyeglass and camera lenses, to solar panels and optoelectronic devices, to name just a few. Our study examines several factors that affect the quality of antireflective coatings created by the self-assembly of alternating layers of SiO2 and/or TiO2 nanoparticles and poly(diallyldimethylammonium chloride) polycation on glass substrates. We use a factorial design to investigate the effects of the molarity of the nanoparticle solution, the size of the nanoparticles, the pH of the nanoparticle and polycation solutions, and the number of nanoparticle-polycation bilayers on the optical properties of the films. The first order effects of these factors, as well as their interactions, on the reflectance, transmittance, and uniformity of the coatings are reported.

S1.00278 Magnetic domain configuration of $La_{0.7}Sr_{0.3}MnO_3$ patterned elements , CARLOS A.F. VAZ, JAN RHENSIUS, ANDRE BISIG, MATHIAS KLÄUI, LAURA HEYDERMAN, Paul Scherrer Institut, Switzerland, MIGUEL NIÑO, ANDREA LOCATELLI, Sincrotrone Trieste, Italy, F. GAUCHER, ALICE GALDI, LAURENCE MÉCHIN, Universite de Caen Basse-Normandie, France — The magnetization configuration in small $La_{0.7}Sr_{0.3}MnO_3$ elements is investigated as a function of geometry, film thickness, magnetic field, and temperature using x-ray magnetic circular dichroism photoemission electron microscopy (XMCD-PEEM). The patterned elements were defined by focused ion beam (FIB) lithography, and consist of elements varying in shape (from circular, triangular and quadrangular) and size, from 200 nm up to 10 μm. A strong magnetic contrast is observed for all thicknesses (10-50 nm). The magnetic state in the larger elements tends to be multidomain, with complex configurations that are determined by the presence of local pinning sites. These pinning sites are overcome with increasing temperature, and the magnetic configuration evolves into lower energy states. In contrast, the magnetic configuration of the smaller elements are largely determined by the magnetostatic energy contribution, which gives rise to highly symmetric states as found in 3d ferromagnetic structures. Our results show that the magnetism of small LSMO elements is robust nearly up to the critical temperature, with magnetic configurations that can be controlled by suitable geometrical design.

S1.00279 Visible light photoreactivity from Carbon nitride bandgap states in Nb and Ti oxides , HOSIK LEE, TAKAHISA OHNO, NIMS, ICNSEE TEAM — Lamellar niobic and titanic solid acids (HNb_3O_8, $H_2Ti_4O_9$) are photocatalysts which can be used for environmental cleanup application and hydrogen production through water splitting. To increase their efficiency, bandgap adjustment which can induce visible light reactivity in addition to ultraviolet light has been one of hot issue in this kinds of photo-catalytic materials. Nitrogen-doping was one of the direction and its microscopic structures are disputed in this decade. In this work, we calculate the layered niobic and titanic solid acids structure and bandgap. Bandgap reduction by carbon nitride absorption are observed computationally. It is originated from localized nitrogen state which is consistent with previous experiments.

S1.00280 Statistical Analysis of Biotissues Mueller Matrix Images in Cancer Diagnostics , ROMAN TSYLYAK — This work is directed to the investigation of the scope of the technique of laser polarimetry and polarization spectrometry of oncological changes of the human prostate tissue under the conditions of multiple scattering, which presents real experimental clinical situation. Statistic moments of the first (M), second (σ), third (A) and fourth (E) orders were used as the analytical tool for estimating the ensemble of random values of z, that characterize the image of biological object (intensity I, polarization azimuths α and ellipticities β) and its optical-geometrical structure (orientation directions of the protein fibrils and birefringence index of their substance Δn). It was shown that the difference between the values of average and dispersion of distributions I (0 - 0), I (0 - 90), the intensities of images of various types of prostate tissues are insufficient and are within 10%-25%. The values of the excess of intensity distribution of the images of oncologically changed prostate tissues differ from the similar parameter of a sound tissue by 1-2 times. The third statistic moment proved to be the most sensitive because it's value in the intensity distribution of polarization image I (0 - 90) of oncologically changed tissue is 21 times higher if compared with healthy tissue.

S1.00281 The Itinerant Electron and Local Moment Hybrid Model of Iron-based Superconductors , YIZHUANG YOU, Institute for Advanced Study, Tsinghua University, FANG YANG, Physics Department, Beijing Institute of Technology, SHUPENG KOU, Physics Department, Bejing Normal University, ZHENGYU WENG, Institute for Advanced Study, Tsinghua University — An itinerant electron and local moment hybrid model for iron-based superconductors is studied, with the band structure modeled simply by two pockets. Reasonable phase diagram is obtained on the mean field level. The spin and charge dynamics are further studied by the random phase approximation (RPA). The dynamic spin susceptibility displays a Goldstone mode of the collective itinerant electron and local moment excitations in the SDW phase, and a resonance mode in the superconducting phase which persists all the way to the normal state phase. It is found that the scattering with local moment always tends to reduce the pocket depth of the itinerant electron. The study also suggests that, to correctly account for the features in transport experiments, the multi-band effect that give rise to the nodal SDW should be included.

S1.00282 Synthesizability of Superhard Carbon by Cold Compression of Graphite[1] , SALAH EDDINE BOULFELFEL, ARTEM OGANOV, Stony Brook University SUNYSB, STEFANO LEONI, Technical University Dresden — We present an efficient scheme combining Monte Carlo walk in the space of transition pathways with molecular dynamics simulations for predicting matter modification under high pressure. If crystal structure prediction is a top-interest field for science and technology, the quest is even more exciting for elements such as boron and carbon. While under pressure above 15 GPa and at high temperatures (1600-2500 K) graphite is converted into diamond, room temperature compression gives a new superhard modification of carbon. Its nature remained unresolved until recent theoretical investigations predicted two candidate structures, M-Carbon and BCT4. Both structures have comparable physical properties and refine well the XRD data. To elucidate the nature of the final product of graphite cold compression we performed molecular dynamics transition path sampling simulations and we determined the energy profile of each transition (graphite to M-carbon and graphite to BCT4). The intrinsic mechanism of the reconstruction and the reasons of the favoring of one structure over the other have been determined. A detailed picture of events of nucleation and growth during the transition is finely reproduced. Our procedure do not only determine the nature of a transition final product but predicts its synthesizability under given conditions of pressure and temperature.

[1]We acknowledge DARPA for funding.

S1.00283 Infrared optical absorption spectra of CuO single crystals: Fermion-spinon band and dimensional crossover of the antiferromagnetic order , E.J. CHOI, JOOYEON KIM, University of Seoul, Y. SEIKO, T. KIMURA, Osaka University, Japan, J. LORENZANA, Università di Roma — We have obtained mid-infrared optical absorption spectra of the $S = 1/2$ quasi one-dimensional CuO using polarized transmission measurement and interpreted the spectra in terms of phonon assisted magnetic excitations. When the electric field is parallel to the main antiferromagnetic direction a Δ shaped peak is observed with the maximum at $\omega = 0.23$ eV which is attributed to spinons along Cu-O chains. At low temperatures in the antiferromagnetic phase another peak appears at $\omega = 0.16$ eV which is attributed to two-magnon absorption but the spinon peak remains. This behavior is interpreted as due to a dimensional crossover where the low temperature three- dimensional magnetic phase keeps short range characteristics of a one- dimensional magnet.

S1.00284 ABSTRACT WITHDRAWN —

S1.00285 Development of Graphene for High Frequency Electronics , JOSHUA ROBINSON, The Pennsylvania State University, DAVID SNYDER, MARK FANTON, MATTHEW HOLLANDER, MICHAEL LABELLA, KATHLEEN TRUMBULL, RANDALL CAVALERO, BRIAN WEILAND, THE PENNSYLVANIA STATE UNIVERSITY TEAM — The practicality and success of a graphene technology depends on the ability to regularly and controllably synthesize graphene; integrate it with metals and dielectrics; and to develop device designs that take advantage of graphene's unique properties. We demonstrate graphene synthesis on SiC(0001) and Sapphire with 1.5% variation in sheet resistance across 100mm wafers. Hall mobility measurements indicate that direct growth of graphene on sapphire leads to a 2x increase in mobility (2200 cm^2/Vs) compared to silicon sublimation from SiC(0001). Additionally, we have developed high quality ohmic contacts to graphene, which improves the contact resistance by nearly 6000x (5x10^{-8} Ohm-cm^2) compared to untreated metal/graphene interfaces. Finally, we discuss integration of ultra-thin high-k dielectrics and their impact on graphene transport. Atomic layer deposited oxide heterostructures (seed not equal to overlayer) have deleterious effects on Hall mobility while homostructures lead to an increase in Hall mobility. Importantly, 5nm thick EBPVD HfO_2 gate dielectrics are successfully demonstrated and show improved Hall mobility, on-off ratio, and transconductance relative to Al_2O_3 gates and heterostructure gates.

S1.00286 Synthesis and properties of artificially layered (Ba,K)BiO_3 and Ba(Bi,Pb)O_3 structures[1] , G.W.J. HASSINK, K. MUNATAKA, R.H. HAMMOND, T.H. GEBALLE, M.R. BEASLEY, Geballe Laboratory for Advanced Materials, Stanford University, Stanford, California 94305, USA — The possibility of superconductivity in a negative U material due to the proximity effect with a normal metal (Berg, Phys.Rev.B 78, 094509), and of doping via charge transfer at interfaces (Ohtomo, Nature 427, 423-426) has led us to investigate the properties of artificially-layered films of $BaBiO_3$ (a negative-U insulator) and $BaPbO_3$ (a normal metal) and of their doped variants (Ba,K)BiO_3 and Ba(Bi,Pb)O_3, both of which are isotropic (3D) and are superconducting over a specific range of doping. Samples were either Ruddlessden-Popper phases of (Ba,K)BiO_3 synthesized by pulsed laser deposition or bi-layers of $BaPbO_3$ and $BaBiO_3$ and their variants by e-beam evaporation. We studied the transport properties of these samples to investigate the presence of superconductivity and the influence of anisotropy.

[1]Work supported by the AFOSR MURI Towards New and Better High Temperature Superconductors

S1.00287 Unique microstructure of $\alpha \rightarrow \varepsilon \rightarrow \alpha$ transition in shock-compressed iron[1] , MAN-LING SUI, Beijing University of technology, SHU-JUAN WANG, Shenyang National Laboratory for Materials Science, Institute of Metal Research, CAS, YONG-TAO CHEN, QING-ZHONG LI, HAI-BO HU, Institute of Fluid Physics, CAEP — Unique microstructure in recovered samples of shock-compressed iron is founded by transmission electron microscope (TEM) research. This confirms that the $\alpha \rightarrow \varepsilon \rightarrow \alpha$ martensitic transformation occurs during shock condition. Based on the specific features we reveal the mechanisms of both the transitions.

[1]This work was supported by the NSFC Grant No. 10776032

S1.00288 Alignment Behavior of Liquid Crystals on Nanoscopically Heterogeneous Surface , KYUNGHEE LEE, HYO KANG, GUIDUK YU, BONG SEOCK KIM, JONG-CHAN LEE, KYUSOON SHIN — We investigated the alignment behavior of liquid crystal molecules (LCs) on highly ordered polystyrene nanorod arrays. The diameter-controlled and height-controlled substrate was obtained from anodized aluminum oxide template. Upon the introduction of 1D nanostructures to the surface, the LC alignment was strongly influenced by the size of surface pattern. When the diameter of nanorods increased, the LC alignment changed from random planar to vertical orientation. The LC orientation was also altered by the increase of the height of nanorods. This transition happened in a small difference of nanorod diameter/height. The orientation change on the variation of nanorod dimension can be explained by the distortion of elastic-energy. The space between adjacent nanorods is sufficiently narrow to impose entropy penalty on LC molecules, and thus the LCs undergo elastic distortion near nanorod surface.

S1.00289 Metal–nanotube interactions – wetting properties[1] , RUZENG ZHU, LNM, IMech, CAS., Beijing, China, SHUWEN CUI, ChaoYang school of HSRUC — The wetting properties of metal nanoparticles in large-diameter single Carbon nanotubes (LDSWNT) is studied by considering the size effect on surface tension of the metal cluster. For the case of macro-nonwetting, we get finite critical atom number N such that the metal cluster with any atom number smaller than it has contact angle π, and so it shrinks into a ball. For an experiential formula of the surface tension of cluster expressed by the number of atoms, we determine the parameters in it for Pd and Pt respectively by density functional theory (DFT). Taking a graphene sheet as a representative of LDSWNT and using the known data of the surface tensions of solid and liquid, we obtain solid-liquid interface tension through Berthelot rule. Based on these results, we obtain N=5 for Pd and N=6 for Pt. For cluster containing 13 Pd atoms and that containing 13 Pt atoms, we use the above mentioned experiential formula to obtain their contact angles in LDSWNT consistent with those shown by the pictures given by DFT (A Maiti and A Ricca, Chem Phys Letters 395 (2004) 7–11), and thus the validity of our method is proved.

[1]Project supported by the National Natural Science Foundation of China (Grant No.11072242).

S1.00290 Magnon spectrum in a spiral magnetic order on the pyrochlore lattice: application to $CdCr_2O_4$, EUNSONG CHOI, GIA-WEI CHERN, NATALIA PERKINS, University of Wisconsin, Madison — Recent neutron scattering measurement on a geometrically frustrated antiferromagnet $CdCr_2O_4$ observed an unusual ground state in which a spiral magnetic order characterized by an incommensurate wavevector $\mathbf{Q} = (0, \delta, 1)$ is accompanied by a tetragonal lattice distortion [1]. These results can be consistently explained by a model of Heisenberg interaction with anisotropic exchange constants perturbed by the Dzyaloshinski-Moriya interaction [2]. Based on this spin Hamiltonian, we numerically integrate the Landau-Lifshitz-Gilbert equation to obtain the linear magnon spectrum [3]. Exact diagonalization based on the conventional Holstein-Primakoff transformation is ineffective in our case due to the lack of translational symmetry in the magnon Hamiltonian. We also compare the numerical spectrum with the experimental results and discuss its implications on the model Hamiltonian.

[1] J.-H. Chung *et al.* Phys. Rev. Lett. **95**, 247204 (2005).
[2] G.-W. Chern, C. J. Fennie, and O. Tchernyshyov. Phys. Rev. B. **74**, 060405 (2006).
[3] M. Mochizuki, N. Furukawa, and N. Nagaosa. Phys. Rev. Lett. **104**, 177206 (2010).

S1.00291 Vortex Confinement in Superconducting/Ferromagnet Hybrid Structures , M. IAVARONE[1], Physics Department, Temple University, Philadelphia, PA 19122, USA, A. SCARFATO, F. BOBBA, M. LONGOBARDI, Physics Department, University of Salerno, Fisciano 84084, Italy, F. GIUBILEO, CNR-SPIN Laboratory, Salerno, Italy, G. KARAPETROV, V. NOVOSAD, V.G. YEFREMENKO, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA, A. CUCOLO, Physics Department, University of Salerno, Fisciano 84084, Italy — Magnetically coupled superconductor-ferromagnet hybrids offer advanced routes for nanoscale control of superconductivity. Scanning tunneling microscopy (STM) and scanning magnetic force microscopy (MFM) coupled to magneto-transport measurements reveal rich vortex phase diagram. The magnetic stripe domain of the ferromagnet induces periodic local magnetic induction in the superconductor, creating a series of pinning and anti-pinning channels for vortices observed with low temperature STM and MFM. Such laterally confined Abrikosov vortices form chains. We also found general equilibrium condition for which vortex-antivortex pairs are spontaneously formed during zero-field cooling. In the non-equilibrium state the strong magnetic pinning of the vortex lattice results in avalanches of antivortices when changing the polarity of the applied magnetic field.

[1]Physics Department, University of Salerno, Fisciano 84084, Italy

S1.00292 Lipid Bilayer Vesicle extrusion through nanopores: a coarse grained molecular dynamics study[1] , MARTIN BERTRAND, BELA JOOS, University of Ottawa — We conducted Coarse-Grained Molecular Dynamics simulations of the pressure extrusion of vesicles in nanopores that confirm and help explain prior experimental observations (Patty, P. and Frisken, B., Biophys. J., 85, 2003). We demonstrate that, to a first approximation, the final size of extruded vesicles can be obtained by considering an invariable inner vesicle volume enclosed by a finitely extensible lipid bilayer. Using our data, we also describe in details the mechanics of vesicle rupture in a nanopore when pushed by various pressure gradients. This is made possible by tracking local variations of the stress in the lipid membrane via changes in surface area using a triangulation algorithm. The simulations are executed using state of the art GPU accelerated software. Our findings could potentially be useful in the design of liposome based drug delivery systems and in getting a better understanding of how the cell nucleus and the cell as a whole react in similar conditions.

[1]Work supported by NSERC and FQRNT

S1.00293 Spin-dependent 8x8 k.p Hamiltonian in silicon[1] , PENGKE LI, HANAN DERY, University of Rochester — Silicon is a promising material choice in spintronics devices due to its long electron spin lifetime and dominant technology. We present a theory that describes the spin properties of conduction electrons in different valleys in silicon. Using the method of invariants, we have developed an 8×8 Hamiltonian with spin-orbit interaction that captures the symmetry of the zone edge states and their spin dependent parameters. We derive analytical results of the energy bands, and more important, of the spin mixing of states. Both are in perfect agreement with the numerical results of an empirical pseudopotential method with spin orbit interaction. The new theory is capable of filling a dominant role in studying spin properties of electrons silicon similar to the way that the Kane model in being used in direct band-gap semiconductors.

[1]AFOSR Contract No. FA9550-09-1-0493 & NSF Contract No. ECCS-0824075.

S1.00294 Polaron formation and multi-band multi-gap superconductivity in layered materials , ANNETTE BUSSMANN-HOLDER, Max-Planck-Institute for Solid State Research, HUGO KELLER, Physik Institut der Universität Zürich — In cuprates and novel layered superconductors electron-lattice interactions are not strong enough to achieve the high transition temperatures. However, polaron formation may occur locally at intermediate sized regions around the dopants thus leaving the surrounding matrix remains almost unaffected. The coexistence of the dynamical polarons and the host matrix represents a multi-component system, where different physics are combined. The consequences of this scenario are manyfold: The strong *local* electron-lattice coupling induces a *local soft mode* which gives rise to divergences in the relative Cu-O, Fe-As squared displacements. The electronic bands are renormalized and experience an exponential reduction which is the origin of unconventional isotope effects. Superconductivity is characterized by multi-components, which can have system dependent different pairing symmetries. Cuprates and other layered superconductors are discussed and comparison to experimental data is made.

S1.00295 Node-node correlations and transport properties in scale-free networks , BIBIANA OBREGON, Posgrado en Ingenieria, UNAM, Mexico, LEV GUZMAN, UPIITA, Instituto Politecnico Nacional, Mexico — We study some transport properties of complex networks. We focus our attention on transport properties of scale-free and small-world networks and compare two types of transport: Electric and max-flow cases. In particular, we construct scale-free networks, with a given degree sequence, to estimate the distribution of conductances for different values of assortative/dissortative mixing. For the electric case we find that the distributions of conductances are affect ed by the assortative mixing of the network whereas for the max-flow case, the distributions almost do not show changes when node-node correlations are altered. Finally, we compare local and global transport in terms of the average conductance for the small-world (Watts-Strogatz) model

S1.00296 Controlling Rotational Molecular Rotor by Selection of Anchoring Sites , HYO WON KIM, Seoul National University, M. HAN, H.-J. SHIN, S. LIM, Y. OH, K. TAMADA, M. HARA, Y. KIM, M. KAWAI, Y. KUK, SEOUL NATIONAL UNIVERSITY TEAM, TOKYO INSTITUTE OF TECHNOLOGY COLLABORATION, RIKEN ADVANCED SCIENCE INSTITUTE COLLABORATION, TOHOKU UNIVERSITY COLLABORATION, THE UNIVERSITY OF TOKYO COLLABORATION — In future nano-electro-mechanical-systems (NEMS), a molecular motor may become a key component to produce nanoscopic dynamical motions. At the level of a single molecule, rotational motions of various molecules have been observed on clean metal or semiconductor surfaces in scanning tunneling microscope (STM) images. Based on the observations, molecular bearings, nanocars, pinwheels, a rack and pinion device, wheels and gears have been proposed using a hindered molecular rotation. Despite extensive studies, the control of rotational motion in a molecular rotor is quite difficult. In this talk we report a controlled rotational-motion of an azobenzene derivative, EtO-Azo-C10, by inducing a reversible hopping motion between an immobile and a mobile site on a Au(111) surface with tunneling electrons in STM geometry.

S1.00297 Entropic transport - a step beyond Fick-Jacobs , STEFFEN MARTENS, Humboldt-University Berlin, Department of Physics, Newtonstr. 15, 12489 Berlin, Germany, GERHARD SCHMID, University Augsburg, Department of Physics, Universitaetsstr. 1, 86135 Augsburg, Germany, LUTZ SCHIMANKY-GEIER, Humboldt-University Berlin, Department of Physics, Newtonstr. 15, 12489 Berlin, Germany, PETER HÄNGGI, University Augsburg, Department of Physics, Universitaetsstr. 1, 86135 Augsburg, Germany — We investigate the transport of point-size Brownian particles under the influence of a constant and uniform force field through a three-dimensional channel with smoothly varying periodic cross-section. We apply the standard long-wave asymptotic analysis and show that the leading order term is equivalent to the Fick-Jacobs approximation. Using the higher order corrections of the probability density we derive an expression for the spatially dependent diffusion coefficient. In addition, we demonstrate that in the diffusion dominated regime the averaged velocity and the effective diffusion coefficient are determined by the product of the Fick-Jacob result and the expectation value of the spatially dependent diffusion coefficient. Analytic findings are confirmed by numerical simulations of the particle dynamics in a reflection symmetric sinusoidal channel.

S1.00298 Thermally activated fragmentation of a homopolymer chain[1] , SIMON FUGMANN, IGOR M. SOKOLOV, Humboldt University Berlin, Department of Physics, Newtonstr. 15, 12489 Berlin, Germany — We consider the thermally activated fragmentation of a homopolymer chain, which can exhibit strongly non-Markovian behavior on the timescale of interest. In our model the dynamics of the intact chain is a Rouse one until a bond breaks and bond breakdown is considered as a first passage problem over a barrier to an absorbing boundary. Using the framework of the Wilemski-Fixman approximation we calculate activation times of individual bonds for free and grafted polymer chains. We show that these times crucially depend on the length of the chain and the location of the bond yielding a minimum at the free chain ends. Going beyond the Wilemski-Fixman approximation we show that a generalized form of the renewal equation for barrier crossings serves to improve the quantitative agreement between numerical simulations and analytical predictions.

[1]The authors thankfully acknowledge financial support by DFG within the SFB 555 research collaboration program.

S1.00299 Non-equilibrium ballistic phonon transport in microstructures , OBAFEMI OTELAJA, JARED HERTZBERG, RICHARD ROBINSON[1], Cornell University — A non-thermal spectral distribution of phonon modes may be excited in silicon microstructures by using the decay of quasiparticles injected into an adjacent superconducting film. [1] We demonstrate generation, ballistic transport and detection of phonons of frequency of order 100 GHz in microstructures of dimension 10 to 50 microns. We describe the fabrication process for the superconducting transducers, the measurement procedure, and plans to extend these techniques to build a nanoscale phonon spectrometer. This work is supported by KAUST (KUS-C1-018-02), NSF (DMR 0520404), and DOE (DE-SC0001086).

[1] W. Eisenmenger, A. H. Dayem, Phys. Rev. Lett. 18, 125 (1967).

[1](corresponding author)

Wednesday, March 23, 2011 2:30PM - 4:54PM –

Session T1 DCMP: Entanglement Spectroscopy Ballroom A1

2:30PM T1.00001 Momentum space entanglement in quantum spin chains , DANIEL AROVAS, University of California, San Diego — I will discuss work performed in collaboration with R. Thomale and A. Bernevig (*Phys. Rev. Lett.* **105**, 116805 (2010)) on entanglement spectra in spin chains. Typically, bipartite entanglement entropy and spectra have been studied in the case of spatial partitions, *i.e.* A denotes the left half of a spin chain, B the right half, $\rho_{\rm A} = {\rm Tr}_{\rm B} |\Psi_0\rangle \langle\Psi_0|$ is the reduced density matrix, and ${\rm spec}(\rho_{\rm A})$ is the entanglement spectrum (ES). We find for the $S = \frac{1}{2}$ Heisenberg model that a remarkable structure in the ES is revealed if the partition is performed in momentum space, *i.e.* A = left-movers and B = right-movers. Further classifying the entanglement eigenstates by total crystal momentum, we observe a universal low-lying portion of the ES with specific multiplicities separated from a higher-lying nonuniversal set of levels by an *entanglement gap*, similar to what was observed by Li and Haldane (*Phys. Rev. Lett.* **101**, 010504 (2008)) for the fractional quantum Hall effect. Indeed, the momentum space ES for the Heisenberg chain is understood in terms of the proximity of the Haldane-Shastry model, which corresponds to a fixed point with no nonuniversal corrections, and whose ground state wavefunction is related to that for the $\nu = \frac{1}{2}$ Laughlin state. We further explore the behavior of the ES as one tunes through the spin-Peierls transition in a model with next-nearest-neighbor exchange. We also discuss entanglement gap scaling and applications to other systems.

3:06PM T1.00002 Identifying Topological Order from the Entanglement Spectrum[1] , F.D.M. HALDANE, Princeton University — The Schmidt decomposition reveals bipartite entanglement of a quantum state. Calculation of the entanglement entropy reduces it to a single number, which can be studied as a function of the size and shape of the entangled regions. However, this reduction discards additional information contained in the full spectrum of the entanglement, which can be presented as a set of (dimensionless) "pseudo-energy" levels spectrum, labeled by quantum numbers such as momentum parallel to the $(d-1)$-dimensional boundary along which the bipartite decomposition of a d-dimensional system is made. The nature of the entanglement is revealed by this spectrum, much as the elementary excitations and collective modes characterizes condensed-matter states. (The von Neumann entropy is equivalent to the the thermodynamic entropy of the system of pseudo-energy levels at a particular fictitious "temperature" $k_B T = 1$.) The previously-unrecognized importance of the spectrum (as opposed to just its entropy) became immediately apparent when the entanglement spectrum of a 2D fractional Quantum Hall state along a 1D cut was first plotted [1]. The gapless spectrum of the conformal field theory related to the topological order of the FQHE can be recognized, and is the only spectrum in model states like the Laughlin or Moore-Read wavefunctions related to cft. For realistic states, corrections due to collective-mode fluctuations give rise to high-pseudo-energy modes that are separated from the gapless (topological) modes by a finite gap. Previously, it had been believed that the extensive O(L) ("area law") part of the entanglement entropy of this spectrum was non-universal, and topological order could only be recognized from the O(1) subleading behavior as the length L of the cut was scaled. However, while the "pseudo-energy" distribution appears to be non-universal, the distribution of the spectrum *as a function of (true) momentum* does not have this drawback, showing that the topological contribution to the O(L) part has a universal character not visible in the numerical value of the entropy itself. In general, (including also systems such as topological or Chern insulators [2]), the signature of topological order is the occurrence of gapless mode in the entanglement spectrum, providing a fingerprint from which this order can be identified.

[1] Hui Li and F. D. M. Haldane, Phys. Rev. Lett. **101** 246806 (2008).
[2] F. D. M. Haldane, BAPS.2009.MAR.T13.13.

[1]Supported in part by NSF MRSEC DMR-0819860.

3:42PM T1.00003 Multiplets in the Entanglement Spectrum , ARI TURNER, UC Berkeley — Often, spin chains do not have any long range order, because of quantum mechanical fluctuations. Surprisingly, there can be phase transitions between two such phases, which suggests the existence of a hidden order. In this talk, I demonstrate that the entanglement spectrum can be used to distinguish between these subtly different phases. The central idea is to reduce a one-dimensional chain to a zero-dimensional imaginary system, called the entanglement Hamiltonian. One can then understand the phases of the original spin chain simply by looking at the spectrum of the entanglement Hamiltonian, just as one deduces the properties of atoms from their spectra. The next question is what the physical meaning of the entanglement Hamiltonian is. Properties of the entanglement Hamiltonian are in fact often reflected in physical properties of the ends of a finite chain, such as the appearance of gapless degrees of freedom or surface charge; I will give some examples in higher dimensional systems such as topological insulators as well as one dimension.

4:18PM T1.00004 Interacting Topological Insulators , LUKASZ FIDKOWSKI, Microsoft Research, Station Q — Topological insulators and superconductors are new phases of matter whose physics is described by non-interacting fermions. They can be understood in terms of the topological "twisting" of the fermion's phase over the Brillouin zone, and using topology one can come up with a full classification of when such phases can occur. Strangely, this classification fails for some one dimensional systems once higher-order interactions are allowed. In this talk I will use the entanglement spectrum to understand the modified interacting classification, in one dimension. I will also discuss general one dimensional gapped models, and how matrix product states allow us to find their phases.

Wednesday, March 23, 2011 2:30PM - 5:30PM –
Session T2 DCMP: Defects and Strain in Graphene Ballroom A2

2:30PM T2.00001 Electron Interactions in Graphene , PHILIP KIM, Department of Physics, Columbia University — Electrons confined in two dimensions (2D) can exhibit strongly correlated states. Recent experimental discovery of integer and fractional quantum Hall effect in graphene amplified interest in correlated 2D electronic systems, owning to presence of the unusual topological phase associated with zero effective mass of charge carriers. In this talk, we will discuss the role of the many-body effects due to the electron-electron interaction in graphene manifested in electron transport phenomena. In particular, we will discuss the nature unusual spontaneous symmetry breaking Landau levels graphene under the extreme quantum condition, the appearance of unique low density insulating states and fractional quantum Hall states. Employing extremely high quality samples obtained by suspending graphene and graphene on atomically flat defect free insulating substrate such as hexa-bron nitride, we now investigate various broken symmetry states under high magnetic field. The nature of these broken symmetry state can be explained generally considering underlying SU(4) symmetry in the single particle level of the Landau levels.

3:06PM T2.00002 Spatially Resolving Spin-split Edge States of Chiral Graphene Nanoribbons[1] , M.F. CROMMIE, U.C. Berkeley Physics Dept. and Lawrence Berkeley National Laboratory — A central question in the field of graphene-related research is how graphene behaves when it is patterned at the nanometer scale with different edge geometries. The most fundamental shape in this regard is the graphene nanoribbon (GNR), a narrow strip of graphene that is characterized by its width and chirality. GNRs have been predicted to exhibit a wide range of behavior that includes tunable energy gaps and unique 1D edge states with unusual magnetic structure. I will discuss a scanning tunneling microscopy and spectroscopy (STS) study of GNRs that allows us to examine how GNR electronic structure depends on the chirality of atomically well-defined GNR edges. Our STS measurements reveal the presence of 1D GNR edge states that closely match theoretical expectations for GNRs of similar width and chirality. We additionally observe width-dependent energy splitting in GNR edge states, providing compelling evidence of their magnetic nature.

[1]This work performed in collaboration with Chenggang Tao, Liying Jiao, Oleg V. Yazyev, Yen-Chia Chen, Juanjuan Feng, Xiaowei Zhang, Rodrigo B. Capaz, James M. Tour, Alex Zettl, Steven G. Louie, and Hongjie Dai.

3:42PM T2.00003 Graphene under a tip[1] , EVA Y. ANDREI, Department of Physics and Astronomy, Rutgers University, Piscataway NJ — The strictly two dimensional structure of graphene results in 2D charge carriers that are readily accessible by surface probes such as scanning tunneling microscopy (STM) and spectroscopy (STS), and in electronic properties that can be controlled through doping, strain and external potentials. At the same time the 2D structure causes graphene to be extremely sensitive to environmental disturbances. I will describe STM, STS and magneto-transport experiments showing that when graphene is decoupled from substrate-induced potential fluctuations the intrinsic properties of the carriers become apparent. This is clearly seen in suspended graphene devices where, in the absence of substrate induced potential fluctuations, electron-electron interactions lead to a fractional quantum Hall effect and to an insulating phase at the Dirac point [1]. We find that even for non-suspended graphene it is possible to find non-invasive substrates on which one can directly observe the sequence of quantized Landau levels [2] and to track their evolution with field and doping down to the Dirac point where interaction effects kick in [3]. When the "substrate" is another graphene layer with relative orientation other than that of the standard Bernal stacking, it can profoundly affect the electronic density of states transforming it from the linear massless Dirac spectrum to one containing prominent Van Hove singularities which are controlled by the degree of twist between the layers [4].

[1] X. Du, I. Skachko, F. Duerr, A. Luican, EYAndrei, Nature **462**, 192 (2009)
[2] G. Li, A. Luican and E. Y. Andrei, Phys. Rev. Lett. 102, 176804 (2009).
[3] A. Luican, G. Li, and E. Y. Andrei, Phys Rev. B (R) (2011)
[4] G. Li, A. Luican and E. Y. Andrei, Nature Physics 6, 109 (2010)

[1]Work supported by DOE DE-FG02-99ER45742 , NSF-DMR-0906711 and Lucent.

4:18PM T2.00004 High Resolution Tunneling Spectroscopy of Graphene in Strong and Weak Disorder Potentials , JOSEPH STROSCIO, Center for Nanoscale Science and Technology, NIST, Gaithersburg, MD 20899 — Using scanning tunneling spectroscopy (STS), the local density of states can be mapped in real space to give insight into the role the local disorder potential plays in determining the 2-dimensional electron gas (2DEG) properties. In this talk I describe studies using scanning tunneling spectroscopy to examine various graphene systems with varying degrees of disorder. The amount of disorder depends on how the graphene was made. In the growth of graphene on the Si-face termination of SiC in UHV, local defects are found which contribute to strong inter- and intra-valley scattering [1]. Medium disorder is found in exfoliated graphene on SiO_2. Using a back-gated exfoliated graphene device on SiO_2 we observe a Landau level spectrum and charging resonances [2] that are completely different from previous STS measurements on weak disorder graphene systems. Applying a gating potential allows us to obtain "STS gate maps" which show the graphene 2DEG breaking up into a network of interacting quantum dots formed at the potential hills and valleys of the SiO_2-induced disorder potential. Graphene grown on the C-face termination of SiC is shown to have weak disorder with Landau level line widths approaching thermal limits at liquid He temperatures [3]. Using a new STM system operating at 10 mK, we are able to resolve a graphene "quartet" of the N=1 Landau level [4]. The quartet structure shows the complete lifting of the valley and spin degeneracies, which we determine as a function of magnetic field.

[1] *Scattering and Interference in Epitaxial Graphene*, G. M. Rutter, J. N. Crain, T. Li, P. N. First, and J. A. Stroscio, *Science* **317,** 5835, 219 (2007).
[2] *Evolution of Microscopic Localization in Graphene in a Magnetic Field: From Scattering Resonances to Quantum Dots*, S. Jung, G. M. Rutter, N. N. Klimov, D. B. Newell, I. Calizo, A. R. Hight-Walker, N. B. Zhitenev, and J. A. Stroscio, (Nature Physics in press DOI:10.1038).
[3] *Observing the Quantization of Zero Mass Carriers in Graphene*, D. L. Miller, K. D. Kubista, G. M. Rutter, M. Ruan,W. A. de Heer, P. N. First, and J. A. Stroscio, Science **324**, 924 (2009).
[4] *High Resolution Tunneling Spectroscopy of a Graphene Quartet*, Y. Jae Song, A. F. Otte, Y. Kuk, Y. Hu, D. B. Torrance, P. N. First, W. A. de Heer, H. Min, S. Adam, M. D. Stiles, A. H. MacDonald, and J. A. Stroscio, Nature **467**, 185 (2010).

4:54PM T2.00005 Influence of edge structure, substrate structure and grain boundaries on the electronic properties of graphene quantum dots and transferred graphene[1] , JOSEPH LYDING, University of Illinois — We have used UHV STM to study the quantum size effect gap and the effects of edge electronic structure on graphene quantum dots (GQDs) and nanoribbons [1]. GQDs on H-Si(100) exhibit the expected size-dependent gap with the exception of those with predominantly zigzag edges, which are metallic. STM spectroscopy elucidates the predicted zigzag metallic edge state, which has a characteristic decay length of 1nm. Monolayer graphene deposited in UHV on cleaved GaAs(110) and InAs(110) substrates exhibits an electronic semitransparency effect in which the substrate electronic structure can be observed 'through' the graphene [2]. This effect is observed when the equilibrium graphene-substrate spacing is reduced by about 0.06nm. We have also studied the grain boundaries in graphene monolayers that have been grown on copper and then transferred to silicon dioxide substrates. On the annealed copper foils, we find many crystallographic facets, grain boundaries, and annealing twins, all of which affect the carbon species nucleation. Graphene does not grow as readily on the foil annealing twins and non-primary crystal facets, leading to varying nucleation and graphene grain boundaries in the transferred film. STM images show graphene misorientation angles of approximately 7°, 23°, and 30° at the grain boundaries. Standing wave patterns with a decay length on the order of 1 nm were observed adjacent to the grain boundaries and depend on the structure of the boundary. Spectroscopy across the boundaries showed enhanced conduction in empty states on the grain boundaries.

[1] K.A. Ritter and J.W. Lyding, Nat. Mat. **8**, 235 (2009).
[2] K.T. He, J.C, Koepke, S. Barraza-Lopez and J.W. Lyding, Nano Lett. **10**, 3446 (2010).

[1]This work is supported by the Office of Naval Research under Grant N00014-06-10120

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T3 DCMP DMP: DCMP/DMP Prize Session: Buckley, McGroddy, Davisson-Germer

Ballroom A3

2:30PM T3.00001 Oliver E. Buckley Condensed Matter Prize Talk I , JUAN CARLOS CAMPUZANO, Argonne National Laboratory — This abstract not available.

3:06PM T3.00002 Oliver E. Buckley Condensed Matter Prize Talk: High-resolution Photoemission Studies of the High Tc Superconductors[1] , PETER JOHNSON, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory — In the last decade, high resolution angle-resolved photoelectron spectroscopy has evolved into one of the most powerful probes of the electronic structure of condensed matter systems. This development reflects new technological advances coupled to the enormous research effort devoted to the study of strongly correlated systems, particularly the high T_c cuprate superconductors. Two decades after their initial discovery the latter still present some of the biggest challenges for materials science. In this talk we review some of the developments in new instrumentation and analysis techniques in photoemission and include discussion of both self-energy effects and Fermi surface studies. In the latter case, the discussion will focus on the pseudogap phase of the underdoped cuprates with particular reference to an observed particle-hole asymmetry and the possibility of hole pockets.

[1]Work at Brookhaven is supported by the U.S. Department of Energy.

3:42PM T3.00003 Oliver E. Buckley Condensed Matter Prize Talk: Energy Gaps and Their Implications on the Phase Diagram of Cuprate Superconductors , ZHI-XUN SHEN, Department of Physics and Applied Physics, Stanford University; Stanford Institute for Materials and Energy Sciences, SLAC, Stanford University — In this talk, I will survey the progress made in understanding the cuprate superconductors using angle-resolved photoemission spectroscopy. I will focus on the discovery and understanding of the anomalous energy gaps, and their implication on the pairing symmetry as well as the phase diagram of cuprate superconductors. This includes the detection of the d-wave superconducting gap structure that contributes to the current consensus of d-wave pairing symmetry, the unexpected discovery of the anisotropic normal state gap in single particle spectra (also known as pseudogap) that has become a defining feature of the cuprate phase diagram, the new progress in demonstrating that the pseudogap state is a distinct phase that breaks the particle-hole (thus translational) symmetry, and the momentum dependent information on the competition between pseudogap and superconducting gap.

4:18PM T3.00004 James C. McGroddy Prize for New Materials Talk: Geometrically Frustrated Materials , ARTHUR RAMIREZ, University of California Santa Cruz — Geometrical frustration occurs when interacting degrees of freedom do not "fit" into the lattice that they occupy and, as a result, are under-constrained at low temperature. While the early ideas behind geometrical frustration originate in Wannier's triangular antiferromagnetic Ising model and Anderson's resonating valence bond model, they are broadened here to define an entire class of magnetic materials whose structures are based on triangular or tetrahedral units. When the degree of misfit is high, conventional long range order is suppressed and thermodynamic spectral weight is pushed to energies much lower than the mean field value. Out of this low energy spectral weight, new states of matter are found to emerge experimentally, such as spin liquid on the kagome lattice and spin ice on the pyrochlore lattice. The concept of geometrical frustration can be broadened beyond magnetism to describe a frustrated soft mode that can lead to persistent negative thermal expansion and giant dielectric constants. A brief review will be given of recent work on excitations in frustrating lattices, including the prediction of, and evidence for, magnetic monopoles in spin ice, and the relevance of frustrated hopping for topological insulators.

4:54PM T3.00005 Davisson-Germer Prize in Atomic or Surface Physics Talk: Soft X-Ray Studies of Surfaces, Interfaces and Thin Films: From Spectroscopy to Ultrafast Nanoscale Movies[1] , JOACHIM STÖHR, SLAC National Accelerator Laboratory — My talk will review the development of soft x-ray spectroscopy and microscopy and its impact on our understanding of chemical bonding, magnetism and dynamics at surfaces and interfaces. I will first outline important soft x-ray spectroscopy and microscopy techniques that have been developed over the last 30 years and their key strengths such as elemental and chemical specificity, sensitivity to small atomic concentrations, separation of charge and spin properties, spatial resolution down to the nanometer scale, and temporal resolution down to the intrinsic femtosecond timescale of atomic and electronic motions. I will then present scientific breakthroughs based on soft x-ray studies in three selected areas: the nature of molecular bonding and reactivity on metal surfaces, the molecular origin of liquid crystal alignment on surfaces, and the microscopic origin of interface-mediated spin alignments in modern magnetic devices. My talk will also cover the use of soft x-rays for revealing the temporal evolution of electronic structure, addressing the key problem of "function," down to the intrinsic femtosecond time scale of charge and spin configuration changes. As examples I will present the formation and breaking of chemical bonds in surface complexes and the motion of the magnetization in magnetic devices.

[1]Work supported by the Office of Basic Energy Science of the US Department of Energy.

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T4 GIMS: Keithly Award Session Ballroom A4

2:30PM T4.00001 Joseph F. Keithley Award For Advances in Measurement Science Talk: Beyond the Fringe: measuring ultrafast optical pulses using spectral interferometry , IAN WALMSLEY, University of Oxford — The ability to completely characterize ultrashort electromagnetic pulses has revolutionized the field of ultrafast optics, enabling both new technology and new science. The aim of pulse characterization is to infer the electric field of the pulse from measurements of quantities that rely on standard (relatively slow) photodetectors. Since the field is a fundamental entity in Maxwell's theory, it contains the most information one may obtain about a system probed by an optical pulse, and is, in this sense, much more valuable set of data than a measurement simply of the pulse energy or even the spectral or temporal intensity, Pulse measurement methods may be categorized as spectrographic and tomographic, by which the time-frequency phase space of the pulse is mapped, or interferometric, by which the phase is determined directly. Interferometry provides a sensitivity and robust approach affording a rapid, direct reconstruction algorithm that gives a provably unique solution to the complete space-time field. An important class of self-referencing interferometric are those based on spectral shearing, whereby two frequency shifter replicas of the test pulse are generated encoding the spectral phase derivative in the spectral interferogram resulting from their superposition. The nonlinear implementation of this approach is called spectral phase interferometry for direct electric-field reconstruction (SPIDER). SPIDER has shown itself to be an adaptable and robust method, gaining widespread application in all areas of ultrafast optics, from nonlinear microscopy to attoscience. Some essential concepts and history of the field will be presented, along with recent developments, illustrating applications in ultrafast source diagnosis and certification, dynamical spectroscopy, coherent control, imaging and materials processing.

3:06PM T4.00002 High-Energy Sub-Cycle Waveform Synthesis and Characterization , FRANZ KÄRTNER, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology — The control of atomic scale electronic motion by ultrafast optical electric field waveforms strong enough to mitigate the atomic Coulomb potential has broken tremendous new ground with the advent of phase controlled high-energy few-cycle pulse sources. Currently, such sources are based on Ti:sapphire amplifiers and hollow-core fiber post-compression or optical parametric chirped pulse amplification, together with optical gating techniques. Significant control of the waveform on sub-cycle time scales, however, requires a fully phase-controlled multiple-octave-spanning spectrum. Here, we present a first fully phase-controlled multi-octave-spanning source that supports gigawatt-peak-power isolated single-cycle waveforms based on pulse synthesis of two carrier-envelope phase (CEP) stable OPCPA systems. It is especially a challenge to fully characterize such ultrawide band waveforms. We apply two-dimensional spectral shearing interferometry (2DSI), which can measure the group delay between all spectral components of the synthesized pulse.

3:42PM T4.00003 Generation, characterization and spectroscopic use of ultrashort pulses fully tunable from the deep UV to the MIR , EBERHARD RIEDLE, LMU München — The impressive work of Ian Walmsley has brought us invaluable new possibilities for the full characterization of ultrashort pulses. Spectroscopy of physical, chemical and biological relevance does, however, need pulses far from the 800 nm Ti:sapphire wavelength used for testing SPIDER and its advanced versions. Fortunately, optical parametric amplification (OPA) allows for easy generation of fully tunable pulses. I will review our efforts, highlighting noncollinear OPA, i.e. NOPA, for visible pulses shorter than 10 fs, mixing into the UV down to below 200 nm at 20 fs duration and novel hybrid schemes to efficiently reach the middle IR. I will show that these schemes can be used equally well from kHz to MHz repetition rates. The tunable ultrafast pulses in turn also demand improvements in characterization. The UV range led us to use difference frequency generation instead of the sum frequency mixing employed in the original SPIDER. The lack of proper beam splitters and auto-referencing led us to the use of two auxiliary pulses and the avoidance of any additional chirp added to the test pulse. We termed this zero-additional-phase SPIDER, i.e. ZAP-SPIDER. Lately, with increased use of UV pulses, we came to the conclusion, that the ubiquitous two-photon-absorption can well serve as nonlinearity, at least in UV autocorrelation measurement. How do we use this for full characterization? Hopefully, Ian will tell us! Since the proof is known to be in the eating, I will demonstrate the success of our technical efforts with examples taken from ultrafast molecular dynamics. Highly pronounced vibronic wavepackets in the product of ultrafast excited state proton transfer and the very primary processes leading to homolytic and heterolytic bond cleavage will serve as easy to comprehend illustrations.

4:18PM T4.00004 Probing Electron Correlation with Sequential Laser–Induced Tunnel ionization , PAUL CORKUM, University of Ottawa — Since 1964 we have known that multiphoton ionization could be approximated by tunnel ionization for long wavelength light. Aside from re-collision, since then multiple ionization has been treated as successive, independent single ionization events. Our results show that this long-held belief is false. Tunnelling is highly directional and highly sensitive to the ionization potential (Ip) of the accessible ionic states (which itself can depend on the direction of ionization). Using rare gas atoms as examples, we show that laser induced tunnelling is suppressed or enhanced depending on how the field is applied. We image the hole left by the first tunnelling electron by measuring in the spatial correlation of the second electron. Laser induced tunnelling gives us experimental access to one of the most difficult to measure properties of matter – electron-electron correlations [1].

[1] A. Fleischer, H.J. Wörner, L. Arissian, L.R. Liu, M. Meckel, A. Rippert, R. Dörner, D.M. Villeneuve, A. Staudte and P.B. Corkum, unpublished results.

4:54PM T4.00005 Pulse Propagation through Dispersive Optical Materials , ROBERT BOYD, University of Ottawa — It is now possible to characterize the complete time-frequency behavior of optical pulses with unprecedented precision [1, 2]. The frequency content of optical pulses determines how they propagate through dispersive optical materials. In this talk, we review recent work on methods for dramatically modifying the velocity with which light pulses propagate through material systems. This modification can be so severe that one speaks of slow light, fast light, and backwards light depending on how the magnitude and sign of the group velocity compares to the vacuum speed of light c. We review the physical processes that can be used to achieve such a strong modification of the velocity of light, and we discuss the conceptual understanding of exotic propagation effects such as backwards propagation. We also review the implications of modified pulse velocities within the context of modern optical technology.

[1] Kane, D.J. and R. Trebino, Opt. Lett., 18 823 (1993)
[2] C. Iaconis and I. A. Walmsley, Opt. Lett., 23 792 (1998).

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T5 GQI: 20 Years of Quantum Information in Physical Review Letters Ballroom C1

2:30PM T5.00001 Theory of entanglement and entanglement-assisted communication , CHARLES H. BENNETT, IBM Research Division — Protocols such as quantum teleportation and measurement-based quantum computation highlight the importance of entanglement as a resource to be quantified and husbanded. Unlike classical shared randomness, entanglement has a profound effect on the capacity of quantum channels: a channel's entanglement-assisted capacity can be much greater than its unassisted capacity, and in any case is given by much a simpler formula, paralleling Shannon's original formula for the capacity of a classical channel. We review the differences between entanglement and weaker forms of correlation, and the theory of entanglement distillation and entanglement-assisted communication, including the role of strong forms of entanglement such as entanglement-embezzling states.

3:06PM T5.00002 Twenty Years of Quantum Error Correction , DAVID DIVINCENZO, Forschungszentrum Juelich & RWTH Aachen — Starting around 1991 It became clear that the emerging quantum computer would need error correction to be sensible. Almost immediately, Berthiaume, Deutsch, and Jozsa announced the first key ideas (e.g., allowed codewords should live in a well-defined subset of the Hilbert space), and in less than ten years, the problem was "solved." This solution had many components, involving insights from quantum teleportation, the concept of noisy entanglement and its improvement, creative borrowings from classical binary and quaternary codes, pure group theory, and the reliable working of noisy automata. Actually, this "solved" problem continues to produce new difficulties and insights up to the present day, and it is increasingly central for the question of what we do next in the progress towards a functioning quantum computer.

3:42PM T5.00003 Less Reality, More Security , ARTUR EKERT, Oxford University and National University of Singapore — Bell's inequality makes a seemingly insane scenario possible — devices of unknown or dubious provenance, even those that are manufactured by our enemies, can be safely used for secret communication. And this is for real! All that is needed to implement such a bizarre form of cryptography is a loophole-free violation of Bell's inequalities. It is on the edge of being technologically feasible. I will provide a brief overview of quantum and post-quantum cryptography and describe how studies of entanglement and the foundations of quantum theory influenced the way we may soon protect information.

4:18PM T5.00004 Twenty Seven Years of Quantum Cryptography! , RICHARD HUGHES, Los Alamos National Laboratory — One of the fundamental goals of cryptographic research is to minimize the assumptions underlying the protocols that enable secure communications between pairs or groups of users. In 1984, building on earlier research by Stephen Wiesner, Charles Bennett and Gilles Brassard showed how quantum physics could be harnessed to provide information-theoretic security for protocols such as the distribution of cryptographic keys, which enables two parties to secure their conventional communications. Bennett and Brassard and colleagues performed a proof-of-principle quantum key distribution (QKD) experiment with single-photon quantum state transmission over a 32-cm air path in 1991. This seminal experiment led other researchers to explore QKD in optical fibers and over line-of-sight outdoor atmospheric paths ("free-space"), resulting in dramatic increases in range, bit rate and security. These advances have been enabled by improvements in sources and single-photon detectors. Also in 1991 Artur Ekert showed how the security of QKD could be related to quantum entanglement. This insight led to a deeper understanding and proof of QKD security with practical sources and detectors in the presence of transmission loss and channel noise. Today, QKD has been implemented over ranges much greater than 100km in both fiber and free-space, multi-node network testbeds have been demonstrated, and satellite-based QKD is under study in several countries. "Quantum hacking" researchers have shown the importance of extending security considerations to the classical devices that produce and detect the photon quantum states. New quantum cryptographic protocols such as secure identification have been proposed, and others such as quantum secret splitting have been demonstrated. It is now possible to envision quantum cryptography providing a more secure alternative to present-day cryptographic methods for many secure communications functions. My talk will survey these remarkable developments.

4:54PM T5.00005 A Brief Prehistory of Qubits , BENJAMIN SCHUMACHER, Kenyon College — In the early 1990's, alongside the early work on quantum cryptography, there existed a considerable body of research on the classical information capacity of quantum channels. The strongest and most general result known was the theorem of Holevo giving an entropic bound for the accessbile information in a mixture of quantum signals. This motivated the problem of whether the Holevo bound could be closely approached by suitable choice of code and decoding observable. If so, then the quantum (von Neumann) entropy had a straightforward informational interpretation. When this question was found to be very difficult to answer, quantum data compression and the idea of a "qubit" was introduced as an alternate framework for thinking about information in quantum systems and interpreting the quantum entropy. However, the mathematical ideas from the new framework proved essential to solving the original problem of showing that the Holevo bound was asymptotically achievable. This was an early example of the interplay between classical and quantum concepts of information – an interplay that has been, to say the least, extremely fruitful.

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T6 FIAP: Theory in Industry Ballroom C2

2:30PM T6.00001 From Atoms to Autos: Adventures of a Theoretical Physicist in Industry , JAN HERBST, GM R&D Center — After earning a PhD in solid state theoretical physics at Cornell and following a post-doc, the author arrived at GM R&D for what has turned out to be his first and only real job. An anecdotal chronicle of his adventures in the auto industry will be presented.

3:06PM T6.00002 Challenging theoretical physics problems in the energy industry , MARTIN-DANIEL LACASSE, Corporate Strategic Research Laboratory, ExxonMobil Research and Engineering Company — Critical reliance on technology is ubiquitous in the energy industry, where considerable resources are dedicated to fundamental research aimed at solving our most challenging problems. For example, technological challenges are found in all aspects of the oil and gas industry ranging from exploration, development, and production of oil fields, to transportation and refining of the raw materials, and all the way to the production of specialty products such as polymers and lubricants. From a scientific perspective, these activities cover a broad range of physical science disciplines. As examples, during the exploration and development of oil and gas fields, sound and electromagnetic waves are used to image the earth's interior, and drilling involves an array of sophisticated tools and detectors at the bore hole, both activities being possible thanks to geophysicists, applied mathematicians, and rock physics specialists. Similarly, the transformation of crude oil to refined products requires a fundamental understanding of physical chemistry, phase transition, and transport processes, while the design of products involves polymer physics, and special disciplines such as tribology. The goal of this talk is to present examples of problems posed by the energy industry in view of encouraging physicists to contribute to finding solution to these problems, either through their academic research, or by pursuing a challenging career as industrial physicists. Many of those problems can benefit from the unique approach provided by a rigorous physics training.

3:42PM T6.00003 Theoretical Physics + Experiments in Superfluid He^4 = Commercial Oilfield Acoustic Service , DAVID JOHNSON, Schlumberger-Doll Research — I will describe a specific project which involved the understanding of the basic physics of acoustics in porous and permeable fluid saturated media. The end product is a commercially available measurement of the fluid-flow resistance of porous rock in a real oil-field borehole using an acoustic technique. One key ingredient of the understanding was obtained by laboratory measurements of the acoustic properties of a porous sample saturated with superfluid He^4. Another key ingredient is the theoretical understanding of the properties of the frequency dependent fluid-flow resistance, and its extension to complex values of the frequency.

4:18PM T6.00004 Industry: Theory Matters , ALEXANDER BRATKOVSKY, Hewlett-Packard Laboratories, Palo Alto, CA 94304 — This talk will try to illustrate on a few examples a significant role that theory and modeling plays in an industrial environment of a diversified company. It is especially clear in case of novel materials and processes that may bring big benefits down the road to those with sufficient time horizon. Relevant global trends will be analyzed in this regards.

4:54PM T6.00005 Technologically relevant, in theory , J. TERSOFF, IBM T. J. Watson Center — This talk will give a personal perspective on the role of theoretical physicists in industry, and in particular at IBM. This role has changed over the decades, and continues to evolve.

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T7 GSNP: Structural and Mechanical Properties of Jammed Amorphous Materials Ballroom C3

2:30PM T7.00001 Length scale of dynamic heterogeneity and its relation to time scales in a glass-forming liquid[1] , CHANDAN DASGUPTA, Indian Institute of Science — The role of the length scale of dynamic heterogeneity in the enormous increase in the relaxation times of glass-forming liquids upon supercooling has received much attention recently. Using molecular dynamics simulations and finite-size scaling for a realistic glass-forming liquid, we establish that the growth of dynamic heterogeneity with decreasing temperature is governed by a growing dynamic length scale. We also perform a computational study of a four-point structure factor, defined from spatial correlations of mobility, for the same liquid and show that estimates of the dynamic correlation length and susceptibility obtained from this study are consistent with the results of the finite-size scaling analysis. However, the observed dependence of the simultaneously growing time scale of the long-time α-relaxation on system size does not exhibit the same scaling behavior as the dynamic heterogeneity: this time scale is instead determined, for all studied system sizes and temperatures, by the configurational entropy, in accordance with the Adam-Gibbs relation. We also investigate the dependence of the time scale of the short-time β-relaxation on temperature and system size. A finite-size scaling analysis of this dependence reveals the existence of a length scale that grows as the temperature is reduced. Surprisingly, the temperature dependence of this length scale is found to be identical to that of the length scale that governs the growth of dynamic heterogeneity at the α-relaxation time scale. This result suggests a close connection between short-time dynamics and dynamic heterogeneity at time scales of the order of the α-relaxation time.

[1]This talk is based on work done in collaboration with S. Karmakar, S. Sastry and S. Sengupta.

3:06PM T7.00002 Point-to-Set as a measure of Correlations during Unjamming in Granular Systems , MITCH MAILMAN, Brandeis University — There is evidence indicating that the unjamming of frictionless, soft grain packings occurs at a critrical point, however, no correlation function associated with a diverging, static length scale has been identified. To better understand the nature of this transition, we consider the soft grain packing problem as a constraint satisfaction problem [1]. Jammed configurations are mechanically stable packings with non-zero pressure. Contact forces on each grain therefore satisfy the equations of mechanical equilibrium, which are a set of local constraints, as well as a global constraint from the pressure. In general when jammed, there are more contact forces than constraints, so that an ensemble of force networks exists [2] which satisfy the constraints. These force networks make up a high-dimensional solution space that shrinks to a point at the unjamming transition, suggesting that the unjamming transition can be considered an entropy vanishing transition. We explore a new type of "point-to-set" correlation function which has been used to identify non-obvious length scales in other constraint satisfaction problems [3], and show that it exhibits a diverging length scale. We compare and contrast this length scale with the well established "isostatic length" of Wyart et. al [4].

[1] F. Krzakala and J. Kurchan, PRE 76, 021122 (2007)
[2] J.H. Snoeijer et. al, PRE 70, 061306 (2004)
[3] A. Montanari and G. Semerjain, Journal of Stat. Phys, 125, 1 (2006)
[4] M. Wyart et. al, PRE 72, 051306 (2005)

3:42PM T7.00003 Protocol Dependence in Jammed Particulate Media: Statistics of the Density Landscape[1] , ASHWIN S. SAMPANGIRAJ, Department of Mechanical Engineering & Department of Physics, Yale University, New Haven CT — The density at which hard-sphere fluids jam into amorphous solids depends strongly on the compression protocol. Extremely fast quenching protocols bring each initial point in configuration space to the closest basin-maximum on the density landscape. In contrast, slower quench protocols allow the system to relax and explore configuration space. The protocol-dependence of the density, other structural quantities, and mechanical properties depends strongly on statistical features of the landscape. In this talk, I describe calculations of the the basin volumes associated with jammed hard sphere packings, and the critical quench rate Γ^* above which the probabilities for obtaining jammed packings are determined by their basin volumes. Basin volumes are exponentially distributed; thus, for $\Gamma > \Gamma^*$, so are jammed packing probabilities. We discuss the implications of this result on the statistical mechanics of jammed systems.

[1]This work was done in collaboration with Corey S O'Hern, Jerzy Blawdziewicz, Mark D. Shattuck. S. S. Ashwin and Corey O'Hern are supported by NSF grant no. CBET-0967262.

4:18PM T7.00004 Vibrational modes identify soft spots in a sheared model glass , M. LISA MANNING, Princeton Center for Theoretical Science, Princeton University — Both solids and fluids can flow under applied stress. In crystalline solids, flow occurs via particle rearrangements controlled by a population of dislocations, while in fluids, particle rearrangements occur everywhere throughout the material. In disordered solids, flow generally occurs via localized rearrangements, but no one has been able to identify a population of flow defects, analogous to dislocations, that are structurally different from the rest of the system and more susceptible to flow. It has therefore remained unclear whether a solid-like or fluid-like description is more appropriate for describing flow in such systems. By analyzing the low-energy vibrational modes in a model glass, we have identified a population of structural "soft spots" and have shown that particle rearrangements are initiated at these spots. Thus, these spots serve as good candidates for flow defects. We analyze statistical and structural features of the spots and find that the density of spots decreases with increasing packing fraction and that the population of spots changes slowly compared to the time between particle rearrangements. These results support a solid-like description of flow controlled by a population of localized flow defects in glassy materials.

4:54PM T7.00005 Jamming Mechanisms and Density Dependence of Dynamic Heterogeneities in a Kinetically-Constrained Model , YAIR SHOKEF, Weizmann Institute of Science — Experiments on granular [1] and colloidal [2] systems show steady growth in dynamic heterogeneities as the relaxation time increases with increasing density. In glass-forming liquids, however, the scale of heterogeneities remains modest even as the relaxation time increases by more than ten orders of magnitude with decreasing temperature [3]. This difference may be attributed to the far greater dynamic range measurable in glass-forming liquids [2]. We introduce a simple lattice model [4] which suggests that this difference signals a fundamental distinction between jamming due to an increase in particle density as opposed to jamming by lowering the temperature, or the strength of external driving forces. The recently proposed spiral model [5] has a kinetic constraint that breaks its ergodicity at a critical density smaller than 1. We add to it relaxation mechanisms that mimic the effect of temperature and non-equilibrium driving. This enables us to explore its jamming phase-diagram and study unjamming by temperature or driving above the critical density, which we relate to the random close packing density in particulate systems. We separate the effects of density, temperature and driving and show that jamming resulting from increasing density gives rise to dynamic heterogeneity that grows unboundedly. Whereas decreasing temperature or driving eventually leads to a saturation of the dynamic correlation length even though the relaxation time diverges.

[1] A.R. Abate and D.J. Durian, Phys. Rev. E 76, 021306 (2007).
[2] G. Brambilla et al., Phys. Rev. Lett. 102, 085703 (2009).
[3] C. Dalle-Ferrier et al., Phys. Rev. E 76, 041510 (2007).
[4] Y. Shokef, A.J. Liu, Europhys. Lett. 90, 26005 (2010).
[5] C. Toninelli, G. Biroli, D.S. Fisher, Phys. Rev. Lett. 98, 129602 (2007).

Wednesday, March 23, 2011 2:30PM - 5:30PM –
Session T8 FIP: Shaping Regional Identities through Research Funding Policies Ballroom C4

2:30PM T8.00001 Europe and research: a multi-speed scenario , LUISA CIFARELLI, University of Bologna & European Physical Society — A review of the European situation concerning physics research facilities, collaborations, networks and funding policies will be sketched, pointing out the diversity among different countries of the enlarged EU. Some special focus will be put on particle physics. The continuing integration of Europe, the higher students' mobility trained in the "Bologna Process" frame, the expansion of the European research infrastructures in physics, the increasing funding from the European Commission, the various research shaping and roadmap attempts, the challenge by Asia in addition to that from the USA, are all issues to be examined.

3:06PM T8.00002 Science, Technology and Innovation in Brazil: Advances and Challenges[1] , CARLOS ARAGAO DE CARVALHO, CNPq and UFRJ — We review the construction of the infra-structure for science and technology in Brazil, its success cases, its major advances, and its challenges, both present and future. We emphasize the budget increases, the new legal framework, new mechanisms of support for S&T, and the plans for the future. Preliminary results of the discussions that took place in the 4^{th} National Conference on Science, Technology and Innovation of May 2010 will also be presented.

[1]CNPq

3:42PM T8.00003 Mega Physics Projects: National and International Initiatives: the Indian Experience , ROHINI GODBOLE, CERN PH/TH Theoretical Physics Department — Indian Physics community is now getting involved in a number of Mega physics projects, both home and abroad, national and International. I will present some information on these efforts.

4:18PM T8.00004 Science and Technology in Africa: The African Union new initiatives and financial support perspectives , JEAN-PIERRE EZIN, Commissioner Human Resources, Science & Technology — Physics, which is widely considered as the most fundamental of the sciences, underpins the progress in all other branches of science and has a wide range of applications in economic development, including in health, energy research, food security, communication technology and climate change. The African Union (AU) Commission articulates the continental vision of its Member States and its programs are designed to directly contribute to its social and economic development and integration efforts. In the area of science and technology the Department has developed *Africa's Science and Technology Consolidated Plan of Action* as a strategic policy document through the AU system of conference of ministers responsible for science to guide the continent on common priority programs. The programs in this plan of action that have been transformed into bankable projects under the Book of "lighthouse projects Phase 1," adequately respond to Africa's challenges and development needs using science. They can be summarized into three main themes: a pan-African university (PAU) initiative (to combine higher education and scientific research as a network of differentiated PAU in each of the five African regions), African research grants (to strengthen the research capacity of the African institutions and upgrading infrastructures, consolidating their accumulated asset of scientific knowledge), popularization of science and technology and promotion of public participation (to build public understanding and raising awareness on science and technology as a driving agent for social and economic progress for Africa and its integration process) and a science and technology institutional capacity building program). This talk will provide a review these programs and their status and impact in Africa.

4:54PM T8.00005 Science for Energy , HARRIET KUNG, Associate Director of Science for Basic Energy Sciences - DOE — This abstract not available.

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T9 DFD: Flow Instabilities, Turbulence and CFD D220

2:30PM T9.00001 ABSTRACT WITHDRAWN –

2:42PM T9.00002 Modal decomposition of free and forced circular jets at low and high Reynolds numbers , MURALIDHAR KRISHNAMURTHY, Professor, TRUSHAR GOHIL, doctoral student, ARUN SAHA, Assistant Professor — Free and forced jets are important in applications such as combustion, propulsion, mixing, and aero-acoustics. Jet control for noise reduction and mixing efficiency can be achieved by manipulating the flow structures. The most energetic structures of a flow field can be objectively recovered by proper orthogonal decomposition. POD extracts a basis for modal decomposition as eigenfunctions from an ensemble of signals. In the present work, the snapshot POD method is applied to data recorded from direct numerical simulation as well as large eddy simulation in three dimensions. Free jets are reported at a Reynolds number of 1000 and 10000 and 4300 for forced jets. Results show that all of the kinetic energy of laminar flow is stored in large-scale structures while for the turbulent jet, a broader distribution of kinetic energy is obtained. At Re = 1000, 40 snapshots of the flow field are adequate to resolve the major flow structures. For Re=10000, at least 100 snapshots are required for a good spectral representation. Blooming jets arising from dual mode forcing show the formation of odd-even pairs. The first pair contains the details of branching. In addition, the higher order modes capture the inherent jet instability mechanisms.

2:54PM T9.00003 Generalized Saffman-Taylor formula for multi-layer Hele-Shaw flows , PRABIR DARIPA, Texas A&M University — Stability theory plays a major role from fundamental science to applied sciences. It is useful in the design of many processes and engineering instruments as well as in explaining many phenomena. In this paper we review some of the author's and his collaborator's recent works on the extension of Saffman-Taylor instability which occurs at an interface between two immiscible fluids in porous media and Hele-Shaw cells when displacing fluid is less viscous than the displaced one. The growth rate of interfacial disturbances is given by a formula called Saffman-Taylor formula which plays a very important role in many areas including flows in porous media and oil recovery among many others. In this talk, we will present our results on the generalization of this formula to multi-layer flows involving many interfaces. As an application of the generalized Saffman-Taylor formula, we will derive necessary conditions for suppressing instability of two-layer flows by introducing arbitrary number of constant viscosity fluid layers in between. The important role that these conditions play in stabilization of hydrodynamic instabilities in Hele-Shaw flows will be discussed.

3:06PM T9.00004 The stability of a droplet suspended in a straight micro-channel , HAIDER HEKIRI, TAKUMI HAWA, School of Aerospace and Mechanical Engineering, The University of Oklahoma, Norman, OK 73019 — CFD simulations of the dynamics of a two-dimensional, incompressible, and two coupled spherical-cap water droplets suspended in a straight micro-channel, whose channel height is D, have been conducted to investigate the stability of the droplet. FLUENT with a 2-D pressure based solver is utilized in this simulation. The suspended droplet states are measured by the location of the central of mass of the droplet. We find that there is a critical volume, Vc(D), where asymmetric droplet states appear in addition to the basic symmetric states when V $>$ Vc(D). Using the CFD it is demonstrated that when V $<$ Vc(D) the symmetric droplet states have a stable mode. However, when V $>$ Vc(D) the symmetric states become unstable and asymmetric states have a stable mode. The bifurcation of asymmetric states at Vc(D) has a pitchfork nature. The simulations clarify the relationship between the linear stability results and the experimental results of the droplet behavior.

3:18PM T9.00005 Liquid-air interface instability due to an in-plane electric field , MIKHAIL PEVNYI, JAKE FONTANA, PETER PALFFY-MUHORAY, Liquid Crystal Institute - KSU — We report observations of an instability at the free surface of a liquid due to an in-plane electric field. The horizontal air-liquid interface in a partially filled sample cell between vertical electrodes exhibited first oscillations, then increasingly turbulent fluctuations as the strength of the horizontal electric field was increased. This behavior was observed in toluene and choloroform; the applied AC field was sinusoidal with f= 60Hz. The dynamics of the interface was probed via dynamic light scattering. We present our experimental observations, as well as a simple model and numerical simulations of the interface dynamics under the influence of the applied electric field.

3:30PM T9.00006 Stretch-induced wrinkles in reinforced membranes , ATSUSHI TAKEI, ESPCI, FABIAN BRAU, Universit de Mons , BENOÎT ROMAN, JOSÉ BICO, ESPCI — We study through model experiments the buckling of a rigid stripe (or fiber) embedded in a soft membrane under compression. The compression is induced through Poisson effect when the membrane is stretched perpendicularly to the stripe. The wavelength of the wrinkles is found to depend on the material properties and the stretching strain. A balance between the bending and stretching energies of both the membrane and the stripes dictates this wavelength: $\lambda \sim (Bd\ /E_S H_S \delta\ )^{1/3}$, where B is the bending stiffness, d the width of the rigid band, δ the strain, and E_S andH_S the Young modulus and the thickness of the membrane, respectively. The characteristic extension of the wrinkled zone is set by the wavelength. This result also applies to fibers imbedded in a thin membrane. However, in-plane buckling is observed when the thickness of the membrane is large compared with the radius of the fiber. In this last regime, we find $\lambda \sim R(E_F\ /E_S\ )^{1/4}$, where $E_F$and R are the Young modulus and the radius of the fiber, respectively.

3:42PM T9.00007 Computational Parametric Study of R-M Instability Growth for an Inclined Interface[1] , JACOB MCFARLAND, DEVESH RANJAN, Texas A&M University, JEFF GREENOUGH, Lawrence Livermore National Labratory — An inclined interface perturbation is studied for an RM instability to model upcoming experiments in the Texas A&M inclined shock tube facility. Simulations were created using the ARES code developed at Lawrence Livermore National Lab. A parametric study was performed for inclination angles from 30 to 60 degrees, incident Mach numbers of 1.5 to 2.5, and high Atwood number gas pairs air-SF6 and helium/SF6. Qualitative results are examined to show the relative effects of these parameters. Interface growth rates are calculated and compared to the existing linear growth regime models. A new model is proposed based on the interface geometry and compared to the simulation results.

[1]This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

3:54PM T9.00008 Drop Splashing on a Smooth Surface at Low Velocities , CACEY STEVENS, SIDNEY NAGEL, University of Chicago — When a low viscosity liquid drop impacts on a smooth, dry surface, a thin fluid sheet is emitted which subsequently breaks up into a distribution of secondary droplets. Ambient gas pressure is crucial in creating this splash: splashing is completely suppressed below a threshold pressure [1]. There are several regimes that occur as the velocity and liquid viscosity are varied [2]. Here, we discuss splashing in the low velocity, low viscosity regime. We explore how the threshold pressure scales with drop size, as well as liquid viscosity. We also characterize the dependence of threshold pressure with molecular weight of the surrounding gas.

[1] L. Xu, S. Nagel, and W. Zhang. Phys. Rev. Lett. 94, 184505 (2005).
[2] L. Xu. Phys. Rev. E 75, 056316 (2007).

4:06PM T9.00009 Elastic effects on the shear flow instabilities in viscoelastic fluids , AHMED KAFFEL, Department of Mathematics Virginia Tech, DEPARTMENT OF MATHEMATICS VIRGINIA TECH TEAM, DEPARTMENT OF MATHEMATICS TEAM — A linear stability analysis was applied and the stability equation is derived and solved numerically using the spectral Chebyshev collocation method. The objective is to study the elastic effects on the instability of inviscid parallel shear flows. We focus on the upper convected Maxwell model in the limit of infinite Weissenberg and Reynolds numbers. Specifically, we study the effects of elasticity on the instability of a few classes of simple parallel flows, specifically plane Poiseuille and Couette flows, the hyperbolic-tangent shear layer and the Bickley jet. The algorithm is computationally efficient and accurate in reproducing the discrete eigenvalues. We consider flows bounded by walls as well as flows bounded by free surfaces. In the inviscid, nonelastic case all the flows we study are unstable for free surfaces. In the case of wall bounded flow, there are instabilities in the shear layer and Bickley jet flows. In all cases, the effect of elasticity is to reduce and ultimately suppress the inviscid instability. The numerical solutions are compared with the analysis of the long wave limit and excellent agreement is shown. We found flows which are long wave stable, but nevertheless unstable to wave numbers in a certain finite range. While elasticity is ultimately stabilizing, this effect is not monotone; there are instances where a small amount of elasticity actually destabilizes the flow.

4:18PM T9.00010 Thermal convection in multiphase systems , LUCA BIFERALE, University of Rome "Tor Vergata", PRASAD PERLEKAR, TUE, Eindhoven, MAURO SBRAGAGLIA, ANDREA SCAGLIARINI, University of Rome "Tor Vergata", FEDERICO TOSCHI, TUE, Eindhoven, ICTR COLLABORATION — We present preliminary results of a numerical study of two dimensional and three dimensional multiphase thermal convection close to the phase transition and in presence of phase coexistence. The numerical algorithm is based on a suitable implementation of multiphase Lattice Boltzmann scheme with non-ideal pressure tensor. We discuss the effects of droplets and bubbles formation on the global heat flux from bottom to top boundaries.

4:30PM T9.00011 Vortex Sheet Model for a Turbulent Mixing Layer , UJJAYAN PAUL, RODDAM NARASIMHA, MEHEBOOB ALAM, JNCASR, Jakkur, Bangalore 64 — The primary aim of this work is to study instability induced roll up of a slightly perturbed vortex sheet in an Euler fluid. A point vortex model tends to evolve into a chaotic cloud of point vortices instead of smooth double branched spirals. The present model uses linear splines to interpolate the vortex sheet. Computer simulation of this vortex sheet is numerically prohibitive. However, the evolution of the vortex sheet can be performed conveniently using a closed form equation of motion which derived from the basic equations of vortex dynamics. The vortex sheet rolls up into a smooth double branched spiral. A vortex core is formed by regular windings of the vortex sheet and irrotational fluid in between the layers. Various statistical quantities like the growth rate and mean velocity profiles are computed along with the evolution of the vortex sheet. The problem of spontaneous appearance of singularity in an evolving vortex sheet is treated in detail. The critical time for the present vortex sheet model is calculated analytically and compared to the numerical value.

4:42PM T9.00012 Nonlinear Deformation in Weak Turbulence[1] , NICHOLAS OUELLETTE, DOUGLAS KELLEY, YANG LIAO, Department of Mechanical Engineering & Materials Science, Yale University — Turbulent and chaotic flows are well known to mix efficiently: by repeatedly stretching and folding material volumes, material lines stretch exponentially quickly and gradients of an advected scalar field can become very large. By adapting a technique originally introduced to study plasticity in glassy solids, we explicitly separate stretching (a linear transformation) from folding (a nonlinear transformation) in a quasi-two-dimensional experimental flow and study them independently. We compare results from two forcing schemes: one that is dominated by rotation, and another that is dominated by shear.

[1]This work was supported by NSF Grant No. DMR-0906245.

4:54PM T9.00013 Principal Direction of Scalar Transport in Wall Turbulence[1] , CHIRANTH SRINIVASAN, DIMITRIOS PAPAVASSILIOU, The University of Oklahoma — Lagrangian scalar tracking in conjunction with direct numerical simulation is utilized in an infinitely long channel to study the principal direction of scalar transfer for both forwards and backwards single particle dispersion. Four regions are of interest: the viscous sub-layer, the transition region (between the viscous sub-layer and the logarithmic region), the logarithmic region and the center of channel. Fluctuating velocities of scalar markers released in the flow field are correlated forwards and backwards in time to find the components of the correlation coefficient tensor. Eigenvalues and eigenvectors are obtained for both the forwards and backwards dispersion and for fluids with Prandtl number between 0.1 and 1000. The largest eigenvalues are higher in the case of backwards dispersion compared to the case of forwards dispersion. The eigenvector inclinations relative to the yz plane are different for forwards and backwards dispersion (at times comparable to the Lagrangian timescale).

[1]NSF under grant CBET-0651180.

5:06PM T9.00014 Molecular origins of continuum fluid mechanics: Atomic migrations of single-phase fluid and slip boundary conditions , ALAN GRAHAM, SHIHAI FENG, TONY REDONDO, Los Alamos National Lab — We report the results of molecular dynamics simulations of pressure-driven flows of liquid argon in circular and planar conduits. We find that in inhomogeneous shear flows the molecules migrate to the center of the conduits and establish large radial density gradients under conditions that were previously assumed to be incompressible. These are the first predictions of shear-induced migration in pure fluids subjected to inhomogeneous shear flows. These density gradients increase monotonically with Péclet number. They result in a blunted velocity profile that deviates from the parabolic profile predicted by the Navier-Stokes equations for an incompressible fluid. Comparisons with simulations where the flow exhibits zero or linear shear indicate that this phenomenon is the result of the nonlinear shear flows and the finite size of the molecules.

5:18PM T9.00015 Search for Euler Singularity using Vortex Filaments , SAHAND HORMOZ, MICHAEL BRENNER, Harvard University — A promising mechanism for generating a finite-time singularity in the incompressible Euler equations is stretching of vortex filaments. An exhaustive search of all possible initial conditions involving filaments, however, is not practically feasible. In this talk, I will show that two interacting vortex filaments can not generate a singularity for any initial conditions, by analyzing the asymptotic self-similar limit of their collapse. Essentially, our approach entails a separation of the dynamics of the filament shape, from the shrinking of its core. We solve for the dynamics using a self-similar ansatz and show that the core does not shrink fast enough for a self-consistent collapse. The similarity solution allows for many different collapse geometries, consistent with the tireless effort in the past of investigating new initial conditions. Potential for a singularity at higher number of filaments is also discussed.

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T10 DMP: Focus Session: Growth, Structure, Dynamics, and Function of Nanostructured Surfaces and Interfaces – Oxides D221

2:30PM T10.00001 Cross-sectional scanning tunneling microscopy and spectroscopy of fractured oxide surfaces and heterostructure interfaces[1] , TEYU CHIEN, Argonne National Laboratory — Recently, interfaces between novel oxide materials have become a playground for manipulation of new functionalities. At interfaces, the broken symmetry and the spatially confined environment have been shown to modify the local interactions and generate wholly new electronic phases (e.g. magnetism, metallicity, superconductivity etc.) distinct from the composite bulk materials. However, to date our understanding of these interface driven phases is still limited. While there exists powerful spatially resolved tools for visualizing the chemical and magnetic structure of an interface, a direct observation of electronic behavior across the interface presents a major experimental challenge. After the success of creating flat fractured surfaces on Nb-doped $SrTiO_3$ (Nb:STO) accessible to scanning tunneling microscopy (STM) [1-3], we have further harnessed the high-sensitivity to electronic local density of states (LDOS) of the scanning tunneling spectroscopy (STS) in cross-sectional geometry to visualize complex oxide interface electronic properties. By extending XSTM/S to the interface between colossal magnetoresistant manganite $La_{2/3}Ca_{1/3}MnO_3$ (LCMO) and semiconducting Nb:STO, we were able to map the LDOS across the boundary to unambiguously visualize the interface by the location of the valence band and elucidate the fundamental issue of band alignment at a complex oxide heterointerface [4].

[1] TeYu Chien *et al.*, *Appl. Phys. Lett.* **95**, 163107 (2009).
[2] Nathan P. Guisinger *et al.*, *ACS nano* **3**, 4132 (2009).
[3] TeYu Chien *et al.*, *J. Vac. Sci. Technol. B* **28**, C5A11 (2010).
[4] TeYu Chien *et al.*, *Phys. Rev. B* **82**, 041101(R) (2010).

[1]Use of the Center for Nanoscale Materials was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

3:06PM T10.00002 Electrical-stress-induced transport and surface potential characterizations of metal/TiO_2/metal planar junctions , HAERI KIM, DONG-WOOK KIM, Ewha Womans University — Electric-field-induced resistive switching (RS) phenomena in metal oxides have attracted considerable research interest due to their potential use in nonvolatile memory device applications. Intensive investigations have revealed that coupled electron ion dynamics play a key role the RS mechanism. Metal/single crystal junction can be an ideal model system to study how the ionic drift and diffusion can affect the resistance. We investigated transport and local electrical properties of Pt/TiO_2 single crystal/Ti planar junctions with micron- sized gaps between the electrodes. Scanning Kelvin probe microscopy (SKPM) showed that negative (positive) electrical stress to the Pt electrodes significantly reduced (hardly affected) the Pt/TiO_2 contact resistance. The SKPM results also revealed that the electrical stress caused alteration of the local work function of TiO_2. The comparative investigations of the transport and SKPM results suggested that the electrical stress induced redistribution of ions, resulting in the change of the junction resistance.

3:18PM T10.00003 ABSTRACT WITHDRAWN –

3:30PM T10.00004 Theoretical study of Ge/$BaTiO_3$ Interfaces , KURT FREDRICKSON, ALEXANDER DEMKOV — It has been shown (McKee *et al.,* Phys. Rev. Lett. **81,** 3014 (1998), and R. McKee, *et al., Science* **293**,468 (2001)) that perovskite oxides $SrTiO_3$ and $BaTiO_3$ (BTO) can be grown epitaxially on Si and Ge, respectively. It would be interesting to achieve the reverse, i.e. to grow for example, Ge on BTO. It is not clear, however, whether one can achieve wetting of BTO by Ge. Theoretically, the energy of the Ge (001) surface is estimated to be anywhere between 591 and 1700 erg/cm^2 and the surface energy of BTO is in the range of 1083-1496 erg/cm^2 depending on termination and environment. The missing piece of information is the energy of the Ge/BTO interface. We examine five possible Ge/BTO interface structures and calculate their energies using density functional theory to determine which one has the lowest energy, and whether wetting can be achieved.

3:42PM T10.00005 Strain relaxation in single crystal $SrTiO_3$ grown on Si (001) , MIRI CHOI, AGHAM POSADAS, RYTIS DARGIS, The University of Texas at Austin, TX, DINA TRIYOSO, Freescale Semiconductor, Austin, TX, DAVID THEODORE, Freescale Semiconductor, Tempe, AZ, CHIH-KANG SHIH, ALEXANDER A. DEMKOV, The University of Texas at Austin,TX, THE UNIVERSITY OF TEXAS AT AUSTIN, TX TEAM, FREESCALE SEMICONDUCTOR, AUSTIN, TX COLLABORATION, FREESCALE SEMICONDUCTOR, TEMPE, AZ COLLABORATION — A layer of $SrTiO_3$ grown directly on Si may be used as a pseudo-substrate in perovskite deposition. As grown, $SrTiO_3$ is compressively strained, however, by subsequent annealing in oxygen at elevated temperature, a strain relieving SiO_x buffer layer can be grown between the substrate and the perovskite layer. We perform a systematic study of strain relaxation in $SrTiO_3$ films grown on Si by molecular beam epitaxy as a function of the process conditions (annealing time, temperature, and oxygen partial pressure). Using a combination of X-ray diffraction, reflection high energy electron diffraction, and transmission electron microscopy we explore the oxidation and strain relaxation of $SrTiO_3$. We compare the kinetics of the buried oxide growth to that predicted by the conventional Deal-Grove model. An understanding of strain relaxation of $SrTiO_3$ on silicon can potentially be used to control the $SrTiO_3$ lattice constant for lattice matching with functional oxide overlayers.

3:54PM T10.00006 X-ray 3D atomic imaging of Pt nanocrystals supported on $SrTiO_3$(001) , ZHENXING FENG, Department of Materials Science and Engineering, Northwestern University, ALEXANDER KAZIMIROV, CHESS, Cornell University, MICHAEL BEDZYK, Department of Materials Science and Engieneering, Northwestern University — Ultrathin metal or metal-oxide layers deposited onto oxide surfaces have wide applications in catalysis, chemical sensing and electronics. For sub-monolayer Pt deposited on the 2x1 $SrTiO_3$(001) surface, atomic-force microscopy shows the formation of nanoparticles and X-ray standing wave (XSW) atomic imaging shows that these nanoparticles are composed of Pt face-centered-cubic nanocrystals with cube-on-cube epitaxy coherent to the substrate unit cell. The phase sensitivity of the XSW allows for a direct measurement of the interface offset between the two unit cells along the c-axis. Different Pt coverages lead to differences in the observed XSW image of the interfacial structure, which is explained by the Pt-Pt interaction becoming stronger than the Pt-substrate interaction as the coverage is increased from 0.2 to 0.6 ML. Proposed atomic-scale interface models are based on a published double-layer TiO_2 terminated structure for the 2x1 $SrTiO_3$(001) surface and density functional theory.

4:06PM T10.00007 Dynamics of early stage nano-oxidation by *in situ* UHV-TEM[1] , JUDITH YANG, University of Pittsburgh — Environmental stability is one of the most important properties for materials exposed to air. As dimensions of engineered systems approach nanoscale, fundamental understanding of reactions with oxygen at this length scale is critical for environmental stability as well as for processing oxide nanostructures, where surface reactions are commonly utilized. The nanoscale stages of oxidation from the nucleation of the metal oxide to the formation of the thermodynamically stable oxide represent a scientifically challenging and technologically important terra incognito. The kinetics of early stage oxidation of Cu, Cu-Au and Cu-Ni alloys were visualized using in situ ultra-high vacuum transmission electron microscopy (UHV-TEM), where the initial oxidation stages can be observed in real-time under well-controlled surface conditions. We examined the dynamic responses of thin films to variations in thermodynamic variables such as temperature, oxygen pressure, strain, and crystallographic orientation. The kinetics of the nucleation and growth of three-dimensional oxide islands demonstrate that oxygen surface diffusion is the primary mechanism for oxide growth during initial oxidation in dry oxygen, and thus bears a striking resemblance to heteroepitaxy. Compared with the behavior of Cu films, the oxidation of Cu-Au alloys revealed more complexity. For example, the oxidation of (100)-oriented Cu-Au alloys with low Au content at $\sim$ 600C results in the formation of Cu2O oxide islands with a dendritic morphology and a non-uniform lateral distribution of Au around the islands. For Cu-Ni oxidation, the addition of Ni causes the formation Cu2O and/or NiO where the oxide type(s) and the relative orientation with the film depend on the Ni concentration, oxygen partial pressure and temperature. Evolution of the shape and size of the oxide islands can be quantitatively analyzed and provide fundamental insights into the complex kinetics and energetics of oxidation. Models based on surface orientation, strain development, and diffusion will be discussed to explain the formation of some of the novel oxide nano-structures.

[1]This research is supported by the NSF-DMR (0706171) and DOE-BES Materials Division (1041032).

4:42PM T10.00008 Controlled surface reorganization of complex oxides by laser MBE , MIKHAIL KAREEV, B. GRAY, JIAN LIU, E.J. MOON, J. CHAKHALIAN, University of Arkansas — We report on the fabrication of ultra-thin layers of complex oxide perovskites, which display a variety of high-order surface reconstructions. In order to obtain the observed complex surface reconstructions (e.g. 6x2, 4x2, 4x4, etc.), nearly stoichiometric complex oxide material are found to be re-arranged into specific combinations of long-ordered periodic structures. We examine details of homo- and heterogeneous growth of SrTiO3 (STO) and LaNiO3 respectively on TiO2 terminated and mixed TiO2/SrO termination STO substrates by the combination of high-pressure RHEED and AFM to investigate mechanisms behind the high order surface reconstruction. J.C. was supported by DOD-ARO under the Contract No. 0402-17291 and NSF Contract No. DMR-0747808.

4:54PM T10.00009 Quantum confinement effects in nanocrystals of SnO_2 in MgO matrix , M.B. SAHANA, Wayne State University, C. SUDAKAR, Indian Institute of Technology Madras, India, A. DIXIT, J.S. THAKUR, R. NAIK, Wayne State University, V.M. NAIK, University of Michigan-Dearborn — We have studied the nanocrystal formations of SnO_2in$x$$SnO_2$-(1-$x$)MgO composite thin films (x =0 to 1 and thickness 0.5 to 1 μm) prepared by metal-organic decomposition method. We find a direct relationship between the size of SnO_2 nanocrystals and the annealing temperature. Similarly, higher concentration of Mg in $x$$SnO_2$-(1-$x$)MgO leads to smaller size nanocrystals of SnO_2. Under the controlled choice of composition and annealing conditions, the bandgap of SnO_2 can be continuously increased from 3.89 eV to 4.5 eV thus providing a generic approach for tuning the bandgap in nanocomposite systems over a wide range of energy. We discuss this behavior in terms of the quantum confinement effect arising from particle size being comparable to the order of Bohr radius of the material.

5:06PM T10.00010 Detection of Dielectric Trap States in Hafnium Oxide By Single Electron Tunneling Force Spectroscopy[1] , DUSTIN WINSLOW, JON JOHNSON, CLAYTON WILLIAMS, Department of Physics, University of Utah — Atomic scale detection and imaging of electronic trap states in dielectric films has recently been demonstrated.[2] Standard methods typically provide characterization over a much larger scale. Single Electron Tunneling Force Spectroscopy has been employed to measure the energy levels of trap states in HfO_2 with sub-nanometer spatial resolution. Analysis of individual spectra obtained at different locations shows variation in the density of defect states. When multiple spectra taken from 40 different locations are averaged, a broad peak 0.3 eV below the conduction band is observed, which agrees with data obtained over large areas by standard measurements.[3] Additional peaks, not seen by the standard methods, are also observed. The method will be described and the data discussed.

[1]This research was supported by the Semiconductor Research Corporation

[2]J.P. Johnson et al, Nanotechnology **20** (2009) 055701

[3]G. Ribes et al, IEEE Trans. Dev. Mat. Reliability **6**, 132 (2006).

5:18PM T10.00011 Charge Injection and Relaxation in HfO_2 Films Measured by Single Electron Tunneling Force Spectroscopy[1] , CLAYTON WILLIAMS, DUSTIN WINSLOW, JON JOHNSON, Department of Physics, University of Utah — Detection and imaging of individual trap states in dielectric materials with atomic scale spatial resolution has been recently demonstrated.[2] Spectroscopic measurements on HfO_2 films by Single Electron Tunneling Force Spectroscopy have now shown evidence of both reversible and irreversible tunneling to and from these electronic trap states. The irreversibility is small near the middle of the band gap, becoming larger at $\sim$ 0.7 eV below the conduction band and 1.3 eV above the valence band. The irreversibilty of tunneling is likely due to charge relaxation. The evidence of charge relaxation in the film and a description of this new nanometer scale spectroscopic capability will be presented. The possible mechanisms by which the relaxation takes place will also be described.

[1]This research was supported by the Semiconductor Research Corporation.

[2]J.P. Johnson et al, Nanotechnology **20** (2009) 055701.

Wednesday, March 23, 2011 2:30PM - 4:30PM –

Session T11 FIAP: Spin and Transport in Low Dimensional Semiconductors D222

2:30PM T11.00001 Noble Metals and Transition Metals Adsorbed on Graphene: The Pursuit of Graphene Spintronics , MATHEUS PAES LIMA, Univeristy of Sao Paulo, ADALBERTO FAZZIO, University of Sao Paulo — Via first-principles simulations we study the structural, magnetic and electron transport properties of 2D graphene in the presence of single atoms. We consider Cu, Ag and Au, as well as Mn, Fe, Co and Ni adsorbed on pristine and defective graphene containing vacancies and divacancies. To obtain the transport properties we perform ab-initio calculations based on Density Functional Theory (DFT) coupled to Non-Equilibrium Greens' Function (NEGF) formalism using the Landauer-Büttiker formula within the Meir-Wingreen approach. Our results show that graphene+noble metals systems have a gate controllable spin polarized current, allowing the fabrication of switchable spin filters with a moderated efficiency. In the particular case of Gold adsorbed on pristine graphene, a positive gate leads to a polarized current with excess of up electrons, while a negative gate the converse. Despite the high-spin configuration of Mn, the d levels are very far from the Fermi level. The Ni atom prefers a non-magnetic configuration. Therefore, graphene+transition metals systems present a polarized current only for Fe and Co atoms, allowing the fabrication of spin filters with very high efficiency.

2:42PM T11.00002 ABSTRACT WITHDRAWN –

2:54PM T11.00003 Hole-induced Dynamic Nuclear Polarization in Quantum Dots[1] , WEN YANG, L.J. SHAM, Department of Physics, University of California San Diego — We present a microscopic theory showing that through the non- collinear hole-nuclear dipolar hyperfine interaction, an optically excited heavy hole in a quantum dot can induce a steady-state nuclear polarization. The preferential direction of the nuclear spin flip is set by the energy mismatch of relevant transitions instead of thermal relaxation. The induced nuclear polarization shows a sign dependence on the product of the nuclear Zeeman splitting and the frequency detuning of the pumping laser, leading to bidirectional hysteretic locking of the optical absorption peak onto resonance or bidirectional hysteretic shift of the peak away from zero detuning. This sheds light on a puzzling observation of bidirectional hysteretic locking of the neutral exciton absorption peak in Faraday geometry [C. Latta et al., Nature Phys. 5, 758 (2009)]. By solving the Fokker-Planck equation for the nuclear polarization distribution, we found a 10-fold suppression of the steady- state nuclear fluctuation, in reasonable agreement with the single pump experiment in Voigt geometry [X. Xu et al., Nature 459, 1105 (2009)].

[1]This research was supported by NSF (PHY 0804114) and U. S. ARO MURI award W911NF0910406.

3:06PM T11.00004 Beating of Friedel Oscillations in Spin-Orbit Coupled System[1] , SAMVEL BADALYAN, Department of Physics, University of Regensburg, 93040 Regensburg, Germany, ALEX MATOS-ABIAGUE, University of Regensburg, GIOVANNI VIGNALE, Department of Physics and Astronomy, University of Missouri, Columbia, Missouri 65211, USA, JAROSLAV FABIAN, Department of Physics, University of Regensburg, 93040 Regensburg, Germany — The interplay of different spin-orbit interaction mechanisms induces highly anisotropic modifications of the static dielectric function of a two-dimensional electron system. One of the main changes of the static polarization function is the induced shift of its singularity position, which is in opposite directions for orthogonal momentum orientations. More interestingly, we have found that in certain situations the polarization function exhibits a *doubly-singular* behavior. This new property generates a novel phenomenon–*the beating of Friedel oscillation*s, which can be controlled by an external electric field. This effect is a general feature of systems with Bychkov-Rashba and Dresselhaus spin-orbit fields and should be directly observable through tunneling microscopy imaging of the density distribution around an impurity.

[1]The work is supported from EU Grant No. PIIF-GA-2009-235394 (S.M.B.), SFB Grant No. 689, and NSF Grant No. DMR-0705460 (G.V.).

3:18PM T11.00005 Cyclotron resonance in graphene and Kohn's theorem , KESHAV SHRIVASTAVA, University of Malaya — In 1961 Kohn has shown [1] that the cyclotron frequency is independent of the interaction. In the case of graphene there is some effort to suggest that the electron dispersion is linear in k, instead of $(h/2\pi)^2k^2/2m$ so that the Kohn theorem may not apply [2]. We find that the Kohn theorem does not use the dispersion relation and applies to graphene the same way as in some other material. We find that if e is replaced by $e^*=(1/2)ge$, the Kohn theorem applies with the cyclotron frequency $(h/2\pi)\omega_c = (1/2)geB/mc$. Hence there is no interaction and all of the interaction is contained in $g = (2j+1)/(2l+1)$ which is used only in the unperturbed Hamiltonian. The degeneracy of the levels is found to be related to the flux quantization. We have explained [3] the plateaus observed in the Hall effect resistivity of graphene without the use of interaction. Hence the Kohn's them applies to graphene.

[1] W. Kohn, Phys. Rev. 123, 1242-1244 (1961);
[2] E. A. Henriksen, et al., Phys. Rev. Lett. 104, 067404(2010).
[3] K. N. Shrivastava, AIP Conf. Proc. 1150, 59-67(2009); 1017,422-428(2008); Proc. SPIE 7155, 71552F(2008).

3:30PM T11.00006 Fluctuation-dissipation theorem for chiral systems in nonequilibrium steady states[1] , DIMA FELDMAN, CHENJIE WANG, Brown University — We consider a three-terminal system with a chiral edge channel connecting the source and drain terminals. Charge can tunnel between the chiral edge and a third thermal. The third terminal is maintained at a different temperature and voltage than the source and drain. We prove a general relation for the current noises detected in the drain and third terminal. It has the same structure as an equilibrium fluctuation-dissipation relation with the nonlinear response $\partial I/\partial V$ in place of the linear conductance. The result applies to a general chiral system and may be useful for detecting "upstream" modes on the quantum Hall edges.

[1]This research was supported in part by NSF grant No. DMR-054116.

3:42PM T11.00007 Spontaneous Quantum Hall States in Chirally-Stacked Few-Layer Graphene Systems , FAN ZHANG, JEIL JUNG, GREGORY FIETE, QIAN NIU, ALLAN MACDONALD, PHYSICS DEPARTMENT, UNIVERSITY OF TEXAS, AUSTIN COLLABORATION — Chirally stacked N-layer graphene systems with $N \geq 2$ exhibit a variety of distinct broken symmetry states in which charge density contributions from different spins and valleys are spontaneously transferred between layers. We explain how these states are distinguished by their charge, spin, and valley Hall conductivities, by their orbital magnetizations, and by their edge state properties. We argue that valley Hall states have [N/2] edge channels per spin-valley.

3:54PM T11.00008 Re-entrant Negative Coulomb Drag in a 1D Quantum Circuit , DOMINIQUE LAROCHE, GUILLAUME GERVAIS, McGill University, MIKE P. LILLY, JOHN L. RENO, Sandia National Laboratories — We report Coulomb drag measurements between tunable vertically- coupled quantum wires. The wires are fabricated in a GaAs/AlGaAs double quantum well heterostructure with a 15 nm barrier separating the quantum wells and are non-ballistic. The Coulomb drag signal is mapped out versus the number of subbands occupied in each wire, and regions of both positive and negative drag are observed. Negative Coulomb drag signals are measured in two regimes: one at low electronic density when the drag wire is close to or beyond depletion, and one at higher electronic density when the drag wire has more than a single 1D subband occupied. A discussion of the negative drag signal in terms of electron-hole asymmetry and localization is presented. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04- 94AL85000.

4:06PM T11.00009 Dynamic control over nanoparticle plasmon resonance through variation of refractive index[1] , HARI P. PAUDEL, MICHAEL N. LEUENBERGER, University of Central Florida — In a semiconductor material it is possible to vary the index of refraction by exciting electron-hole pairs through a laser pulse. Generally the change in refractive index changes linearly with the carrier density and also increases with the lattice temperature. We present our results on the variation in index of refraction in the TiO2 shell of an Ag/TiO2 core-shell nanoparticle by exciting electron-hole pairs in TiO2 through a laser pulse. We performed bandstructure calculations using VASP to determine the variation of the optical dielectric tensor as a function of photon frequency. This change in refractive index not only affects the refraction of photons with frequency below bandgap, but also affects strongly the resonance peaks of the surface plasmons due to the Ag core. This effect can be used to dynamically control the plasmon resonance of a hybrid metal-semiconductor nanoparticle, for example for use in cancer therapy or nanoplasmonic circuits.

[1]We acknowledge support from NSF Grant No. ECCS-0901784 and AFOSR Grant No. FA9550-09-1-0450.

4:18PM T11.00010 Transport in Coherent Quantum Hall Bilayers[1] , ALLAN MACDONALD, DMYTRO PESIN, The University of Texas at Austin, Austin, TX — We develop an approach to describe transport in bilayer quantum Hall systems in which coherence is established spontaneously between layers. We use Landauer-Buttiker theory with phenomenological parameters which can be fit to experimental data to describe quasiparticle transport in bilayers with strong coherence. We use the above approach to calculate two-probe conductances for various experimental configurations. We also apply the formalism to describe high-current transport in a bilayer with a time-dependent condensate. To describe the transition from strong to weak coherence, we use a pheonomenological single "relaxation length" ansatz for contact-to-contact transmission coefficients. As an application, we consider longitudinal drag, and find a good agreement with experiment in the regime of well- developed Quantum Hall Effect.

[1]Supported by Welch Foundation grant F1473, and by the ARO MURI on bioassembled nanoparticle arrays

Wednesday, March 23, 2011 2:30PM - 5:18PM –
Session T12 FIAP: Atomic Structures and Mechanical Properties in Semiconductors D223/224

2:30PM T12.00001 A dual approach to quantum fluctuations in frustrated lattice spin models[1] , ANIRBAN GANGOPADHYAY, VICTOR GALITSKI, University of Maryland, College Park — We develop a dual approach to describe quantum dynamics in lattice spin models, which allows us to describe nonperturbative *quantum* trajectories in the spin path integral. The spin path integral takes the form of a combination of traces of "dynamic density matrices", which belong to either special linear group $SL(2,C)$ for a quantum ferromagnet or $SU(2)$ for an antiferromagnet. We analyze the latter model of a highly frustrated quantum antiferromagnet and find a class of non-perturbative trajectories that contribute to thermodynamics of the model at low temperatures.

[1]Research supported by DOE

2:42PM T12.00002 Potassium-induced semiconducting to metallic transition on the β-SiC(100) c(4x2) surface , BARRY HAYCOCK, Dublin Institute of Technology / West Virginia University — We present new data on the potassium-induced semiconducting to metallic transition of the silicon-terminated β-SiC(100) c(4x2) surface, resulting from density functional theory simulations. In our calculations we have analysed many different K-SiC(100) structures, corresponding to K coverages ranging from 0.08 to 1.25 monolayers (ML), paying special attention to the 2/3 ML and 1 ML cases where the transition has been reported. We find that the K-SiC(100) surface is metallic in all the cases. In spite of that, the K layer shows a semiconducting density of states (DOS) up to K coverages of $\sim$1ML, beyond which the potassium layer undergoes a transition to metallic behaviour, explaining the experimental observation. We propose a new atomic model for the surface reconstruction of the 1ML case which has far lower total energy than the previously suggested model based on linear K chains after simulated annealing studies.

2:54PM T12.00003 The role of structural ordering in the semiconducting behavior of Cr_3Al[1] , ZOE BOEKELHEIDE, UC-Berkeley, D.A. STEWART, Cornell, F.J. WONG, Y. SUZUKI, F. HELLMAN, UC-Berkeley — $Cr_{1-x}Al_x$ displays unexpected semiconducting behavior for x $\sim$ 0.25; an ordered Cr_3Al structure has been proposed to explain it.[1, 2] In this work, density functional theory calculations and nonequilibrium thin film growth were used to study the role of ordering on the transport properties. The atoms in Cr_3Al occupy the sites of a bcc lattice, like Cr. Calculations comparing possible structures show that the proposed chemically ordered, rhombohedrally distorted Cr_3Al structure, with ordering along the <111> direction, is the lowest energy of those considered. In addition, the band structure shows a pseudogap, consistent with experimentally observed transport properties. Thin films of $Cr_{1-x}Al_x$ were grown with various growth and annealing temperatures to vary the properties. Samples with the most rhombohedral ordering are semiconducting. Decreased rhombohedral ordering leads to lower resistivity. Samples with a tetragonal distortion due to the $C11_b$ (Cr_2Al) structure have metallic resistivity. References: [1] D. J. Chakrabarti and P. A. Beck, J. Phys. Chem. Solids 32, 1609 (1971) [2] F. J. A. den Broeder et al, Phys. Status Solidi A, 67, 233 (1981)

[1]Supported by the DOE under Contract No. DE-AC02-05CH11231.

3:06PM T12.00004 Raman Investigation of Ru_2Si_3 Single Crystals and Thin Films , A. GLEN BIRDWELL, U.S. Army Research Laboratory, Adelphi, MD 20783 USA, DANIEL LENSSEN, DELO Industrial Adhesives, 86949 Windach, Germany, CONIN B. VINING, ZT Services, Inc., Auburn, AL 36830 USA, FRANK CROWNE, U.S. Army Research Laboratory, Adelphi, MD 20783 USA, ROBERT GLOSSER, Department of Physics, University of Texas at Dallas, Richardson, TX 75080 USA — Raman spectra were obtained from Ru_2Si_3 single crystals and thin films. The spectra were taken with the incident light polarization parallel and perpendicular to each axis of the single crystal. When inspecting all the spectra of multiple geometric configurations, we were able to observe a total of thirteen phonon modes. To the best of our knowledge, there are very few published results with which to compare. However, the encouraging point of this work is that when spectra were obtained on thin film material composed of multiple crystal orientations, we have a very close correspondence to the modes found from the experiments on the single crystal.

3:18PM T12.00005 Long-range-order and Short-range-order Structures in Sn-doped Ge Thin Films[1] , YUN-LIANG SOO, S.L. CHANG, National Tsing Hua University, J.F. LEE, National Synchrotron Radiation Research Center, H.H. CHENG, National Taiwan University — The Sn-doped Ge semiconductor thin films have shown direct bandgap and many other interesting physical properties with great potential for technological applications. To understand the underlying mechanism for the unique properties of these materials, information on the locations of Sn atoms in the matrix and the effects of Sn doping on the crystal structure of Ge host is an important prerequisite. Samples of Sn-doped Ge thin films of thickness around 300Å and Sn concentration 4 at.% to 28 at.% have been prepared by molecular beam epitaxy (MBE) method. Long-range-order and short-range-order structures in these films have been probed by using x-ray diffraction (XRD) and extended x-ray absorption fine structure (EXAFS) techniques, respectively. Our x-ray results demonstrate that Sn impurity atoms are located on the substitutional sites in the Ge films with Sn concentration up to 20 at.%. Variation of lattice constant as a result of Sn doping in the Ge host will also be presented.

[1]The present research has been supported by NSC in Taiwan under project number 97-2112-M-007-023-MY3.

3:30PM T12.00006 Wurtzite-derived polytypes of kesterite and stannite quaternary chalcogenide semiconductors , SHIYOU CHEN, Lab of Polar Materials and Devices, East China Normal University, YE LUO, XIN-GAO GONG, Fudan University, ARON WALSH, University College London, SU-HUAI WEI, National Renewable Energy Lab — The $I_2-II-IV-VI_4$ quaternary chalcogenide semiconductors (*e.g.*, Cu_2ZnSnS_4, $Cu_2ZnGeSe_4$) have been studied for more than 40 years, but the nature of their crystal structures has proved contentious. Literature reports exist for the stannite and kesterite structures, which are zincblende-derived structures, and wurtzite-stannite, which is a wurtzite-derived structure. In this talk we report a new wurtzite-derived structure, wurtzite-kesterite (space group Pc), which is the ground state for some $I_2-II-IV-VI_4$ compounds, but is easily confused with the wurtzite-stannite structure. We show that there is a clear relationship between the properties of the wurtzite-kesterite and zincblende-derived kesterite structures,, as well as between wurtzite-stannite and stannite. The energy stability of different structures are studied according to the strain and Coulomb energy contributions, showing a dependence on the size and ionicity of the component atoms. Electronic structure of the wurtzite-derived structures will also be discussed.

3:42PM T12.00007 Spontaneous symmetry breaking in two coupled nanomechanical electron shuttles[1] , CHULKI KIM, University of Wisconsin-Madison, Physics, JONGHOO PARK, ROBERT BLICK, University of Wisconsin-Madison, Electrical & Computer Engineering — We present spontaneous symmetry breaking in two coupled nanomechanical electron shuttles. The electron shuttles are realized as silicon nanopillars and placed between two capacitor plates in a homogeneous electric field. Instead of being mechanically coupled through a spring they exchange electrons, i.e., they shuttle electrons from the source to the drain capacitor plate. The nonzero dc current through this system by external ac excitation is caused via dynamical symmetry breaking. The oscillation frequencies of the shuttling system are mode locked to the applied voltage frequency.

[1]The authors like to thank DARPA fro support through the NEMS-CMOS & CSAC programs (N66001-07-1-2046) and the Graduate School of the University of Wisconsin-Madison for support through a Draper-TIF grant.

3:54PM T12.00008 ABSTRACT WITHDRAWN –

4:06PM T12.00009 Vibrational Modes of thin Silicon Membranes , REIMAR WAITZ, University of Konstanz, OLIVIER SCHECKER, now Robert Bosch GmbH, Gerlingen-Schillerhoehe, Germany, ELKE SCHEER, University of Konstanz — Membranes with thicknesses in the range of hundred nanometers and macroscopic lateral size are interesting systems to study the mechanical properties of solids on various length scales. In our experiment a piezo is used to couple in vibrations, which can be observed with a phase-shift interferometer using stroboscopic light. With this technique we image transverse modes of frequencies up to 12 MHz. In general, the observed wave pattern of the membrane deflection will be a superposition of the mode corresponding to the excitation frequency and several higher harmonics. Using a Fourier transformation in time, it is possible to separate these contributions. This way eigenmodes up to the 8th harmonic of the excitation frequency can be imaged. The influence of strain on the dispersion relation is investigated by applying a pressure difference between both sides of the membrane. The results are compared to finite-elements simulations.

4:18PM T12.00010 Phonon-imaging measurements of $CaWO_4$ Elastic Constants[1] , TIMOTHY HEAD, Abilene Christian University, MADELEINE MSALL, Bowdoin College — Recent use of $CaWO_4$ in phonon-mediated detectors for a dark matter interactions by the Cryogenic Rare Event Search using Superconducting Thermometers (CRESST) collaboration have increased interest in precise measurements of $CaWO_4$ elastic constants. Phonon-imaging simulations based on continuum elasticity theory show that position and shape of phonon caustics depend sensitively on the elastic constants. Spatial and Temporal phonon flux distributions arising after point heat-pulse excitation have been measured for [001] and [010] oriented $CaWO_4$ crystals. We report elastic constants derived from time of flight measurements along symmetry directions, and calculated by matching experimental phonon images to simulations based on continuum elasticity theory.

[1]Thanks to the ACU Math/Science Grant for partial support of this work.

4:30PM T12.00011 Kinetic Monte Carlo simulation of GaAs homoepitaxy and droplet epitaxy , KRIS REYES, DENIS NOTHERN, JOANNA MILLUNCHICK, PETER SMEREKA, University of Michigan — We present a new model for atomistic simulation of III-V semiconductors that is based on the solid-on-solid model and allows for multiple species, atom exchanges, and local considerations for atom bonding energies. The model is validated by comparison with experimental observations of GaAs homoeptiaxial growth. In particular the simulated surface concentration and growth modes agree with experiments over a wide range of growth conditions. An important feature of this model is that Ga and As atoms are treated explicitly, resulting in the ability to realistically model Ga droplet formation under low As overpressure and their recrystallization upon exposure to As.

4:42PM T12.00012 First principles determination of vibrational and elastic properties of quaternary compounds Cu_2ZnSnS_4 and $Cu_2ZnSnSe_4$, TANJU GUREL, CEM SEVIK, TAHIR CAGIN, Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX — Recently, the quaternary compounds, Cu_2ZnSnS_4 and $Cu_2ZnSnSe_4$, have been attracted pretty much attention because of their potential use in the field of energy harvesting applications. Several theoretical calculations have been reported about their first principles electronic, optic and transport properties. However, no lattice dynamic calculations have been published yet despite the discussions about their possible ground state crystal structures and measured low thermal conductivity values. In this systematical study, we examined the vibrational and elastic properties of the two different crystal phases, kesterite (KS) with space group $I\overline{4}$ and stannite (ST) with space group $I\overline{4}2m$, of this quaternary compounds by using density functional perturbation theory. In addition, we predicted the relaxation time dependent lattice thermal conductivity within the solution of phonon Boltzmann transport equation by making use of the acquired vibrational frequency data.

4:54PM T12.00013 Measuring graphene's thermal coefficient of expansion with bimetallic cantilevers , HIRAM CONLEY, Vanderbilt University, NICKOLAY LAVRIK, CNMS Oak Ridge National Lab, DHIRAJ PRASAI, KIRILL I. BOLOTIN, Vanderbilt University — We developed a method for probing the thermal coefficient of expansion of 2D materials by measuring the deflection of a bimetallic cantilever. We fabricate suspended bimetallic cantilevers composed of single-layer or multilayer graphene and either gold or silicon nitride. Because of the mismatch of the thermal expansion coefficients, these cantilevers bend when heated. We employ laser interferometry to measure the bending and to extract the thermal expansion coefficient from -170 C to 250 C. We find that this technique provides a reliable measurement of the thermal expansion coefficient for graphene. Through comparison of the coefficient of expansion obtained from our bimetallic cantilevers and that of suspended graphene we demonstrate how graphene's dimensionality is perturbed by contact with other materials.

5:06PM T12.00014 Temperature Dependence of Cyclotron Decoherance Time in a High Mobility Two-Dimensional Electron Gas , J.A. CURTIS, J.D. MOORE, Department of Physics, University of Alabama, Birmingham, Alabama 35294, T.T. TOKUMOTO, National High Magnetic Field Lab, Florida State University, Tallahassee, Florida 32310, J.G. CHERIAN, Department of Physics, Florida State University, Tallahassee, Florida 32310, X. WANG, Department of Electrical Engineering, Rice University, Houston, Texas 77005, J.L. RENO, Sandia National Laboratories, Albuquerque, New Mexico 87185, A. BELYANIN, Department of Physics, Texas A&M University, College Station, Texas 77843, J. KONO, Department of Electrical Engineering, Rice University, Houston, Texas 77005, S.A. MCGILL, National High Magnetic Field Lab, Florida State University, Tallahassee, Florida 32310, D.J. HILTON, Department of Physics, University of Alabama, Birmingham, Alabama 35294 — Using time-domain THz magneto-spectroscopy, we studied the dynamics of a 2DEG ($\mu = 3.4 \times 10^6 \mathrm{cm}^2\,\mathrm{V}^{-1}\,\mathrm{s}^{-1}$) as a function of temperature (0.4K-100K).The decoherence lifetimes increase monotonically as temperature decreases below 1 K, which we have fit to a power law ($\tau \sim T^{0.29}$). We will discuss the mechanisms that contribute to the lifetimes. The transmitted pulse amplitude increases from 0.4K-1.2K, saturates from 1.5K-25K, and decreases from 50K-100K. J. A. Curtis is supported by a US Dept. Education GAANN Fellowship (P200A090143).

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T13 GSNP: Focus Session: Transport and Diffusion in Non-equilibrium Systems D225/226

2:30PM T13.00001 Thermodiffusion (Ludwig-Soret Effect) in Geological Systems[1] , CHARLES LESHER, UC Davis — Since its discovery more than a century and a half ago, the Ludwig-Soret effect (development of concentration gradients in response to a temperature gradient) has been documented in a large variety of inorganic and organic solutions, and exploited as an industrial tool for chemical and isotopic refinement. Theoretical treatments are numerous based on kinetic and thermodynamic principles, but none adequately explains the phenomenon operating in complex naturally occurring fluids. In the geological sciences, the Ludwig-Soret effect has received extraordinary attention as an agent for small (and large) scale chemical differentiation and a probe of fundamental fluid properties of the Earth's hydrosphere, and silicate (crust-mantle) and alloy (core) interior. In particular, silicate liquids show significant isotope fractionation by thermodiffusion at temperatures greatly exceeding those where equilibrium fractionation effects are vanishingly small, and this can persist to lower temperatures even with concomitant crystallization. We review these recent findings and present new experimental work on silicate and Fe(FeS) melts, considering the underlying causes towards reconciling observed mass-dependent isotope and mass-independent chemical effects.

[1]Work supported by NSF EAR 0943992 and 1019887.

3:06PM T13.00002 Galilean thermodynamics of a multicomponent fluid and its induced electromagnetic fields , SYLVAIN BRECHET, JEAN-PHILIPPE ANSERMET, EPFL — The phenomenological theory of irreversible processes in fluid systems has been successfully applied to new research fields, for example spintronics and spincaloritronics (arXiv:1011.2323). We include the electromagnetic interaction into the thermodynamic description of a multicomponent fluid. Our analysis is performed in the Galilean limit of electromagnetism. The tensorial part of the Onsager relations accounts in particular for mutliferroic effects.

3:18PM T13.00003 Thresholds, memory, and self-similarity on river deltas , MEREDITH REITZ, Dept Physics and Astronomy, University of Pennsylvania, DOUGLAS JEROLMACK, Dept Earth and Environmental Science, University of Pennsylvania — The bulk dynamics of river deltas and alluvial fans result from several physical processes acting on a wide range of scales. We study a series of experimental alluvial fans to sort the relevant processes and determine the way in which their interaction drives fan behavior. We find a timescale of channel movement that depends on mass conservation, as sediment fills a wedge of space determined by a separation between conditions of grain entrainment and distrainment, in a manner analogous to the separation between static and dynamic angles of repose in dry granular systems. Channel path selection behavior shows a marked tendency for flow to reoccupy abandoned paths, in a way that can be abstracted with a random walk model in a system with absorbing states, and resulting in a predictable self-similar shoreline growth pattern. Because we isolate the processes that drive the evolution of our experimental fans, we are able to translate our findings to the study of natural fans and deltas in which the same processes operate.

3:30PM T13.00004 Tailoring Polymer Nanocomposite Properties by Nanoparticle Assembly[1] , SANAT KUMAR, Columbia University — Novel materials based on polymer-grafted nanoparticles (NP) are the focus of this talk. Since inorganic NPs and organic polymers typically "dislike" each other, these "hairy" particles behave like block-copolymers or amphiphiles. They can, therefore, self-assemble into a range of superstructures when placed in an organic matrix. Understanding the factors controlling this this assembly state and how it affects the properties of the resulting material are our central interests in this area. As part of this global effort, here we address three questions: (i) Can we direct NP assembly using external fields, e.g., shear, with the ultimate goal of designing membranes with directional transport properties? (ii) Can we assemble grafted NPs at interfaces with the aim of compatibilizing immiscible polymer blends? (iii) Can NP assemblies result in simultaneous improvements in the Young's modulus, the yield stress and strain-to-break of an amorphous polymer in the solid-state? As with all of our work we combine theory and experiments to understand these concepts that underpin our nascent understanding in this area.

[1]Supported by NSF-DMR.

4:06PM T13.00005 Thermodynamic Analysis of Nanoporous Membrane Separation Processes[1] , DAVID ROGERS, SUSAN REMPE, Sandia National Laboratories — We give an analysis of desalination energy requirements in order to quantify the potential for future improvements in desalination membrane technology. Our thermodynamic analysis makes it possible to draw conclusions from the vast array of equilibrium molecular dynamics simulations present in the literature as well as create a standardized comparison for measuring and reporting experimental reverse osmosis material efficiency. Commonly employed methods for estimating minimum desalination energy costs have been revised to include operations at positive input stream recovery ratios using a thermodynamic cycle analogous to the Carnot cycle. Several gaps in the statistical mechanical theory of irreversible processes have also been identified which may in the future lead to improved communication between materials engineering models and statistical mechanical simulation. Simulation results for silica surfaces and nanochannels are also presented.

[1]Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

4:18PM T13.00006 Geometric Phase Effect in Heat Transport , JIE REN, National University of Singapore, PETTER HANGGI, University of Augsburg, BAOWEN LI, National University of Singapore — Nonlinear molecular heat-pumping devices, which operate via explicitly modulating at least two parameters, are crucial for energy control in low dimensional nano-scale systems. We have applied slow two-parameter modulations on such a molecular junctions and consequently uncovered an intrinsic heat flux contribution, additional to the known, usual dynamical heat flux (from hot to cold). This additional heat flux derives from a nontrivial geometric origin that relates to a non-vanishing, so termed finite Berry phase. It provides a free lunch for the pumped heat and even can direct heat flux against the temperature bias. In addition we are able to show that this so pumped energy exhibits a novel robust fractional quantization phenomenon. Interestingly, this additional geometric heat pump mechanism is also shown to cause a breakdown of the heat-flux fluctuation theorem, which holds true for the non-driving, stationary heat flux transfer. The validity of this theorem is guaranteed whenever (i) the geometric phase contribution vanishes and (ii) the cyclic protocol preserves the detailed balance symmetry.

4:30PM T13.00007 Contact processes in crowded environments , J.M. SCHWARZ, Syracuse University, BISMAYAN CHAKRABARTI, Indian Institute of Technology, Kanpur — A nonequilibrium absorbing state phase transition with conserved particle number has been realized in a periodically sheared particle suspension. A diffusing (active) particle in the suspension collides with a stationary (inactive) particle and activates it. As the strain amplitude is increased, the fraction of active particles per shear cycle becomes nonzero only above some critical strain amplitude. To further study this system at higher densities, we construct a lattice model with active and inactive particles occupying some fraction of the lattice sites with each site being occupied by at most one particle. The active particles hop to empty neighboring sites and activate k neighboring inactive particles at some rate λ_k. Also, active particles become inactive at some rate γ. We investigate this model for $\lambda_{k=1} = 0$ and $\lambda_{k>1} > 0$ to study the effects of multi-particle collisions which are likely to occur at higher densities, i.e. crowded environments.

4:42PM T13.00008 Mixing of Diffusing Particles , ELI BEN-NAIM, Los Alamos National Laboratory — We study how the order of N independent random walks in one dimension evolves with time. Our focus is statistical properties of the inversion number m, defined as the number of pairs that are out of sort with respect to the initial configuration. In the steady-state, the distribution of the inversion number is Gaussian with the average $\langle m \rangle \simeq N^2/4$ and the standard deviation $\sigma \simeq N^{3/2}/6$. The survival probability, $S_m(t)$, which measures the likelihood that the inversion number remains below m until time t, decays algebraically in the long-time limit, $S_m \sim t^{-\beta_m}$. Interestingly, there is a spectrum of $N(N-1)/2$ distinct exponents $\beta_m(N)$. We also find that the kinetics of first passage in a circular cone provides a good approximation for these exponents. When N is large, the first-passage exponents are a universal function of a single scaling variable, $\beta_m(N) \to \beta(z)$ with $z = (m - \langle m \rangle)/\sigma$. In the cone approximation, the scaling function is a root of a transcendental equation involving the parabolic cylinder equation, $D_{2\beta}(-z) = 0$, and surprisingly, numerical simulations show this prediction to be exact.

4:54PM T13.00009 Crossover behavior in models of depinning , YAN-JIUN CHEN, LASSP, Cornell Univ., LASSE LAURSON, ISI in Torino, Italy and Department of Applied Physics, Aalto University, Helsinki, Finland, STEFANOS PAPANIKOLAOU, LASSP, Cornell Univ., STEFANO ZAPPERI, IENI-CNR, Milano, Italy and ISI in Torino, Italy, JAMES P. SETHNA, LASSP, Cornell Univ. — We explore the behavior of models describing driven interfaces in random media. These models are useful in describing a wide range of real-world systems: disordered magnets, fluids in porous medium, pinning of flux lines in superconductors, and fluid imbibition in paper. Variations of these models have been numerically studied and classified into distinct universality classes at the depinning transition, however the exact structure of the phase space is still not known. We are investigating the crossover behavior in between various linear and nonlinear models with short-range and long-range interactions, and will report on their respective scaling functions of height-height correlation and size distributions of avalanches.

5:06PM T13.00010 An Information-Theoretic Order Parameter for Non-Equilibrium Systems , MARTIN TCHERNOOKOV, ILYA NEMENMAN, Emory University — In non-equilibrium statistical physics, symmetry and free energy are difficult to define, preventing application of classical machinery for analysis of phase transitions. Can one define a "universal" order parameter that would be measurable from experimental data, would allow identification of an onset of a phase transition, and would be meaningful independently of the underlying systems dynamics? We suggest that predictive information, which is the mutual information between the sequence of the observed past states of a system and its future states, introduced by us in 2001,[1] may serve as such order parameter. We study this suggestion in the context of a model non-stationary Langevin process. We show analytically that the predictive information attains its maximum value at the phase transition, diverging logarithmically with the length of the observed past. We demonstrate that the speed of divergence is related to traditional critical exponents. Finally, we show how the onset of a phase transition can be found empirically from data, independently of its parameterization.

[1]W Bialek, I Nemenman, N Tishby. Neural Computation (2001),13,2409

5:18PM T13.00011 Classical nucleation theory explains the critical cooling rate of cryoprotectant solutions , MATT WARKENTIN, ROBERT THORNE, Cornell University — We have measured critical cooling rates for a range of concentrations of different solutes in aqueous solutions. Our results show that the glass formability of aqueous solutions is exponential in the concentration for all solutes tested, with a different characteristic concentration for each solute. This characteristic correlates with the Stokes radius of the solute. A simple modification of critical droplet theory relates the characteristic concentration to the critical nucleation radius in pure water, and explains the relationship between the Stokes radius and the exponential characteristic. This simple, general theory of glass formability in aqueous solutions is important at a fundamental level, and will also have broad consequences for the field of cryobiology.

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T14 GSNP: Focus Session: Extreme Mechanics: Elasticity and Deformation II D227

2:30PM T14.00001 Elasto-capillarity: The role of stretching , DOMINIC VELLA, OCCAM, University of Oxford — Elasto-capillarity, the interaction between elasticity and surface tension or surface energies, has been much studied in recent years. However, to date the focus has been almost exclusively on situations where the bending stiffness of an object resists deformation by the surface tension of a liquid. In this talk I will consider some situations in which it is instead the stretching stiffness of an elastic object that resists its deformation by surface tension. I will focus on explaining recent experiments that demonstrate the wrinkling of floating elastic membranes [J. Huang *et al.*, *Science* **317**, 650 (2007)] but will also discuss related fundamental problems in wrinkling as well as other situations that involve an interaction between the stretching of an elastic object and capillarity.

3:06PM T14.00002 Building blocks for the shapes of confined elastic sheets[1] , ROBERT SCHROLL, UMass Amherst, ELENI KATIFORI, Rockefeller University, BENNY DAVIDOVITCH, UMass Amherst — Several configurations, such as d-cones, minimal ridges, and developable patches, occur regularly in the configuration of elastic sheets. We dub such features "building blocks." Here, we study elastic sheets confined in a manner that prohibits the sheet from taking on a single-buckle shape. We find not only building blocks where stress focuses, reminiscent of d-cones, but also "diffuse-stress" regions. The former is characterized by a geometrical constraint (inextensibility) while the latter is governed by a mechanical constraint: the dominance of a single component of the stress tensor. We characterize how boundary conditions and applied tension select which building blocks appear and discuss implications for the curtain problem.

[1]We acknowledge support from the NSF-supported MRSEC on Polymers at UMass (DMR-0820506).

3:18PM T14.00003 Droplet Formation and Scaling in Dense Suspensions , MARC MISKIN, HEINRICH JAEGER, University of Chicago — A drop detaching from a nozzle is a prototypical example of scaling behavior. For a pure fluid, this scaling is contingent on the fact that the material parameters remain invariant throughout the detachment. However, for a dense suspension, this assumption is invalid. We use high-speed photography to examine the formation of suspension droplets. We find that the minimum neck radius, R_m, near breakup can be described by a power law $(t_b - t)^{2/3}$, with a material independent exponent. By considering how particles deform the surface and appealing to topological constraints, we develop a modified version of the Laplace-Young equation relating the surface pressure to the macroscopic Gaussian curvature. This model, combined with a scaling argument, allows us to collapse all of our data for R_m near breakup. These results open a new territory for modeling suspensions by asserting that a major stress resides at the boundary, and that it can be calculated using strictly macroscopic parameters.

3:30PM T14.00004 Surface patterns in thermally responsive elastomeric gels , SHAWN CHESTER, LALLIT ANAND, MIT — Many stimulus responsive elastomeric gels operate in non-isothermal, chemically saturated environments in a variety of applications. We have recently developed a three dimensional continuum level theory to describe the coupled fluid permeation and large deformation response of thermally responsive elastomeric materials. In this work, we apply our theory and numerical simulation capability to the specific case of surface wrinkles induced via swelling of a thermally responsive gel bonded on top of a compliant impermeable elastic substrate. We show that we can numerically model the swelling behavior and subsequent surface pattern formation. Also, we examine the effect of substrate thickness by varying the ratio of gel to substrate thickness. Further, we show that it is possible to modulate the amplitude of the surface wrinkles by taking advantage of the thermally responsive nature of this class of materials.

3:42PM T14.00005 Morphologies of Equibiaxially Wrinkled Surfaces , DEREK BREID, University of Massachusetts, SHENGQIANG CAI, ZHIGANG SUO, JOHN HUTCHINSON, Harvard University, ALFRED CROSBY, University of Massachusetts — The morphological characteristics of a wrinkled film are largely determined by the state of stress at the onset of the instability. For surfaces compressed equibiaxially, it is well established that ridge-based structures, including herringbone or labyrinth patterns, provide the lowest energy state for stresses far exceeding critical buckling. For near-critical stresses, the equilibrium morphology is less understood. Using surface-oxidized poly(dimethylsiloxane) as a model wrinkling material, we control the applied stress by swelling the oxide film with a compatible vapor-phase solvent. The extent of swelling is controlled by the vapor pressure of the solvent and the thickness of the oxide layer, and the generated overstress in turn dictates the observed morphology. Analytical and numerical models are used to determine the deformation morphologies that provide the lowest energy state with increasing overstress. Comparison of experimental observations and theoretical predictions provides insight into the importance of substrate curvature in determining final equilibrium morphologies.

3:54PM T14.00006 Revisiting the curvature cancellation in forced thin sheets[1] , JIN WANG, THOMAS WITTEN, University of Chicago — We revisit the numerically observed spontaneous vanishing of mean curvature [1] on a developable cone or "d-cone" [2] made by pushing a thin elastic sheet into a circular container. The deflection of the d-cone is the distance by which the sheet is pushed into the container. We investigate the ratio of the two principal curvatures versus sheet thickness h over a wider dynamic range than was used previously, holding the deflection and radius fixed. Instead of tending towards 1 as suggested by previous work, we find that the ratio scales as $h^{1/3}$. Scaling arguments and geometric variants support this $h^{1/3}$ finding. Thus the mean curvature does not vanish for very thin sheets as previously claimed.

[1] T. Liang and T. A. Witten, *Phys. Rev. E* **73**, 046604 (2006).
[2] E. Cerda, S. Chaieb, F. Melo, and L. Mahadevan, *Nature* **401**, 46 (1999).

[1]Supported by NSF award DMR 0820054.

4:06PM T14.00007 Mechanics of Geometrically-Tuned pH-Responsive Polymers , LIFENG WANG, Massachusetts Institute of Technology, LIN HAN, KHEK-KHIANG CHIA, ROBERT COHEN, MICHAEL RUBNER, MARY BOYCE, CHRISTINE ORTIZ — Stimuli-responsive polymer materials have been extensively explored over the past two decades because of their promising applications. We consider the mechanics of mechanomutable polyelectrolyte multilayers (PEMs), which undergo reversible pH-responsive transition from a condensed, ionically crosslinked state (small pH) to a hydrated, ionized state (large pH). Instrumented indentation and micro-structurally-based finite element analysis are conducted on the PEM thin films and PEM tube forests to determine the effective elastic properties and further the mechanomutability as a result of the coupling between inherent responsive material properties and geometry. We demonstrate that geometry can be used to introduce and tailor different deformation mechanisms as a means to tune mechanomutabilibility of stiffness and dissipation in addition to the constitutive material properties. The rate-dependent stimulus-responsive mechanomutability can be finely controlled within a wide range from $\sim$ 2 – 100 times by tailoring the tube geometrical factors at different indentation rates. These studies provide fundamental understanding and mechanics of indentation of PEM thin films and tube forests and show the tremendous potential for dynamically tuning surface and bulk properties of novel complex structured materials.

4:18PM T14.00008 Stretch-induced compressive stresses and wrinkling in hyperelastic thin sheets , RUI HUANG, University of Texas at Austin, VISHAL NAYYAR, K. RAVICHANDAR, CENTER FOR MECHANICS OF SOLIDS, STRUCTURES AND MATERIALS TEAM — Wrinkles are commonly observed in stretched thin sheets. This paper presents a study on stretch-induced wrinkling of hyperelastic thin sheets using the finite element method. The model problem is set up for uniaxial stretching of a rectangular sheet with two clamped ends and two free edges. A two-dimensional stress analysis is performed first under the plane-stress condition to determine stretch-induced stress distributions in the elastic sheets, assuming no wrinkles. As a prerequisite for wrinkling, the development of compressive stresses in the transverse direction is found to depend on the length-to-width aspect ratio of the sheet and the applied stretch. A phase diagram is constructed with a set of different distribution patterns of the compressive stress spanning a wide range of aspect ratios and up to moderately large tensile strain ($\sim$150%). Next, an eigenvalue analysis is performed to find the potential buckling modes of the elastic sheet under the prescribed boundary conditions. Finally, a nonlinear post-buckling analysis is performed to show evolution of the stretch-induced wrinkles. In addition to the aspect ratio and the applied stretch, it is found that the critical condition for wrinkling and the post-buckling behavior both depend sensitively on the sheet thickness.

4:30PM T14.00009 Elastic Instabilities of Nematic Liquid Crystals in Spherical Geometries , VINZENZ KONING, Leiden University, TERESA LOPEZ-LEON, K.B.S. DEVAIAH, ALBERTO FERNÁNDEZ-NIEVES, Georgia Institute of Technology, VINCENZO VITELLI, Leiden University — We investigate elastic instabilities of nematic liquid crystals confined in spherical shells characterized by extreme thickness inhomogeneity. For shells with a uniform thickness there exists an equilibrium defects structure containing two pairs of boojums at the north and south poles. By minimizing the elastic free energy (subject to tangential boundary conditions on both bounding surfaces), we determine the locations of the defects as a function of thickness inhomogeneity. We find that the defects make an abrupt confinement transition to the thinnest hemisphere from the initial antipodal arrangement, when the thickness inhomogeneity exceeds a critical value. Our results agree well with recent experimental studies on nematic double emulsions and suggest design criteria to engineer micron scaled particles with directional binding capabilities.

4:42PM T14.00010 Near critical phenomena in amorphous smart materials , EDUARD OBERAIGNER, University of Leoben, Institute of Mechanics, MICHAEL FISCHLSCHWEIGER, Materials Center Leoben Forschung GmbH — The importance of smart materials e.g. shape memory alloys (SMAs) for technological applications has been growing during the last 20 years. Especially modeling SMAs behavior has become of high interest in materials science for the prediction of macroscopic effects like pseudoelasticity. The key for their behavior is a displacive solid - solid phase transformation, called martensitic phase transformation. However, such a critical phenomenon requires investigations for deep relations between physical quantities nearby the region of phase transformation. The present study is focusing on a statistical mechanics approach for the description of relations between heat capacity, pseudoelasticity, volume fraction compressibility, alternatively fraction expansion coefficient, and a compressibility tensor, leading to the compliance tensor in the case of elasticity. Also a heat expansion tensor along the line of magnetic phase transitions and transformations has been formulated for shape memory alloys. The work discusses martensitic variants (which occur due to a subgroup relation between the austenitic and martensitic phase) and their asymmetry, which influences the above mentioned quantities as well and gives ideas and suggestions for model improvements.

4:54PM T14.00011 The role of membrane viscosity in the relaxation dynamics of fluid membranes , MARINO ARROYO, Universitat Politecnica de Catalunya, Spain, LUCA HELTAI, ANTONIO DESIMONE, SISSA, Italy — Fluid membranes made out of lipid bilayers are the fundamental separation structure in eukaryotic cells. Many physiological processes rely on dramatic shape and topological changes (e.g. fusion, fission) of fluid membrane systems. Fluidity is key to the versatility and constant reorganization of lipid bilayers. Here, we study the role of the membrane intrinsic viscosity, arising from the friction of the lipid molecules as they rearrange to accommodate shape changes, in the dynamics of morphological changes of fluid vesicles driven by curvature elasticity. In particular, we analyze the competition between the membrane viscosity and the viscosity of the bulk fluid surrounding the vesicle as the dominant dissipative mechanism. We consider the relaxation dynamics of fluid vesicles put in an out-of-equilibrium state, but conclusions can be drawn regarding the kinetics or power consumption in regulated shape changes in the cell. On the basis of numerical calculations, we find that the dynamics arising from the membrane viscosity are qualitatively different from the dynamics arising from the bulk viscosity. When these two dissipation mechanisms are put in competition, we find that for small vesicles the membrane dissipation dominates, with a relaxation time that scales as the size of the vesicle to the power 2. For large vesicles, the bulk dissipation dominates, and the exponent in the relaxation time vs. size relation is 3.

5:06PM T14.00012 The star shaped pattern on broken thin sheets , NICOLAS VANDENBERGHE, ROMAIN VERMOREL, EMMANUEL VILLERMAUX — We study transverse impacts of rigid objects on a thin elastic sheet made of acrylic. After impact, a transverse wave propagates on the sheet and orthoradial stresses lead to the formation of radial cracks. The result of this fragmentation process is the star shaped pattern frequently observed on broken windows. We investigate the variation of the pattern and in particular the number of radial cracks with impact speed and material properties. The formation of rayed craters by meteorite impacts will be briefly discussed.

5:18PM T14.00013 How to make sticky tapes stickier , LAURENT PONSON, Institut d Alembert, CNRS - Universite Pierre et Marie Curie Paris VI, SHUMAN XIA, GURUSWAMI RAVICHANDRAN, KAUSHIK BHATTACHARYA, California Institute of Technology, CALIFORNIA INSTITUTE OF TECHNOLOGY TEAM — Thin film adhesives have become increasingly important in various applications such as packaging and coating, and we benefit daily of their adhesion properties by using various kinds of tapes. Despite the apparent simplicity of these systems, a certain number of questions remain open. In particular, important efforts have been deployed recently to understand the effect of the complex tridimensional and highly heterogeneous structure at the interface of some adhesives, such as the one encountered in nature like the geckos toes. Although inspired by these natural adhesives, we studied a much simpler system, and however largely unexplored: a thin film with spatially varying adhesion energy and elastic properties. We will show how these heterogeneities introduced at the microscale can generate quite unexpected macroscopic behaviors, and that one can this way design stronger adhesives with new properties. Beyond their practical interests, these systems involve long range elastic interactions and heterogeneities resulting in a rich and complex physics that will be illustrated through experimental examples and their theoretical interpretation.

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T15 DMP GMAG FIAP: Focus Session: Spins in Semiconductors - III-V Magnetic Semiconductors D171

2:30PM T15.00001 Valence-band structure of the ferromagnetic semiconductor GaMnAs investigated by resonant tunneling spectroscopy , SHINOBU OHYA, Dept. of Electrical Eng. and Information Systems, The Univ. of Tokyo — The origin of ferromagnetism in the prototype ferromagnetic semiconductor GaMnAs is still controversial due to the insufficient understanding of its band structure and Fermi level position. Here, we investigate the valence-band (VB) structure of GaMnAs by analyzing the resonant tunneling levels of the GaMnAs quantum well (QW) in double-barrier heterostructures. The resonant levels including the heavy-hole first state (HH1) are clearly observed in the metallic GaMnAs QW with the Curie temperature (T_C) of 60 K, which indicates that no holes reside in the VB of GaMnAs in the equilibrium condition. Clear enhancement of tunnel magnetoresistance induced by resonant tunneling is demonstrated. We find that the resonant levels formed in the GaMnAs QW are well explained by using the transfer matrix method with the 6x6 *kp* Hamiltonian and small $p-d$ exchange Hamiltonian. The VB structure of GaMnAs is well reproduced by that of GaAs with a small exchange splitting energy of 3-5 meV and with the Fermi level lying at $\sim$30 meV higher than HH1 in the bandgap. Furthermore, we show our more recent results of resonant tunneling spectroscopy on various surface GaMnAs films (Mn concentration: 6-15%, T_C: 71-154 K) grown on an AlAs layer, where the resonant levels are formed by confinement of the VB holes by the surface Schottky barrier and the AlAs barrier. We systematically investigate the thickness dependence of the resonant levels in GaMnAs by precisely etching the surface of GaMnAs. We find that the p-d exchange interaction is negligibly small (3-5 meV) and that the Fermi level exists in the bandgap. This work was performed in collaboration with I. Muneta, P. N. Hai, K. Takata, and M. Tanaka, and partly supported by Grant-in-Aids for Scientific Research, the Special Coordination Programs for Promoting Science and Technology, and FIRST Program by JSPS.

[1] S. Ohya et al., Phys. Rev. Lett. 104, 167204 (2010).
[2] S. Ohya et al., arXiv:1009.2235.

3:06PM T15.00002 On magnetism and the insulator-to-metal transition in p-doped GaAs , BRIAN CHAPLER, University of California San Diego, R.C. MYERS, Ohio State University, S. MACK, University of California Santa Barbara, A. FRENZEL, B.C. PURSLEY, University of California San Diego, K.S. BURCH, University of Toronto, E.J. SINGLEY, California State University East Bay, A.M. DATTELBAUM, Los Alamos National Laboratory, N. SAMARTH, Pennsylvania State University, D.D. AWSCHALOM, University of California Santa Barbara, D.N. BASOV, University of California San Diego — Although $Ga_{1-x}Mn_xAs$ is often described as the prototypical ferromagnetic semiconductor, many aspects of the electronic structure and nature of mediating carriers remain open. A central question in this regard is whether the insulator-to-metal transition (IMT) in p-doped GaAs is significantly modified when dopants are magnetic. We address this through an infrared spectroscopic study of GaAs doped with either non-magnetic Be or magnetic Mn acceptors. Through our comparison, we are able to isolate effects of magnetic dopants in GaAs from those associated with disorder and proximity to the IMT. Here we show Mn-doped samples exhibit an unusual electronic transport regime, combining elements of both metallic and insulating behavior, at doping concentrations far beyond the onset of the IMT. Be-doped films however, reveal genuine metallicity just above the IMT boundary. These results underscore the pivotal role of magnetism in transport and optical phenomena of $Ga_{1-x}Mn_xAs$.

3:18PM T15.00003 Magnetic properties of narrow gap $In_{1-x}Mn_xSb$ semiconductor films with x>0.10 , CAITLIN FEESER, JOHN PETERS, BRUCE WESSELS, Northwestern University — Narrow gap $In_{1-x}Mn_xSb$ magnetic semiconductors with x $<$ 0.05 have been recently shown to have interesting magnetotransport properties at room temperature.[1] Calculations based on the field dependence of the magnetoresistance indicate that the carriers are highly spin polarized. To increase both the saturation magnetization and potentially the Curie temperature Tc of the alloys, we have investigated MOVPE epitaxial layers with 0.10 $<$ x $<$ 0.22. Films were ferromagnetic at room temperature, showing clear hysteresis in field dependent measurements from 5 to 300 K. Alloys with magnetization values as high as 83 emu/cm^3 for x=0.22 were measured at 5 K. Temperature dependent magnetization indicated that the Curie temperature of the films was above 400 K. These measurements indicated the presence of two magnetic species both with Curie temperatures above 300 K. The high Tc is attributed to carrier mediated ferromagnetism involving Mn and its complexes that form shallow or resonant electronic states with the valence band through correlated substitution.

[1]J. A. Peters et al, PRB **82** 2010.

3:30PM T15.00004 Cyclotron Resonance in InMnAs and InMnSb Ferromagnetic Films[1] , GITI KHODAPARAST, Department of Physics, Virginia Tech, Blacksburg, VA, USA, Y.H. MATSUDA, R. SHEN, S. TAKEYAMA, Institute for Solid State Physics, University of Tokyo, Kashiwa, Japan, X. LIU , J. FURDYNA, Department of Physics, University of Notre Dame, Notre Dame, IN, USA, B.W. WESSELS, Materials Research Center, Northwestern University, Evanston, IL, USA — Ferromagnetic semiconductors are important materials for development of spintronic devices. While effort in this area was made primarily on GaMnAs, other ferromagnetic III-Mn-V alloys have also been developed, including the narrow gap ferromagnetic alloys such as InMnAs and InMnSb. Investigation of the electronic structure of III-Mn-V alloys by techniques such as the cyclotron resonance (CR) can shed important light on the origin of ferromagnetism and the p-d exchange interaction in III-Mn-V systems. In this work we report on CR experiments carried out on the ferromagnetic InMnAs and InMnSb films, on which clear resonance signals have been successfully observed in high magnetic fields generated by a single turn coil technique. The CR in ferromagnetic InMnSb was observed for the first time and we compare our observations with the Landau levels calculations on the basis of an 8-band $k\cdot p$ model.

[1]Supported by: NSF-DMR-0507866, AFOSR YIP 06NE231, NSF-Career Award DMR-0846834, NSF DMR 0804479, NSF DMR-1005851.

3:42PM T15.00005 Visualizing Critical Correlations Near the Metal-Insulator Transition in $Ga_{1-x}Mn_xAs$, ANTHONY RICHARDELLA[1], Department of Physics, Princeton University — Semiconductors have long been an ideal class of materials for studying the metal-insulator transition. Samples of the dilute magnetic semiconductor $Ga_{1-x}Mn_xAs$ with Mn doping levels near to the metal-insulator transition have been studied using low temperature cross-sectional scanning tunneling microscopy (STM). This allows us to visualize the electronic states near the Fermi level which display unique critical properties. Strong modifications to the density of states around the Fermi energy due to electron-electron interactions are observed. In this energy range, the electronic states show a diverging correlation length approaching E_F, where the correction to the density of states due to interactions is strongest. The distance dependence of the correlations at E_F is consistent with a power law decay, expected for multifractal states near criticality in the metal-insulator transition, while away from E_F the correlations fall off exponentially. These results highlight the importance of electron-electron interactions and represent some of the first experimental observations of states near the Mott-Anderson metal-insulator transition, where both disorder and interactions are important for the localization of electronic states.

[1]Currently at Penn State University.

4:18PM T15.00006 Time resolved spectroscopy of MOVPE grown narrow gap III-Mn-V ferromagnetic semiconductors[1] , T. MERRITT, M. BHOWMICK, G.A. KHODAPARAST, Department of Physics, Virginia Tech, Blacksburg, VA, C. FEESER, B.W. WESSELS, Materials Research Center, Northwestern University, Evanston, IL, S. MCGILL, National High Magnetic Field Laboratory, Tallahassee, FL — The emergence of III-Mn-V magnetic semiconductors, has led to a number of exciting results relevant to the spin and charge based applications. Important advances have now been made in the MOVPE growth of the narrow gap ferromagnetic structures with the Tc above room temperature. As the switching rates in electronic and optoelectronic devices are pushed to higher frequencies, understanding the dynamical behavior of non- equilibrium carriers/spins can provide valuable information about different scattering mechanisms, carrier phonon coupling, and band structures. In this work, we report several time-resolved and magneto-optical measurements on $In_{1-x}Mn_xAs$ and $In_{1-x}Mn_xSb$ ferromagnetic films with the Mn content of 4%. Our measurements on the basis of several time resolved differential transmission techniques in NIR and MIR demonstrate unique and complex dynamics in these material systems where photo-induced absorption and bleaching can co- exist.

[1]Supported by: NSF-DMR-0507866, NSF-DMR-0804479, AFOSR YIP06NE231, NSF-Career Award DMR-0846834.

4:30PM T15.00007 Structural and Magnetic Characteristics of p-GaAs/MnAs Nanocluster Hybrids , DAVID RENCH, PETER SCHIFFER, NITIN SAMARTH, Department of Physics and Materials Research Institute, The Pennsylvania State University, University Park, Pennsylvania 16802, USA — A possible route towards semiconductor spintronic devices involves the controlled synthesis of hybrid materials that combine ferromagnetic (FM) nanoclusters within a doped semiconductor host lattice. We use molecular beam epitaxy of (Ga,Mn,Be)As followed by in situ annealing to synthesize a systematic set of samples wherein FM nanoclusters are embedded in a p-GaAs matrix. High resolution transmission electron microscopy (HRTEM) and magnetometry demonstrate our ability to reproducibly synthesize two distinct classes of materials: (a) type I samples consisting of uniformly distributed, small clusters ($\sim$6 nm); (b) type II samples consisting of a bimodal distribution of small ($\sim$6 nm) and large ($\sim$25 nm) clusters. HRTEM studies show that while the large clusters are clearly MnAs with NiAs structure, the smaller clusters are possibly zinc blende in structure but with a more complex composition. We analyze the magnetic behavior of these two classes of samples and show measurements of their transport properties. Supported by the ONR-MURI program.

4:42PM T15.00008 Magnetoresistance due to inelastic spin-flip cotunneling within Coulomb blockade regime in III-V semiconductor / MnAs nanoparticle heterostructures , RYOTA AKIYAMA, SHINOBU OHYA, PHAM NAM HAI, MASAAKI TANAKA, Dept. of Electrical Eng. and Information Systems, The Univ. of Tokyo — Inelastic spin-flip cotunneling is a key to understand the spin-dependent single-electron transport in the ferromagnetic nanoparticles systems. We fabricated a heterostructure consisting of Al/ AlAs/ ferromagnetic zinc-blende (ZB) MnAs nanoparticles embedded in GaAs / GaAs:Be on a GaAs(001) substrate, where electrons are expected to go through only one nanoparticle during tunneling. By analyzing the $I-V$ data at various temperatures T, we found that inelastic cotunneling is dominant when T <60 K. The ratio of the inelastic cotunneling energy E to the thermal energy kT, estimated by the $I-V$ data, was remarkably increased with decreasing T. We observed clear magnetoresistance (MR) up to ∼3% (at 1T), and MR was also increased with decreasing T. The shape of the *MR-T* curve was quite similar to that of the *E/kT - T* curve, which strongly suggests that MR is induced by the spin-flip process due to inelastic cotunneling. From the *E/kT - T* curve, the energy needed for the spin-flip process is estimated to be ∼0.04 meV, which corresponds to ∼3.3% of the inelastic cotunneling energy. This work was partly supported by the Grant-in-Aids for Scientific Research, Special Coordination Programs by JST, FIRST Program, and JSPS Fellowship.

4:54PM T15.00009 Magnetism in Cr doped Si nanowires , MICHAEL SHAUGHNESSY, UC Davis/ LLNL, C.Y. FONG, UC Davis, LIN YANG, LLNL — We carry out first principles calculations of magnetic and electronic structures of single and multiple Cr atom dopants in Si nanowires. Both unsupported isolated wires and supported wires on Si 110 surfaces are studied. The relative stability and underlying physical picture of the ferromagnetic and antiferromagnetic configurations of the local moments on the Cr atoms are studied. Results are also presented for fully noncollinear calculations.

5:06PM T15.00010 GaMnAs-based Core-Shell Nanowires Grown by Molecular Beam Epitaxy[1] , R. PIMPINELLA, X. LIU, K. TIVAKORNSASITHORN, J.K. FURDYNA, M. DOBROWOLSKA, Department of Physics, University of Notre Dame, Notre Dame, IN 46556, USA, T. WOJTOWICZ, Institute of Physics, PAS, Al. Lotnikow 32/46, 02-668 Warsaw, Poland — We have successfully fabricated GaMnAs/GaAs core-shell nanowires (NWs) by molecular beam epitaxy (MBE), by first growing Au-assisted GaAs NWs, and subsequently depositing the GaMnAs shells on the Gaas NW side facets under low temperature conditions. Scanning electron microscopy (SEM) and scanning transmission electron microscopy (STEM) show that GaMnAs grows epitaxially on the GaAs NWs, retaining good crystalline quality. SQUID magnetometry shows that the shells obtained so far are ferromagnetic below 20 K. Studies by high resolution transmission electron microscopy (HRTEM) and energy-dispersive X-ray spectroscopy are planned for the future, in order to allow us to relate the observed magnetic properties of these one-dimensional magnetic wires to their chemical and structure profiles, in the hope of designing strategies for increasing the Curie temperature of the GaMnAs shells.

[1]Supported by NSF Grant DMR1005851.

5:18PM T15.00011 Magnetic Nanostructures in the Mn-Si system[1] , PETRA REINKE, KIRIL SIMOV, University of Virginia, CATHERINE JENKINS, Advanced Light Source, LBNL — Magnetic doping of group IV semiconductors is coveted for spintronics building blocks. Theoretical assessment of magnetism in Mn-Si is promising, but many of these structures have not been realized yet. Our STM study combines the study of Mn-nanostructure growth on Si(100)(2x1) with the investigation of the magnetic signature with X-ray magnetic circular dichroism and magnetometry. Mn self-assembles into monoatomic chains on the Si(100) surface. The mechanism of chain-formation and its competition with cluster growth will be presented. The nanostructures are capped with a 10 ML Si-or Ge- layer to form delta-doped layers, and protect the Mn-nanostructure. The Mn-chains are preserved, and the growth process for the cap was studied by STM and is now well understood. The magnetic signature is presented for nanowires and nanocluster structures below about 50 K, and a dense array of Mn-chains shows the highest saturation magnetization with 2-3 $\mu_B$ger Mn. The hysteresis loops indicate a superparamagnetic behavior. We will discuss the relative spin-orbital contributions and the directional dependence of the magnetic signature in relation to the Mn-nanostructure geometry.

[1]This work is supported by: NSF CHE-0828318 and DMR-0907234.

Wednesday, March 23, 2011 2:30PM - 5:18PM –

Session T16 DMP GMAG: Focus Session: Magnetic Nanostructures, Materials & Effects D173

2:30PM T16.00001 Magnetocaloric effect and refrigerant capacity in $Eu_8Ga_{16}Ge_{30}$ clathrates and $Eu_8Ga_{16}Ge_{30}$-EuO composites , H. SRIKANTH, A. CHATURVEDI, M.H. PHAN, S. STEFANOSKI, G.S. NOLAS, University of South Florida, V. FRANCO, University of Sevilla — $Eu_8Ga_{16}Ge_{30}$ clathrates are widely known for their excellent thermoelectric properties. Recently, we have discovered the giant magnetocaloric effect (MCE) in $Eu_8Ga_{16}Ge_{30}$ type-VIII clathrates. The tunable MCE and refrigerant capacity (RC) have also been achieved in $Eu_8Ga_{16}Ge_{30}$type-I clathrates by partial substitution of Eu with non-magnetic Sr. As an interesting host matrix the type-I clathrates are combined with EuO at different portions (80%/20%, 70%/30%, 65%/35%, 60%/40%, 40%/60%) for making novel composites with enhanced RC over a tunable temperature range (10-100K). We have achieved a very large RC of 794 J/kg at 5T over a 70K in the clathrate type I – EuO (40%/60%) composite, which is the largest value ever achieved among the existing materials for magnetic refrigeration around 70K. This composite is very attractive for magnetic refrigeration for nitrogen liquefaction. A new potential of using the type VIII clathrate – EuO composite (50%-50%) to produce refrigeration in two different temperature ranges has been proposed.

2:42PM T16.00002 Exploration of thermal conductivity, Seebeck coefficient, and Lorenz number deviations in Ni-Fe alloy films[1] , B.L. ZINK, A.D. AVERY, R. SULTAN, D. BASSETT, G. COTTERIL, University of Denver — As electronic and spintronic systems continue to shrink, exploration of the fundamental physics affecting thermal transport in prospective materials becomes increasingly essential. For example, the potential use of spin-torque driven domain wall motion in ferromagnetic nanowires as a memory element requires application of large current densities to these tiny structures. The resulting heating could have both helpful and harmful effects, and is in general not yet well-understood. This is partly due to a gap in the fundamental knowledge of thermal properties of nanoscale systems that is due to the challenging nature of the necessary measurements. We have recently developed a micromachined thermal isolation platform that allows measurement of thermal conductivity, electrical conductivity, and thermopower (or Seebeck effect) in thin film systems. In this talk we present our recent data on thermal conductivity, resistivity, and Seebeck coefficient, for Ni-Fe alloy films with thicknesses varying from 25-100 nm. We compare our results to the predictions of the Wiedemann-Franz law and discuss variations represented by deviations from the Sommerfeld value of the Lorenz number, and conclude with our plans to extend the technique to yet smaller structures.

[1]We thank the NRI-WIN and the NSF CAREER program for support

2:54PM T16.00003 Thermodynamics and Magnetocaloric properties of Fe/Cr Superlattices[1]

T. MUKHERJEE, S. MICHALSKI, R. SKOMSKI, D.J. SELLMYER, CH. BINEK, Department of Physics & Astronomy and the Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE, 68588-0111 — We explore MC properties of tailored Fe/Cr superlattices involving simple 3d metals. Our multilayers are fabricated by pulsed laser deposition with emphasis on maximizing magnetic entropy changes near room temperature. We use nanostructuring[2] to tailor magnetic interaction and exploit geometrical confinement in order to fit the FM to paramagnetic transition temperature of the FM constituent films. In concert this leads to an optimized global metamagnetic transition maximizing the isothermal entropy change. Thermodynamic and MC properties of such Fe/Cr superlattices are studied with the help of SQUID magnetometry. Entropy changes are deduced via the Maxwell relation in single phase regions and via the Clausis-Clapeyron relations at first order metamagnetic transitions, X-ray diffraction and X-ray reflectivity are used to correlate structural data with the magnetic properties.

[1]Financial support by NRI, and NSF through EPSCoR, Career DMR-0547887, and MRSEC Grant No. 0820521.
[2]Phys. Rev. B **79**, 144406 (2009).

3:06PM T16.00004 Magnetocaloric effect in heterostructures of $Ni_xCu_{(1-x)}$ alloys[1]

C.A. BAUER, P.B. JAYATHILAKA, R.V. RUPANI, D.D. BELYEA, CASEY W. MILLER, University of South Florida — We used 99.9% compound targets to co-sputter $Ni_xCu_{(1-x)}$ thin film multilayers composed of sub-layers with differing alloying compositions on silicon and oxidized silicon substrates. Each system had a Ta underlayer and capping layer. XRD was used to determine structural properties, showing a (111) preferred orientation for all $Ni_xCu_{(1-x)}$ layers. In-Plane XRD was used to check polycrystallinity. Energy-dispersive X-ray scattering is used to determine the relative concentrations of Nickel and Copper, with XRD data corroborating the EDX results from Vegard's law. The magnetic properties of the systems are characterized and the magnetic entropies are calculated near the relevant critical temperature.

[1]Supported by NSF-CAREER.

3:18PM T16.00005 Thermal conductivity behaviour of magnetic fluids[1]

R.A. MEDINA-ESQUIVEL, J. MENDEZ-GAMBOA, J. TAPIA, FIUADY, J.J. ALVARADO-GIL, CINVESTAV-Merida — We study the thermal conductivity of five kinds of Magnetic Fluids (MFs) by varying the magnetic material volume fraction and the direction and intensity of an homogeneous magnetic field: The studied MFs are: Magnetorheological fluids (MRF), carbon coated and uncoated Fe nanofluids (CcFeNF, FeNF), ferrofluis (FF); and two kind of composed fluids; ferrofluids loaded with carbon nanotubes (FFCNTs) and ferrofluids loaded with carbon nanofibers (FFCNFs). MRF and FFCNFs fluids increase its thermal transport along the field direction; the thermal enhancement in MRF was dramatically overtaken by the FFCNFs, but in contrast; the rest of the fluids did not present thermal conductivity enhancement under the field. Theoretical models show that thermal resistance at the nanoscale level presents a very important role in the thermal transport among linked particles, this is the reason why FFCNTs, FF, FeNF, and CcFeNF did not present an increase in its thermal conductivity under the action of the magnetic field, although its chain-like structuring. We believe that these experimental finding may have significant application in the area of thermally tailored materials.

[1]Ruben Medina wants to acknowledge the continuous help and support received throughout this project from PROMEP 2010 proyect.

3:30PM T16.00006 Large Seebeck coefficient in frustrated doped Mott insulators

LOUIS-FRANÇOIS ARSENAULT, Université de Sherbrooke, B. SRIRAM SHASTRY, University of California, Santa Cruz, PATRICK SÉMON, ANDRÉ-MARIE TREMBLAY, Université de Sherbrooke — Since calculations based on the standard Kubo formula have proven extremely difficult for electric and thermal transport, Shastry and co-workers [1] suggested two novel approximate ways to obtain the thermopower (S) in interacting systems. One method is based on the high-frequency limit. The other, based on ideas of Kelvin, is purely thermodynamical. With these we study the Hubbard model on a 3d FCC lattice, a frustrated lattice. The high dimensionality of the problem justifies the use of dynamical mean field theory (DMFT). CTQMC in the hybridization expansion and the fast IPT are the impurity solver. The Seebeck coefficient is obtained as a function of doping and temperature for different U. Within DMFT, vertex corrections vanish for transports coefficients, hence the bubble suffices. This enables us to further assess how both approximate methods compare with each other and with the DC Kubo approach. At low T, results can be interpreted in terms of effective Fermi temperatures and carrier number.

[1] B.S. Shastry, Rep. Prog. Phys. 72, 016501 (2009)

3:42PM T16.00007 Spin dynamics simulations for a nanoscale Heisenberg antiferromagnetic film[1]

ZHUOFEI HOU, DAVID LANDAU, Center for Simulational Physics, The University of Georgia, G. MALCOLM STOCKS, Center for Defect Physics, Oak Ridge National Laboratory — Thermoinduced magnetization(TiM) is a novel response predicted to occur in nanoscale antiferromagnetic (AF) materials. Extensive Monte Carlo simulations[2] have shown that TiM is an intrinsic property of the AF classical Heisenberg model. To obtain a fundamental understanding of TiM, spin dynamics (SD) simulations are performed to study the spin wave behavior, which seems to be the cause of TiM. A classical Heisenberg model with an AF nearest-neighbor exchange interaction and uniaxial single-site anisotropy is studied. Simple-cubic lattices with two free-surfaces and periodic boundaries parallel to the surfaces are used. We applied fast SD algorithms with 4th-order Suzuki-Trotter decompositions of the exponential operator. Discrete spin wave modes due to spin wave confinement[3] are found in transverse $S(q,\omega)$ in the perpendicular direction to free surfaces.

[1]Research supported by UT-Battelle, and Office of Science, DOE.
[2]G. Brown, A. Janotti, M. Eisenbach, and G. M. Stocks, Phys.Rev.B **72**, 140405(2005)
[3]*Spin Wave Confinement*, edited by S. O Demokritov (Pan Stanford Publishing, Singapore, 2008)

3:54PM T16.00008 Thermomagnonic spin transfer in textured magnets[1]

ALEXEY A. KOVALEV, YAROSLAV TSERKOVNYAK — We study interplay between the spin-energy transport and magnetization dynamics in ferromagnetic insulators with magnetic textures. With the help of the Onsager reciprocity principle we construct a phenomenological theory capable of describing various thermomagnonic effects. Motion of domain walls by thermal gradients and generation of heat flows by magnetization dynamics are suggested. By estimating the kinetic coefficients (such as β like viscous coupling) for realistic materials (e.g. Yttrium iron garnet), we analyze the feasibility of mentioned effects for energy related applications.

[1]Supported in part by the Alfred P. Sloan Foundation, DARPA and NSF under Grant No. DMR-0840965.

4:06PM T16.00009 Rotating magnon wavepackets in ferromagnets and thermal Hall effect , RYO MATSUMOTO, Department of Physics, Tokyo Institute of Technology, SHUICHI MURAKAMI, Department of Physics, Tokyo Institute of Technology, PRESTO, Japan Science and Technology Agency — We theoretically construct the semiclassical equation of motion of the magnon wavepacket in an insulating ferromagnets, in analogy with the electron systems. We find that the magnon wave packet has nonzero angular momentum, which consists of two parts: the self-rotational motion and the revolving motion (edge current). We show that these are expressed in terms of the Berry curvature in **k**-space, i.e., these arise from the magnon band structure. Furthermore, we find that the thermal Hall effect of the magnon is totally due to the magnon edge current, and present an intuitive picture of the thermal Hall effect. We also construct the linear response theory for the thermal Hall effect, and compare the results with the previous works with an example of $Lu_2V_2O_7$.

4:18PM T16.00010 Magnetocaloric Properties of Thin Film Heterostructures[1] , H. KIRBY, C. BAUER, University of South Florida, Department of Physics, B.J. KIRBY, J. LAU, NIST, C.W. MILLER, University of South Florida, Department of Physics — In an effort to understand the impact of nanostructuring on the magnetocaloric (MC) effect, we have studied gadolinium in MgO/W(50 Å)/[Gd(400 Å)/W(50 Å)]$_8$ heterostructures [Miller et al., J. Appl. Phys. 107, 09A903 (2010)]. The entropy change peaks at a temperature of 284 K with a value of 3.4 J/kg K for a 0–30 kOe field change. Polarized neutron reflectometry was used to determine the depth profile of the magnetic moment per Gd atom, m_{Gd} in a Gd/W multilayer. Our results suggest that creating materials with Gd-ferromagnet interfaces may increase the m_{Gd}, leading to enhanced MC properties. Therefore SiOx/Fe(50 Å)/Gd(300 Å)/Fe(50 Å) heterostructures have been investigated.

[1]This work was supported by AFOSR-YIP. Use of the Center for Nanoscale Materials was supported by the U. S. Department of Energy, O?ce of Science, O?ce of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

4:30PM T16.00011 Antiferromagnetism in $BaF_2/Fe_xNi_{1-x}F_2$ bilayers , FELIO PEREZ, TRENT JOHNSON, DAVID LEDERMAN, West Virginia University, MULTIFUNCTIONAL MATERIALS LABORATORY TEAM — A series of crystalline BaF_2/epitaxial (110) $Fe_xNi_{1-x}F_2$ samples were deposited on MgF_2 (110) via molecular beam epitaxy. The Fe concentration x was determined from x-ray diffraction measurements of the [110] lattice parameter. The actual thickness of each layer and the roughness of each interface were determined by fitting x-ray reflectivity data. The antiferromagnetic ordering of samples with x = 0.04, 0.27, 0.40, 0.46, 0.50, and 0.85 were studied and compared with BaF_2/NiF_2 (x=0) and BaF_2/FeF_2 (x=1) bilayers, via standard magnetometry measurements. A significant enhancement of the Néel temperature in alloys and evidence of spontaneous magnetization along c-axis were found.

4:42PM T16.00012 $MnCu_4In$: a new high temperature ferromagnet , ALESSIA PROVINO, Department of Chemistry, University of Genova (Italy), DURGA PAUDYAL, Ames Laboratory, Ames (Iowa), SUDESH K. DHAR, CMP & MS Dept, TIFR, Mumbai (India), MARIA LUISA FORNASINI, PIETRO MANFRINETTI, Department of Chemistry, University of Genova (Italy), VITALIJ K. PECHARSKY, KARL A. GSCHNEIDNER JR., Ames Laboratory, Ames (Iowa), THE AMES LABORATORY, US DEPT OF ENERGY, IOWA STATE UNIVERSITY, AMES, IA 50011, USA COLLABORATION, DEPT OF CHEMISTRY, UNIVERSITY OF GENOA, VIA DODECANESO 31, 16146 GENOA, ITALY COLLABORATION, CMP & MS DEPT, TIFR, HOMI BHABHA ROAD, MUMBAI 400 005, INDIA COLLABORATION, CNR-SPIN, CORSO PERRONE 24, 16152 GENOA, ITALY COLLABORATION — The new intermetallic compound $MnCu_4In$ has been synthesized and investigated. The crystal structure, studied by single crystal and powder X-ray diffractions, shows that the compound crystallizes into its own hexagonal prototype ($hP12$-$P6_3mc$) derived from the $MgZn_2$-type. The measured magnetic and physical properties indicate that, in contrast to the antiferromagnetic $MnCu_4Sn$ ($MgCu_4Sn$-type), $MnCu_4In$ is a high temperature ferromagnet with T_C = 540°C. In order to understand the physics involved, the first principles calculations have been performed and compared with the $MnCu_2Al$-type $MnCu_2In$(Sn) phases and the rare earth representatives $GdCu_4In$ and $GdCu_2In$. Work partially supported by the US DOE, Division of Materials Science and Engineering (Office of Basic Energy Sciences).

4:54PM T16.00013 The layer-by-layer growth of ferromagnetic τ phase MnAl thin films by Bias Target Ion Beam[1] , YISHEN CUI, WENJING YIN, JIWEI LU, STUART WOLF, Univ of Virginia — It is well known that the metastable τ phase of MnAl has a L10 structure (chemical ordering along [001] directions) and is the only ferromagnetic phase of this binary intermetallic. In our study, alternating Al/Mn quasi-monolayer deposition was developed using a novel Bias Target Ion Beam deposition technique, that enabled precise control of the microstructural growth. We have obtained epitaxial τ phase MnAl thin films ($\sim$10 nm thick) on single crystal MgO substrates with improved saturation magnetization and anisotropy in comparison with co-sputtered ultra thin films. We will discuss the microstructure and magnetic behaviors of MnAl films in detail.

[1]We acknowledge the support from DARPA.

5:06PM T16.00014 Field induced first order phase transition in the antiferromagnet Yb_3Pt_4[1] , L.S. WU, Stony Brook University, Y. JANSSEN, M.S. KIM, Brookhaven National Lab, C. MARQUES, Stony Brook University & Brookhaven National Lab, K.S. PARK, M. BENNETT, Brookhaven National Lab, M.C. ARONSON, Stony Brook University & Brookhaven National Lab, S.X. CHI, J.W. LYNN, NIST Center for Neutron Research — Yb_3Pt_4 is an antiferromagnet that orders at T_N=2.4K. Magnetic fields B suppress T_N, and the B-T phase line T_N(B) terminates almost vertically at T=0, B_C=2.0 T. Specific heat measurements find a mean-field transition at T_N(B), and the magnetocaloric effect shows that the antiferromagnetic transition is continuous at all fields, with no associated latent heat. However, neutron diffraction measurements performed for B$\sim B_C$ find that a distinct step in the magnetization ΔM occurs near the transition, with a magnitude that increases for T<1 K. The field dependent magnetization M(B) similarly has a metamagnetic-like step at T_N(B) below 1 K, accompanied by a sharp peak in the susceptibility whose magnitude increases but does not diverge as T$\rightarrow$0. We argue that a nonzero magnetization step ΔM is required to give ΔS=0 for T=0, since the vertical phase line at T=0 implies dT_N/dB=-$\Delta M/\Delta S \rightarrow -\infty$. We argue that T_N (B) terminates at B_C in a T=0 first order transition.

[1]Research of Stony Brook is supported by NSF.

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T17 GMAG DMP: Focus Session: Magnetic Oxide Thin Films - Manganite Thin Films

2:30PM T17.00001 Tunable Percolative Transport in Manganite Thin Films using Strain and Exchange Fields[1]

, T. ZAC WARD, Oak Ridge National Laboratory — Strongly correlated electronic systems are often sensitively dependent on spin-charge-orbital-lattice interactions. We will discuss recent work on manganites that have led to some fascinating new discoveries on the role of these interactions in driving electronic phase separation in strongly correlated systems. We demonstrate that substrate induced anisotropic strain effects and surface exchange coupled magnetic nanodots can be used to preferentially seed electronic domains. These effects have led to a new understanding of how order parameter tuning can lead to highly controllable electronic and magnetic properties. We find that even strain frustrated ultrathin manganite films—where no metal-insulator transition is present—can be selectively tuned with the application of magnetic nanodots at the film surface. Both the magnetoresistance and the metal-insulator transition temperature can be tuned through dot density and dimension. The strain frustrated film's metal-insulator transition and magnetoresistivity can be driven to bulk levels. We expect these results to be applicable in many other systems in which order parameters are tightly correlated.

[1]Supported by the US DOE Office of Basic Energy Sciences.

3:06PM T17.00002 STM study on the electronic phase separation of manganites[1]

, MIN GAO, Oak Ridge National Laboratory, USA; Institute of Physics, Chinese Academy of Sciences, China, ZHENG GAI, PAUL C. SNIJDERS, HANGWEN GUO, THOMAS Z. WARD, Oak Ridge National Laboratory, USA, H.-J. GAO, Institute of Physics, Chinese Academy of Sciences, China, JIAN SHEN, University of Tennessee, USA — Phase separation is a key problem in understanding the exotic properties of complex oxide materials. Combing pulsed laser deposition with in situ scanning tunneling microscopy, we can investigate the electronic phase separation of$La_{5/8-x}Pr_xCa_{3/8}M\ nO_3$. Current imaging tunneling spectroscopy reveals both local domain contrast and global conductivity evolving when the temperature crosses over the metal-insulator transition temperature. The domain size can be several hundred nanometers. This result confirms other experimental results and shows that the surface electronic properties of complex oxide materials can represent their bulk properties.

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

3:18PM T17.00003 Nonlinear optical imaging of antiferromagnetic domains in orbital-ordered $Pr_{0.5}Sr_{0.5}MnO_3$ thin films

, KENJIRO MIYANO, NAOKI OGAWA, Univ of Tokyo, CREST, YASUSHI OGIMOTO, Univ of Tokyo, CREST, Fuji Electric HD — Perovskite manganites develop various ordering patterns of charge, orbital, and spin, whose geometrical correlation brings out a new order, e.g., electronic polarization. As an example in pseudo-cubic systems, the CE-type charge/orbital order (CO/OO) was predicted to be multiferroic. With the use of nonlinear optics, we show that $Pr_{0.5}Sr_{0.5}MnO_3$ thin films exhibit symmetry breaking in the OO phase without CO. Ultrathin films prepared on LSAT(110) substrates reproduce bulk-like properties, showing successive phase transitions from paramagnetic metal, to ferromagnetic metal, and finally to A-type antiferromagnetic (AF) insulator upon cooling. Below T_{OO}=T_N, we detect SHG from these films and visualize the formation of AF domains with the size of several μm, which is much larger than that of phase-separated manganites. With careful examination of the magnetic point group, we can ascribe the broken symmetry to the AF spin order under the monoclinic lattice distortion concomitant with the OO, which also manifests the direction of the AF vector.

3:30PM T17.00004 Novel Resistive Switching Behavior in Phase Separated Manganites[1]

, HANGWEN GUO, The University of Tennessee, Knoxville & Oak Ridge National Laboratory, T. ZAC WARD, DALI SUN, PAUL C. SNIJDERS, Oak Ridge National Laboratory, ZHENG GAI, Oak Ridge National Laboratory & Center for Nanophase Materials Science, JIAN SHEN, The University of Tennessee, Knoxville & Fudan University — Electronic phase separation plays a key role in many novel phenomena in complex materials. Manganites are a prime example of this class of materials and have recently come under increase scrutiny for possible application in resistive random-access memory (RRAM) technology. Here, we will discuss our recent work on spatially confined La5/8-xPrxCa3/8MnO3. We have discovered that it is possible to drive single electronic domain formation/annihilation through electric field pulsing. By measuring the I-V curve, we find such resistive switching is different from normal RRAM mechanisms in manganites and is closely related to the nature of electronic phase separation. These findings open these systems to a new understanding of the nature of electronic phase separation and begin the development of manganites for future applications in RRAM devices.

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

3:42PM T17.00005 Mesoscopic orientation-ordered percolating network in a strained manganite thin film

, KEJI LAI, Stanford University — Many unusual behaviors in complex oxides are deeply associated with the spontaneous emergence of microscopic phase separation. Recent studies on these strongly correlated materials have shown that multiple states can coexist near certain phase boundaries. In this work, a cryogenic microwave impedance microscope [1] is implemented to investigate the microscopic origin of the colossal magnetoresistance effect in manganite thin films. In a strained $Nd_{0.5}Sr_{0.5}MnO_3$ thin film grown on (110) $SrTiO_3$ surface, the filamentary ferromagnetic metallic domains emergent from the antiferromagnetic charge/orbital-ordered insulating background as increasing magnetic fields align preferentially along certain crystal axes of the substrate [2]. Such an orientation ordering is missing in a relaxed sample with partial loss of the epitaxial coherency. The mesoscopic glassy orders with a period of 100nm indicate that the substrate-induced anisotropic strain rather than the Coulomb interaction plays the dominant role in the phase separation. The microwave images also revealed drastically different domain structures between the zero-field-cool and field-cool processes, consistent with the macroscopic transport measurements in both bulk and thin film materials.

[1] W. Kundhikanjana *et al.*, arXiv 1010.1509.
[2] K. Lai *et al.*, *Science* **329**, 190 (2010).

4:18PM T17.00006 Room Temperature Resistive Switching in Manganite Thin Films

, LUIS PEÑA, LUIS GARZON, ZORIÇA KONSTANTINOVIC, LLUIS BALCELLS, CARMEN OCAL, BENJAMIN MARTINEZ, ICMAB - CSIC, INSTITUTO DE CIENCIA DE MATERIALES DE BARCELONA. CSIC TEAM — Resistive switching (RS), i.e. the switching between two distinct resistive states electrically controlled, is currently a subject of major interest because of its very promising properties for the implementation of data storage devices. In this work we report on the reversible transitions from low resistive (LR) to high resistivity (HR) states in high quality manganite thin films (LSMO) prepared by RF sputtering on top of (001) oriented STO substrates. The transitions between the LR and HR states are induced by the application of a bias voltage by means of the conducting tip of a scanning force microscope [1]. The experimental setup is arranged in order to avoid parasitic interfacial phenomena (e.g., metal diffusion) or electrode interconnections (e.g., filamentary formation). These RS experiments have been performed on few microns wide patterned LSMO structures. The magnetotransport properties and thermal stability of these LR and HR states are investigated in order to gain a deeper insight into the nature of the structural/electronic modifications generated by the application of high electric field by means of the AFM tip on the manganite film.

[1] C. Moreno et al. *Nanoletters 10, 3828 (2010)*

4:30PM T17.00007 Magnetic and Transport Properties of Heterostructured Films of Prussian Blue Analogues and Manganites , P.A. QUINTERO, H. JEEN, E.S. KNOWLES, A. BISWAS, M.W. MEISEL, Dept. Physics and NHMFL, Univ. Florida, M.J. ANDRUS, D.R. TALHAM, Dept. Chemistry, Univ. Florida — The magnetic and transport properties of heterostructured films consisting of Prussian blue analogues, $A_j M'_k[M(CN)_6]_\ell \cdot n H_2O$ (M′M-PBA), where A is an alkali ion and M′,M are transition metals, and manganites have been studied. Specifically, NiCr-PBA and CoFe-PBA films[1] of ∼100 nm thickness have been deposited on perovskite $(La_{1-y}Pr_y)_{0.67}Ca_{0.33}MnO_3$ (LPCMO) manganese films[2] of ∼30 nm thickness. The effect of the ferromagnetic NiCr-PBA, $T_c \sim 70$ K, and the photo-controllable ferrimagnetic CoFe-PBA, $T_c \sim 20$ K, on the I-V properties of the LPCMO will be reported, where special attention will be given to the changes of the transition temperatures of the ferromagnetic metallic (FMM) and the charge-ordered insulating (COI) phases in the LPCMO substrate.
* Supported by NSF DMR-0701400 (MWM), DMR-0804452 (AB), DMR-1005581 (DRT), DMR-0654118 (NHMFL), and by scholarship from the Organization of American States (PAQ).

[1]D.M. Pajerowski *et al.*, J. Am. Chem. Soc. **132** (2010) 4058.
[2]T. Dhakal, J. Tosado, A. Biswas, Phys. Rev. B **75** (2007) 092404.

4:42PM T17.00008 Interfacial phase separation in $La_{2/3}(Sr/Ca)_{1/3}MnO_3$ thin films with different complex oxide capping layers , SERGIO VALENCIA, Helmholtz-Zentrum-Berlin, ZORIÇA KONSTANTINOVIC, ICMAB - CSIC, SCHMITZ DETLEF, Helmholtz-Zentrum-Berlin, LLUIS BALCELLS, BENJAMIN MARTINEZ, ICMAB - CSIC, INSITUT FOR COMPLEX MAGNETIC MATERIALS, MI-1 (BESSY) TEAM, INSTITUTO DE CIENCIA DE MATERIALES DE BARCELONA - CSIC TEAM — Interfacial effects in sputtered manganite thin films with different capping layers (MgO, LAO, STO, NGO and Au) have been investigated. The interfaces have been chemically and magnetically characterized by means of local probes such as X-ray absorption spectroscopy (XAS) and X-ray magnetic circular (XMCD) and linear dichroism (XLD). Total electron yield detection at the Mn L-edge guarantees that the spectroscopic information originates from those regions closer to the film/capping interface. A complex phase separated scenario at the interface arises from the spectroscopic data. XAS shows departure of the Mn valence from bulk like values in case of STO and Au capping (Mn2+ presence) and in case of MgO and NGO (Mn4+ increase). XMCD shows concomitant depressed interface magnetization suggesting coexistence of ferromagnetic and non-magnetic phases. Finally XLD proves the presence of an antiferromagnetic (AFM) and orbital ordered (OO) phase.

4:54PM T17.00009 Photoinduced effects in ferromagnetic state of manganites , VERA SMOLYANINOVA, GRACE YONG, RAJESWARI KOLAGANI, Department of Physics, Astronomy and Geosciences, Towson University, Towson, MD 21252, AMLAN BISWAS, Department of Physics, University of Florida, Gainesville, Florida 32611, KILHWAN WANG, Department of Physics, Astronomy and Geosciences, Towson University, Towson, MD 21252 — Rear-earth manganese oxides have a rich phase diagram. Transitions between different magnetic, electronic and structural states can be induced by application of external fields. Light-induced destruction of the charge ordering in some compositions of manganites, which results in significant increase of conductivity, is a well known example of such transition. Significant change in conductivity of these materials makes them attractive for photonic and opto-electronic device applications. We report a study of photoinduced properties of manganites in ferromagnetic metallic state. Since light penetration depth in these materials is small, thin films of manganites were used in this study. Photoinduced resistivity changes in these materials will be reported. Photoinduced effects in compositions with different temperatures of metal-insulator transition will be discussed. This work is supported by the NSF grant DMR-0348939.

5:06PM T17.00010 Bulk-like electronic structure at the surface of epitaxial $La_{1-x}Sr_xMnO_3$ films , ERIC MONKMAN, CAROLINA ADAMO, DANIEL SHAI, DAWEI SHEN, JOHN HARTER, Cornell University, ILYA ELFIMOV, University of British Columbia, DARRELL SCHLOM, KYLE SHEN, Cornell University — We present direct measurements of the electronic structure of $La_{1-x}Sr_xMnO_3$ (LSMO) using a combined molecular beam epitaxy and angle-resolved photoelectron spectroscopy system. Our results allow for the first comparison between theory and experimental results over the entire Fermi surface in the ferromagnetic-metallic phase. We observe both of the predicted Fermi surface sheets, and find that the evolution of the Fermi surface shape with doping is consistent with a rigid-band shifting of the chemical potential. Measurements in the antiferromagnetic phase at x $>$ 0.5 allow us to determine the changes in the low energy electronic structure linked to the magnetic phase transition. The ability of this surface sensitive technique to probe the bulk electronic structure of LSMO limits the possible depth of a surface dead layer. This conclusion is supported by density functional theory calculations for LSMO slabs, which indicate that the polarity of the (001) surface is efficiently screened within ∼1 unit cell.

5:18PM T17.00011 Hall effect on strain-released $La_{0.67}Ca_{0.33}MnO_3$ thin films , LIUQI YU, XIAOHANG ZHANG, S. VON MOLNÁR, P. XIONG, Florida State University, LINGFEI WANG, W.B. WU, University of Science and Technology of China — It has been demonstrated that releasing the in-plane anisotropic strain in thin films of $La_{0.67}Ca_{0.33}MnO_3$ grown on orthorhombic $NdGaO_3$ (001) substrates can induce a charge ordering state below the Curie temperature.[1] Three LCMO films on NGO, (PLD at 735^{o}C and 45 Pa O_2 pressure, 45 nm thick) were annealed at 780^{o}C in flowing O_2 for 1, 10 and 20 hours to increase degrees of strain relaxation. Hall measurements were performed. In all three samples, the Hall resistivity takes on two distinct slopes in the paramagnetic phase: a negative slope at low fields, which varies with temperature, and a temperature-independent positive slope at high fields. Notably, the switching field for the Hall slope decreases linearly with temperature and extrapolates to the paramagnetic Curie temperatures of the samples. The observation is similar to the behavior of the nonlinear Hall effect in EuB_6 and suggests that the switches occur at a *constant critical magnetization*.[2] In strain-released samples, peaks in the Hall resistivity emerge near T_C and become more pronounced with decreasing temperature. The origins and implications of these observations will be discussed. Work supported in part by NSF DMR-0908625. [1]Z. Huang et al., JAP 105, 113919 (2009) [2]X. Zhang et al., PRL **103**, 106602 (2009)

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T18 GMAG DMP: Focus Session: Low D/Frustrated Magnetism - Molecular Magnets II D172

2:30PM T18.00001 Recent developments in Molecular Magnetism , EUGENIO CORONADO, Instituto de Ciencia Molecular (ICMol). Universidad de Valencia (Spain) — Two hot topics in this area are highlighted namely the design of new multifunctional magnetic materials, and the study of mononuclear single-molecule magnets. In the first topic I will present the attempts to design materials exhibiting coexistence of superconductivity and magnetism using a chemical approach [1]. In the second topic I will show that single-molecule magnets based on lanthanides provides the opportunity to tune quantum tunneling effects and to use these systems as qubits in quantum computing [2]. Finally, I will highlight the relevance of these magnetic systems in molecular spintronics.

[1] E. Coronado, C. Martí-Gastaldo, E. Navarro-Moratalla, A. Ribera, S. J. Blundell, P. J. Baker Nature Chem. 2010, 2, 1031.
[2] F. Luis, M. J. Martínez-Pérez, O. Montero, E. Coronado, S. Cardona-Serra, C. Martí-Gastaldo, J.M. Clemente-Juan, J. Sesé, D. Drung, T. Schurig, Phys. Rev. B 2010, 82, 060403 R.

3:06PM T18.00002 Random Exchange Antiferromagnetic Heisenberg Chains[1] , CHRISTOPHER LANDEE, FAN XIAO, BRIAN WELLS, BRIAN KOOPMAN, MARK TURNBULL, Department of Physics and Carlson School of Chemistry, Clark University, MATTHIAS THEDE, ANDREY ZHELUDEV, Laboratorium für Festkörperphysik, ETH, Zürich, Switzerland — Copper *bis*pyridine dichloride (CPC) and copper *bis*pyridine dibromide (CPB) are isostructural Heisenberg S = $1/2$ linear chains in which the copper atoms are bridged by two halides with the pyridine molecules in the axial sites. The exchange strengths are 27 K (CPC) and 45 K (CPB). We have prepared mixed halide versions $Cu(py)_2[Cl_{1-x}Br_x]_2$ for values of x from 0 to 1. We will report on the effect of the exchange randomness on the susceptibilities and Néel temperatures of this family of compounds, as determined by dc-magnetometry, muon spin relaxation, and low-temperature calorimetry.

[1]Partially supported by the Swiss National Science Foundation, under Project 6 of MANEP.

3:18PM T18.00003 Magnetic dilution in the cadmium-doped spin ladder compound $Cd_xCu_{1-x}(quinoxaline)Br_2$, BRIAN KEITH, CHRIS LANDEE, MARK TURNBULL, Clark University — Both $Cu(quinoxaline)(Br_2)$ and $Cu(quinoxaline)(Cl_2)$ are examples of molecule-based magnets where the CuX_4 dimers are linked into ladders by quinoxaline molecules, where X is either Cl or Br. The rung exchange occurs through the bridging halides while the rail exchange occurs through the quinoxaline rings. Introducing random rung interactions into the system $[Cu(quinoxaline)(Br_2)_{1-x}(Cl_2)_x]$ has caused the spin gap to close, in contrast with the gapped pure spin ladder parents. Crystal growth of non-magnetic-doped molecular magnets, $Cd_xCu_{1-x}(2,3-dimethylpyrazine)Br_2$, have been performed for several values of the nominal conentration, x, and have been confirmed. The magnetizations and susceptibilities of the magnetically diluted ladder assemblage are presented along with a comparison of the effects of dilution from the pure case (x=0).

3:30PM T18.00004 Electron and Spin Transport in Mn_{12} Single Molecule Magnets Bridging Gold Electrodes: How to Determine the Easy Axis Orientation Experimentally[1] , FATEMEH ROSTAMZADEH RENANI, GEORGE KIRCZENOW, Simon Fraser University, Burnaby, Canada — We present a tight-binding theory of Mn_{12} single molecule magnets thiol-bonded to gold electrodes. The model includes both the spatial and spin aspects of the electronic states. Spin-orbit coupling is included explicitly in the Hamiltonian and magnetic anisotropy values in agreement with experiment are obtained. We demonstrate that Mn_{12} single molecule magnets strongly coupled to gold electrodes should exhibit strong spin filtering under appropriate conditions. In experiments, the orientation of the molecule's easy axis relative to leads is not controllable and it has not been feasible to measure it. Our calculations reveal the possibility of determining the easy axis orientation experimentally by means of current measurements: In the molecular junction with the easy axis parallel to leads the current is predicted to be at least two orders of magnitude larger than if the easy axis is perpendicular to the leads, for molecules thiol-bonded to the leads with similar gold-sulfur distances in the two cases.

[1]This work was supported by CIFAR and NSERC.

3:42PM T18.00005 Hall magnetometry measurements of the susceptibility of variants of Mn_{12}-ac[1] , PRADEEP SUBEDI, A.D. KENT, NYU, B. WEN, M.P. SARACHIK, CCNY, Y. YESHURUN, Bar-Illan, A.J. MILLIS, Columbia U, S. MUKHERJEE, G. CHRISTOU, UF-Gainsville — The temperature dependence of the inverse magnetic susceptibility of both Mn_{12}-ac and Mn_{12}-ac-MeOH is found to give finite temperature intercepts, indicating a ferromagnetic phase at low temperature [1, 2]. A magnetic field applied transverse to the Ising axis suppresses the Curie temperature, T_{CW}, to a T = 0 quantum critical point. However, the decrease of T_{CW} with transverse field, $H_\perp$, in Mn_{12}-ac does not agree with mean field calculations performed with a spin Hamiltonian that includes dipolar interactions between molecules and $H_\perp$ effects. We attribute the pronounced suppression of T_{CW} of Mn_{12}-ac to the effect of random fields arising from a distribution of molecular easy axis tilts due to ligand disorder [1]. Mn_{12}-ac-MeOH is of interest in this regard because it appears to have no ligand disorder. We discuss these experiments as well as ongoing studies of Mn_{12}-toluate, a faster relaxing variant of Mn_{12}, which has a lower effective anisotropy barrier that permits the study of the susceptibility in larger $H_\perp$ at very low temperature.
[1] Wen et.al PRB **82**, 014406 (2010)
[2] Li et.al PRB **82**, 174405 (2010)

[1]Supported by NSF-DMR-0506946,DMR-0451605,DMR-0705847,CHE-0910472, ARO W911NF-08-1-0364 and German Research Foundation

3:54PM T18.00006 Local magnetic susceptibility study of long-range order in Mn_{12}-ac[1] , BO WEN, CCNY, P. SUBEDI, NYU, Y. YESHURUN, Bar-Ilan U., Israel, M.P. SARACHIK, CCNY, A.D. KENT, NYU, A.J. MILLIS, Columbia U., S. MUKHERJEE, G. CHRISTOU, U. of Florida — The magnetic susceptibility of single crystals of Mn_{12}-ac obeys a Curie-Weiss law, indicating a transition to a ferromagnetic phase below 1 K [1]. Measurements by Hall magnetometry have yielded different temperature intercepts ranging from 0.4 K to 0.9 K. Moreover, these values differ from those obtained for the same crystals in a SQUID-based MPMS. We have proposed two possible origins: (1) the effect of crystal's aspect ratio, reported in [2]; (2) the possibility that the local ordering temperature differs from the global average value. Here we report an ongoing study of the longitudinal magnetic susceptibility at different locations of a single crystal, performed on a Hall sensor array in both zero and finite transverse magnetic field. Preliminary results yield temperature intercepts that are lower near the end of the crystal than in the middle.

[1] Bo WEN et al., PRB 82, 014406 (2010).
[2] Shiqi LI et al., PRB 82, 174405 (2010).

[1]Funded by NSF-DMR-0506946, ARO W911NF-08-1-0364, NSF-DMR-0705847, NSF-DMR-0451605, NSF-CHE-0910472 and Deutsche Forschungsgemeinschaft

4:06PM T18.00007 Magneto-structural study of M(TCNE)(NCMe)]X molecule-based magnets[1] , KONSTANTIN POKHODNYA, CHRIS OLSON, CHRIS HETH, North Dakota State University, JOHN SCHLUETER, GREGORY HALDER, Argonne National Laboratory — In M^{II}(TCNE)$(NCMe)_2$]X (M=Fe, Mn, Ni; TCNE = tetracyanoethylene; X = monovalent anion) the magnetic properties can be tuned by systematic altering of transition metal from Mn to Ni, as well as adjusting the inter-plane distances via changing the anion volume (e.g., PF_6, AsF_6 and SbF_6). The magnetic properties of the molecule-based magnets are highly responsive to structural perturbations. For the series of M[TCNE]X magnets the synchrotron-based powder diffraction experiments in combination with magnetic susceptibility, all under hydrostatic pressure, were performed revealing the correlations between metal-ligand bonding and magnetic exchange and allowing the structure-magnetic property correlations to be established. The pathways toward important conductivity and band spin polarization improvements substantial for spin-polarized current injection in microelectronic applications are discussed.

[1]This work was supported by NSF and North Dakota EPSCoR grants.

4:18PM T18.00008 Experimental determination of the Weiss temperature of several variants of Mn12-ac[1] , SHIQI LI, CCNY & GC-CUNY, LIN BO, BO WEN, CCNY, P. SUBEDI, NYU, Y. YESHURUN, Bar-Ilan U., Israel, A.D. KENT, NYU, M.P. SARACHIK, CCNY, A.J. MILLIS, Columbia U., C. LAMPROPOULOS, S. MUKHERJEE, G. CHRISTOU, U. of Florida — We report measurements of the susceptibility in the temperature range from 3.5 K to 6.0 K of a series of Mn12-ac and Mn12-ac-MeOH samples in the shape of rectangular prisms. The susceptibility obeys a Curie-Weiss Law, where the temperature intercept varies systematically with sample aspect ratio. Using published demagnetization factors, we obtain the Curie-Weiss intercept for an infinitely long sample corresponding to intrinsic ordering temperatures Tc $\sim$ 0.85 K and $\sim$ 0.74 K for Mn12-ac and Mn12-ac-MeOH, respectively [1]. The difference in Tc for the two materials suggests an additional non-dipolar (exchange) contribution to the Weiss temperature that differs in the two materials because of the difference in ligand molecules. A similar comparison will also be reported for Mn12-toluate.

[1]Supported by NSF-DMR-0506946, ARO W911NF-08-1-0364, NSF-DMR-0705847, NSF-DMR-0451605, CHE-0910472 and German Research Foundation (DFG).

4:30PM T18.00009 Asymmetric Berry-Phase Interference Patterns in a Mn_4 Single-Molecule Magnet , H.M. QUDDUSI, Department of Physics, University of Central Florida, J. LIU, Department of Physics, University of Florida, S. SINGH, Department of Physics, University of Central Florida, K. HEROUX, Department of Chemistry and Biochemistry, University of California at San Diego, E. DEL BARCO, Department of Physics, University of Central Florida, S. HILL, National High Magnetic Field Laboratory and Department of Physics,, D. HENDRICKSON, Department of Chemistry and Biochemistry, University of California at San Diego — We present a low temperature magnetometry study of the quantum interference effect in a Mn_4 single-molecule magnet. Asymmetric modulations of the Berry phase interference patterns upon application of a transverse field are observed for $k > 0$ resonances (i.e. non-zero longitudinal field), contrary to the symmetric patterns obtained at $k = 0$. These asymmetries can be reversed by a full inversion of the total applied field. The observation of a fascinating motion of the Berry-phase minima as a function of both the magnitude and direction of the transverse field can be understood as an outcome of a competition between different intramolecular magnetic interactions. A multi-spin description using non-collinear zero-field splitting tensors and intra molecular dipolar interactions between the manganese ions is employed to explain the results.

4:42PM T18.00010 Observation of double hysteresis in a $MnMn_6(CH_3H_5O_3)_3$ single-molecule magnet , KLAUS GIEB, WOLFGANG KROENER, PAUL MÜLLER, Department of Physics and Interdisciplinary Center for Molecular Materials (ICMM), Universitaet Erlangen-Nuernberg, Germany, CARL-GEORG FREIHERR VON RICHTHOFEN, THORSTEN GLASER, Fakultaet fuer Chemie - Lehrstuhl Anorganische Chemie I, Universitaet Bielefeld, Germany — We report on high field and low temperature magnetization measurements of a novel $MnMn_6(CH_3H_5O_3)_3$ complex. A home-made micro-Hall-probe magnetometer was used to perform the characterization at mK temperatures and fields up to 17 T. Most 3d-ion based single-molecule magnets, known up to now, have a spin ground state well separated from the first excited state, leading to the formation of giant spin at low temperatures. In contrast to this situation, the ground state (S=6) of the present complex can already be exited at moderate magnetic fields. Surprisingly, magnetic hysteresis was observed for both the ground state and the first exited state leading to a double hysteresis in the low temperature magnetization measurements. The blocking temperature was found to be $T_B \approx 1.3$ K. Origin and possible consequences of this unusual behavior will be discussed.

4:54PM T18.00011 A Muon Spin Relaxation Study of NiTCNQ2 , ADAM BERLIE, IAN TERRY, MAREK SZABLEWSKI, Durham University, SEAN GIBLIN, ISIS, RAL — $NiTCNQ_2$ (TCNQ = 7,7,8,8-tetracyanoquinodimethane) is a novel metal-organic material that exhibits a magnetic transition at approximately 20 K. The material was first synthesized by Dunbar *et al* (Chem. Mater. 15, 1840) who identified the low temperature magnetic phase as a glassy ferromagnet. We have investigated this magnetic transition with muon spin relaxation (μSR). We synthesised the deuterated form of the material to minimise hyperfine coupling between the muon and H nuclear moments on TCNQ. Using μSR we probed the transition region to determine whether there was a local or long range coherence of the ferromagnetism. We found that zero field measurements yielded a Lorentzian relaxation along with a nuclear component from the nuclear spins of the nitrogen atoms. A longitudinal field of 0.5 mT decoupled the nuclear component revealing a dynamical Kubo-Toyabe relaxation suggesting that there may be a coexisting static and dynamic field distribution. This may imply a long range static ordering below the transition temperature.

5:06PM T18.00012 Magnetization measurements of a two-leg spin-1/2 ladder with strong leg interactions , K. NINIOS, University of Florida, TAO HONG, Oak Ridge National Laboratory, S.N. HERRINGER, M.M. TURNBULL, C.P. LANDEE, Clark University, Y. TAKANO, University of Florida, H.B. CHAN, The Hong Kong University of Science and Technology — We have measured the magnetization of a single crystal of the spin-1/2 ladder compound bis(2,3-dimethylpyridinium) tetrabromocuprate (DIMPY), using micromechanical force magnetometry down to 30mK. DIMPY undergoes a quantum phase transition from a gapped phase with no long–range magnetic order to a gapless phase, at critical field Hc. Recent specific heat results by Hong et al. show that the gapless phase is a Tomonaga-Luttinger liquid (TLL). Low temperature magnetic susceptibility as a function of field exhibits a maximum near Hc, in consistence with the divergence of the zero temperature susceptibility at Hc expected for an ideal 1-D system. A clear minimum in the magnetization of the gapless phase as a function of temperature is observed, a minimum that marks the limit below which the TLL exists. In addition the field dependence of the TLL parameter K is studied.

5:18PM T18.00013 Field-induced Tomonaga-Luttinger liquid phase of a two-leg spin-1/2 ladder with strong leg interactions[1] , TAO HONG, Oak Ridge National Laboratory, Y.H. KIM, University of Florida, C. HOTTA, Kyoto Sangyo University, Y. TAKANO, University of Florida, G. TREMELLING, M.M. TURNBULL, C.P. LANDEE, Clark University, H.-J. KANG, National Institute of Standards and Technology, N.B. CHRISTENSEN, ETH Zurich and Paul Scherrer Institute, K. LEFMANN, University of Copenhagen, K.P. SCHMIDT, G.S. UHRIG, TU Dortmund, C. BROHOLM, The Johns Hopkins University — We study the magnetic-field-induced quantum phase transition from a gapped quantum phase that has no magnetic long-range order into a gapless phase in the spin-1/2 ladder compound bis(2,3-dimethylpyridinium) tetrabromocuprate (DIMPY) [1]. At temperatures below about 1 K, the specific heat in the gapless phase attains an asymptotic linear temperature dependence, characteristic of a Tomonaga-Luttinger liquid. Inelastic neutron scattering and the specific heat measurements in both phases are in good agreement with theoretical calculations, demonstrating that DIMPY is the first model material for an $S = 1/2$ two-leg spin ladder in the strong-leg regime.

[1] T. Hong et al., Phys. Rev. Lett. 105, 137207 (2010)

[1]The work at ORNL was partially funded by the Division of Scientific User Facilities, Office of BES, DOE.

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T19 GMAG DMP: Focus Session: Spin Transport & Magnetization Dynamics in Metals VII D170

2:30PM T19.00001 Direct observation of strain-induced magnetic domain evolution in Heusler shape memory compounds , C.A. JENKINS, A. SCHOLL, A. DORAN, Lawrence Berkeley National Laboratory, T. OMORI, Graduate School of Engineering, Tohoku University Sendai — The magnetic domain structure in single crystals of a novel Heusler magnetic shape memory (MSM) compound Fe_2MnGa was observed to undergo strain-induced evolution by synchrotron-based photoelectron emission microscopy (PEEM) at Beamline 11.0.1 of the Advanced Light Source. PEEM can produce high resolution, surface-sensitive images reflecting the spatial distribution of magnetism, and a custom flexure rig has been designed for in situ actuation and simultaneous observation of MSM. System energy of an MSM compound is lowered when the volume fraction of the favorably oriented martensitic variant is increased: intermartensitic twin boundary motion is energetically easier than magnetic rotation so magnetic domains evolve not by domain wall motion but by propagation of planar structural defects called twin boundaries. In this ternary MSM intermetallic the direction of tetragonal distortion, which is coupled to the magnetic easy axis, will lie favorably along the axis of compression as defined by the action of the custom rig. The disappearance of unfavorably oriented orthogonal magnetic domains with strain is then observed as expected.

2:42PM T19.00002 Thin film growth and characterization of full Heusler alloys $Rh_{2-x}Co_xFeSn$ and RhCoMnSn , LI GAO, MINGYANG LI[1], MAHESH G. SAMANT, BRIAN P. HUGHES, KEVIN P. ROCHE, CLAUDIA FELSER[2], STUART S.P. PARKIN, IBM Research Division, Almaden Research Center, San Jose, California 95120 — Heusler alloys can be designed and prepared with high spin polarization, high Curie temperature, very low magnetization damping, as well as, tunable magnetic magnetization and anisotropy. Therefore, this family of compounds has great potential for applications such as spin-transfer-torque magnetic random access memory. The growth and characterization of epitaxial thin films of the Rh-based full Heusler compounds, $Rh_{2-x}Co_xFeSn$ and RhCoMnSn, are presented. The magnetization, Curie temperature and crystal structure of these compounds have been investigated and are compared with bulk materials. An important known property of many Heusler alloys is low magnetization damping. Ferromagnetic resonance (FMR) studies using a strip line transmission technique reveals Gilbert damping values of $\sim$0.015 at room temperature in films of RhCoMnSn. These films have Curie temperatures well above room temperature whereas the Curie temperature of Rh_2FeSn is $\sim$350 K.

[1]Physics Department, Stanford University, Stanford, California
[2]Johannes Gutenberg Universität, Mainz, Germany

2:54PM T19.00003 Electronic structure modifications in Cu doped Ni_2MnGa , SUJOY ROY, R. QIAO, P.-A. GLANS, Advanced Light Source, Lawrence Berkeley National Laboratory, USA, A. PATHAK, I.S. DUBENKO, N. ALI, Dept. of Physics, Southern Illinois University Carbondale, USA, E. BLACKBURN, Dept. of Physics and Astronomy, University of Birmingham, UK, W. YANG, Advanced Light Source, Lawrence Berkeley National Laboratory, USA — Ni_2MnGa Heusler alloy is a multifunctional ferromagnetic alloy that exhibits various interesting properties. The compounds typically exhibit a high temperature magnetic and a low temperature martensitic transition. Stoichiometry changes or elemental substitution makes it possible to merge the two transitions to a unique magnetostructural one. We have used resonant inelastic x-ray scattering to study the effects of $d-d$ interactions and charge transfer effects in 25% Cu doped Ni_2MnGa. We find distinct charge transfer effects in the Ni absorption and inelastic x-ray spectrum that are significantly modified by Cu doping. Mn on the other hand shows $d-d$ interaction effects but no charge transfer. Multiplet calculations have been performed and will be compared to the experimental data. These results provide an insight into the origin of multifunctional properties of Ni based Heusler alloys. Work at LBNL is supported by U.S DOE.

3:06PM T19.00004 Approach towards full Heusler alloy based CPP-GMR: from Ag and non-magnetic Heusler to binary intermetallic spacers , OLEG MRYASOV, University of Alabama, Department of Physics, SERGEY FALEEV, S.V. KARTHIK, University of Alabama, MINT — Recently, it has been demonstrated that GMR response can be significantly enhanced by incorporating high spin polarization ferromagnetic (FM) full Heulser alloy into spin valve nano-structures. Experimental results for two types of non-magnetic spacers (i) elemental metal [1] and (ii) non-magnetic Heusler alloy spacers [2] deserve careful comparison. More practical (110) textured combination of Co_2MnGe (CMG) and non-magnetic Heusler alloy Rh_2CuSn (RCS) [2] have been used to build test hard disk drive [3]. In this work, we investigate the mechanism of spin dependent interface scattering for (001) CMG/Ag/CMG (Case1) and (110) CMG/RCS/CMG (Case2) models on the basis of ab-initio electronic structure calculations. We find that in both cases GMR has significant contribution from the spin dependent interface scattering. We propose new binary intermetallic spacer materials Al_2Au and Cu_3Sn as an alternative to Ag and RCS spacers.

[1] T.Iwase et.al. Appl.Phys.Express, **2**, 063003 (2009).
[2] K. Nikolaev et.al. App.Phys. Lett., **94**, 222501 (2009)

3:18PM T19.00005 Spin fluctuations and doping trends in the itinerant magnet Pd_2TiIn_x , JESSICA MISSAGHIAN, ANDREW LAFORGE, DAVID MATTHEWS, GARRETT ROGREN, ZACK SCHLESINGER, ARTHUR RAMIREZ, University of California, Santa Cruz — The intermetallic compound Pd_2TiIn is one of several Heusler-type materials which are remarkable for possessing a significant magnetic moment despite being composed of elements which have no spontaneous local moment. We investigate the nature of the magnetic order and the role of spin fluctuations by studying the magnetic, transport and heat capacity properties of two series of polycrystalline samples derived from Pd_2TiIn_x: one in which the indium content is varied from $x = 0.87$ to 1.22, and another in which 3d and 4d metals are substituted in small quantities for Pd and Ti.

3:30PM T19.00006 Thermal effects on magnetic resonance in single crystal $Co_{1-x}Fe_xS_2$[1] , B. KASTER, M. PECHAN, Department of Physics, Miami University, Oxford, OH 45056, M. MANNO, A. BARUTH, C. LEIGHTON, Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, Minnesota 55455 — Many spintronic applications require spin injection from spin polarized ferromagnetic materials. A promising model system for fundamental studies of such processes is CoS_2, which has -56% spin polarization at the Fermi level and is tunable with Fe doping in $Co_{1-x}Fe_xS_2$ to over 85%. Single crystals of $Co_{1-x}Fe_xS_2$ have been successfully prepared with close to ideal sulfur stoichiometry using chemical vapor transport methods. We have employed variable temperature ferromagnetic resonance (FMR) at 9.2 GHz to investigate the magnetodynamic properties of this system for x=0, 0.05, 0.12 and 0.17. Resonance signals are observed upon cooling to 160 K, well above the Curie temperature, suggesting short-range order enhancements to the susceptibility lead to observable resonances. All concentrations exhibit increasing resonance position, and decreasing damping, with increasing temperature. Both the resonance position and the damping decrease with increasing Fe concentration - the former revealing Fe concentration effects on the moment and anisotropy, while the latter reflects the spin polarization influence on the damping.

[1]Supported by the US Dept. of Energy at MU, NSF MRSEC at UMN.

3:42PM T19.00007 Spin-dependent intergranular hopping transport in very thin highly spin-polarized CoS_2 thin films[1]

, M. MANNO, A. GUNAWAN, A. BARUTH, R. FRAKIE, A. MKHOYAN, C. LEIGHTON, University of Minnesota, DEPARTMENT OF CHEMICAL ENGINEERING AND MATERIALS SCIENCE COLLABORATION — The $Co_{1-x}Fe_xS_2$ alloy system has been shown to exhibit high, composition tunable, spin polarization (-56 % $< \quad P <$ +85 %) in bulk, demonstrating great promise for fundamental studies in spintronics. Incorporation in heterostructures requires reliable thin film deposition routes, which have recently been developed. We present here a detailed study of the thickness (t) dependence of the structural, magnetic, and electronic properties of polycrystalline CoS_2 thin films (70 – 1600 Å). As t is decreased, we observe a suppression in magnetic properties accompanied by a metal-insulator transition. A distinct 3D to 2D crossover is evident in the conductance-voltage curves and intergranular tunneling magnetoresistance. At t of order 70 Å we observe granular metal conduction, in the presence of a Coulomb charging penalty. We demonstrate quantitative agreement between experiment and proposed models. The very thin film data are understood in terms of enhanced grain boundary resistance, due to S accumulation, which is evidenced via several modes of structural characterization.

[1]Work supported by NSF MRSEC

3:54PM T19.00008 Synthesis and basic characterization of the itinerant ferromagnet $Cr_{11}Ge_{19}$[1]

, NIRMAL GHIMIRE, University of Tennessee, MICHAEL MCGUIRE, Oak Ridge National Laboratory, DAVID MANDRUS, University of Tennessee and Oak Ridge National Laboratory — $Cr_{11}Ge_{19}$ is a member of the tetragonal, but structurally complex family of materials known as Nowotny chimney-ladder phases. These materials have composition T_nX_m where $2 > m/n > 1.25$ (T=transition element, X=Si, Ge, Sn or Ga). Although $Cr_{11}Ge_{19}$ was reported to be an itinerant ferromagnet, its basic properties have not been well characterized. Here we present resistivity, magnetization, and heat capacity results on polycrystalline $Cr_{11}Ge_{19}$.

[1]Research supported by DOE BES Materials Sciences and Engineering Division.

4:06PM T19.00009 Unusual magnetism of Gd_5Ge_4 with non magnetic rare earths substitutions[1]

, DURGA PAUDYAL, The Ames Laboratory, US Department of Energy, Iowa State University, Ames, IA 50011-3020, USA, Y. MUDRYK, V.K. PECHARSKY, K.A. GSCHNEIDNER, JR., The Ames Laboratory, U. S. Department of Energy, Iowa State University, Ames, IA 50011-3020, USA — We present first principles and experimental studies on the small substitutions of Gd atoms by Lu, La, Y, and Sc atoms in Gd_5Ge_4. While replacing the Gd atoms located inside the slabs with the Lu or Y atoms leads to a substantial loss of ferromagnetism, the identical substitutions of other Gd locations preferred by La atoms have essentially no effect on the magnetostructural transitions. On the other hand, the Sc atoms prefer the same locations as the Lu and Y atoms. This substitution, however, changes the crystal structure of Gd_5Ge_4 from Sm_5Ge_4 type to Pu_5Rh_4type at 25% of Sc which was not observed with the former substitutions. The Pu_5Rh_4-type has structural parameters that are intermediate between the Gd_5Si_4 and Sm_5Ge_4 types. The exchange interactions in this substitution are positive which indicates that the Sc substituted Gd_5Ge_4 has the ferromagnetic ground state.

[1]This work is supported by U. S. Department of Energy.

4:18PM T19.00010 Examining the AF>FM transition in Fe-Rh thin films through specific heat, photoemission, and Mossbauer spectrometry measurements[1]

, DAVID COOKE, University of California at Berkeley, CATHERINE BORDEL, FRANCES HELLMAN — Iron-rhodium alloys near equiatomic composition undergo a metamagnetic antiferromagnetic-to-ferromagnetic (AF>FM) transition at just above room temperature. This material has been proposed as an exchange layer in thermally-assisted magnetic recording, using the ferromagnetic phase to reduce the switching field of a high-anisotropy storage layer, so clearly being able to control this transition is crucial to implementation. However, theoretically there is still much debate as to the precise mechanism of the AF>FM transition, primarily centered on the contributions of electronic and magnetic entropy differences in the two phases. Through thermodynamic measurements on epitaxially- grown ferromagnetic and antiferromagnetic Fe-Rh alloy films, we test two different thermal fluctuation models of the transition. We also discuss complementary photoemission and Mossbauer spectrometry data above and below the transition to examine the magnetic behavior and electronic densities of state in the two phases and compare these to theoretical calculations.

[1]This work was supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231

4:30PM T19.00011 Transport Spin Polarization of High-Curie Temperature MnBi Films

, PUSHKAL THAPA, Dept. of Physics, Wayne State University, Detroit, MI, 48202, PARASHU KHAREL, Nebraska Center for Materials and Nanoscience (NCMN), Univ. of Nebraska, Lincoln, NE, 68588, PAVEL LUKASHEV, NCMN, Univ. of Nebraska, Lincoln, NE, 68588, RENAT SABIRIANOV, Dept. of Physics, Univ. of Nebraska, Omaha, NE, 68182, EVGENY TSYMBAL, DAVID SELLMYER, NCMN, Univ. of Nebraska, Lincoln, NE, 68588, BORIS NADGORNY, Dept. of Physics, Wayne State University, Detroit, MI, 48202 — We report on the study of the structural, magnetic and transport properties of highly textured MnBi films with the Curie temperature of 628 K. In addition to detailed measurements of resistivity and magnetization, we measure transport spin polarization of MnBi by Andreev reflection spectroscopy and perform first-principles electronic structure calculations. A transport spin polarization of up to 63% is observed, consistent with the calculations and with a recent observation of a large magnetoresistance in MnBi contacts. The band structure calculations indicate that, in spite of almost identical densities of states at the Fermi energy, the large disparity in the Fermi velocities leads to high transport spin polarization of MnBi. The correlation between the values of magnetization and spin polarization observed in MnBi will be discussed.

4:42PM T19.00012 Anomalous electron transport in ferromagnetic MnBi films

, PARASHU KHAREL, D.J. SELLMYER, Nebraska Center for Materials and Nanoscience and Department of Physics and Astronomy University of Nebraska, Lincoln, NE, 68588 — Materials having high spin polarization, large perpendicular magnetic anisotropy and high Curie temperature hold great potential for a range of spintronic applications.[1] MnBi has the hexagonal NiAs structure and possesses strong permanent magnet and magneto-optical properties. Our recent research shows that MnBi exhibits a high transport spin polarization of 63%, so it is useful to investigate the electron transport properties of this material. We have found that MnBi is a metallic conductor but the resistivity shows an anomalous temperature dependence at low temperature. Analysis of the Hall data for various samples shows that the extraordinary Hall effect is the dominant part in the transverse Hall effect and a Hall angle of 2.8% has been measured. An experimental investigation on the origin of the observed large extraordinary Hall effect in MnBi thin films will be discussed. This research is supported by NSF-MRSEC Grant DMR-0820521, the DOE Grant DE-FG02-04ER46152 and NCMN.

[1]S. Mangin, D. Ravelosona, J. A. Katine, M. J. Carey, B. D. Terris and Eric E. Fullerton, Nature Mater. **5**, 210 (2006).

4:54PM T19.00013 $SrMnBi_2$, a new transition metal compound with metallic spacer layer[1] , JIAKUI J. WANG, LIANG L. ZHAO, Department of Physics and Astronomy; Rice University; Houston TX 77005, Q. YIN, G. KOTLIAR, Department of Physics, Rutgers University, Piscataway, NJ 08854, EMILIA MOROSAN, Department of Physics and Astronomy; Rice University; Houston TX 77005 — To explore the correlation between superconductivity and crystal structure in transition metal-pnictides systems, we investigate the band structure and physical properties of $SrMnBi_2$ single crystals. This compound is isostructural with the superconducting Fe-pnictides. In this talk, magnetization, resistivity and specific heat data will be compared with band structure calculations. Both the experimental results and the density functional theory (DFT) calculation are consistent with this material being a bad metal with large residual resistivity, similar to the well-studied Fe-pnictides. The key difference is that the Sr-Bi blocking layer in $SrMnBi_2$ is metallic, which may be more favorable to the occurrence of superconductivity upon doping, likely with a higher transition temperature, commensurate with the high $T_N \approx 280$ K.

[1]This work is supported by MURI AFOSR.

5:06PM T19.00014 Doping - induced Quantum Phase Transition in $Sc_{3.1}In$[1] , ETERI SVANIDZE, EMILIA MOROSAN, Department of Physics and Astronomy, Rice University, Houston, TX 77005 — Sc_3In is a known itinerant ferromagnet with a reported $T_c \approx 6$ K. In this talk we will show that Lu doping induces a quantum phase transition in this compound. Temperature and field - dependent magnetization measurements on $(Sc_{1-x}Lu_x)_{3.1}In$ polycrystalline samples were performed, where $0 \leq x \leq 0.08$. The 3.1 : 1 stoichiometry was chosen because it showed the highest $T_c \approx 10$ K for $x = 0$ when Arrott plots were employed to determine the Curie temperature. In this study we use modified Arrott plots M^2 vs. $(H/M)^{1/\alpha}$. For $\alpha = 1.5$, the corresponding isotherms were linear over larger field ranges, and, for the critical composition $x_c \approx 0.02$, the isotherm was linear down to (M,H) = (0,0). The Curie temperature determined using this method was close to 6 K.

[1]This work was supported by NSF DMR 0847681.

5:18PM T19.00015 On the origin of the magnetic susceptibility anomaly in nearly ferromagnetic alloys , ROMEO DE COSS, Cinvestav, Department of Applied Physics, Cordemex 97310, Mérida, Mexico, AARÓN AGUAYO, Universidad Autónoma de Yucatán, Mérida, Yucatán, México, FILIBERTO ORTIZ-CHI, Cinvestav, Department of Applied Physics, Cordemex 97310, Mérida, Mexico — The magnetic susceptibility of the Ni-Rh and Ni-Cu alloys shows an anomaly near the transition from ferromagnetism to paramagnetism. In order to contribute to understand this phenomenon, we have studied the electronic and magnetic properties of the $Ni_{1-x}Cu_x$ alloy by means of first principles calculations. The ground state properties were obtained using the Full-Potential Linear Augmented Plane Waves method. The alloying was modeled using the self-consistent virtual crystal approximation. The spin magnetic susceptibility is calculated from the total energy as a function of the spin moment, obtained using the Fixed Spin Moment methodology. We found that the calculations predict correctly the reduction of the magnetic moment with the Cu concentration and that the critical concentration where the magnetic moment goes to zero is $x_c = 0.5$, in excellent agreement with the experimental data. The calculated magnetic susceptibility is in good agreement with the experimental data in the whole range of concentrations for the $Ni_{1-x}Cu_x$ alloy, in particular the anomaly present at $x \approx 0.4$ is reproduced by the calculations. This research was supported by Conacyt-México under Grant No. 83604.

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T20 DMP GERA FIAP: Focus Session: Thermoelectric Materials: LAST/TAGS, Heusler, and Silicides D168

2:30PM T20.00001 Charge Neutral Yukawa Lattice Gas on a FCC Lattice , HE HUANG, S.D. MAHANTI, Michigan State University — Structural phase transitions associated with the ordering of Ag and Sb ions in the quaternary systems, $(AgSbTe_2)_x(PbTe)_{2(1-x)}$ (of current thermoelectric interest) has been investigated using an anti-ferromagnetic 3-state Ising model on a FCC lattice with screened Coulomb interaction (Yukawa lattice gas (YLG) model). We have carried out Monte Carlo simulations (MCs) to study phase transitions (PT) in YLG. The nature and the strength of PT depend on the screening parameter κ. The transition is 1^{st} order and the transition temperature T_c is a weak function of the concentration x (excepting when $x \sim 0$ or 1), in agreement with earlier work for $\kappa = 0$. We find $T_c(x,\kappa) = f(x)g(\kappa)$, where $g(\kappa) \rightarrow const$ when $\kappa \rightarrow 0$ and $g(\kappa) \rightarrow 0$ when $\kappa \rightarrow \infty$. For $x = 0.5$, there are two special structures, layered and tubular which have the same ground state energy, independent of κ. This is understood by looking at the connectivity and ordering of ions. Above but near T_c, the generation rates of different micro structures have been analyzed using a simple surface energy density picture. MCs results agree with this analysis and show that the energy barriers decide the generation rates of different micro structures.

2:42PM T20.00002 Effect of doping $Ag_ySb_yGe_{50-2y}Te_{50}$ thermoelectric materials with rare earths , E.M. LEVIN, S.L. BUD'KO, K. SCHMIDT-ROHR, Iowa State University and Ames Laboratory US DOE — The $Ag_ySb_yGe_{50-2y}Te_{50}$ system represents some of the most efficient thermoelectrics, the so-called TAGS materials. In order to understand the effect of doping of $Ag_{6.52}Sb_{6.52}Ge_{36.96}Te_{50}$ ("TAGS-85") with rare earth atoms on the Ge and Te sites, $Ag_{6.52}Sb_{6.52}Ge_{36.96-x}R_xTe_{50}$ and $Ag_{6.52}Sb_{6.52}Ge_{36.96}R_xTe_{50-x}$ materials with R = Gd and Dy (rare earth atoms with large magnetic moments) have been studied by measuring X-ray diffraction (XRD) and ^{125}Te nuclear magnetic resonance (NMR) at 300 K, thermopower and resistivity at 300-760 K, and the magnetization at 1.8-350 K and in magnetic field 0-55 kOe. XRD and ^{125}Te NMR show that some rare earth atoms are incorporated into the lattice and enhance the thermopower by ∼10%. At 700 K, this yields a power factor of up to 36 $\mu W \cdot cm^{-1} \cdot K^{-2}$, which is ∼20% higher than in TAGS-85. All materials studied can be considered as degenerate magnetic semiconductors with non-interacting localized magnetic moments formed by rare earth atoms, with a different effect of rare earths on the Ge and Te sites. Reasons for the thermopower enhancement due to doping with rare earths including magnetic and non-magnetic phenomena are discussed.

2:54PM T20.00003 Nanodopant Induced Band Modulations and Electronic Transport Properties in $AgPb_mSbTe_{2+m}$-type Thermoelectric Nanocomposites[1] , YI ZHANG, CHANGFENG CHEN, Physics Department and HiPSEC, University of Nevada, Las Vegas, XUEZHI KE, Department of Physics, East China Normal University, China, JIHUI YANG, Electrochemical Energy Research Lab, GM R&D Center, PAUL KENT, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — The remarkable performance of many novel thermoelectric materials is attributed to their nanosized inclusions. By extensive first-principles calculations we show the distinct band structure modulation in $AgPb_mSbTe_{2+m}$ (LAST)-type nanocomposites. A band gap widening and conduction band minimum splitting process resulting from the nanodopants is discovered for a series of nanocomposites. Boltzmann transport calculations demonstrate that this process leads to a pronounced change in the high temperature electronic transport. The effects of different substitutional elements and atomistic orderings are discussed. Our results provide new understanding of nanosized doping in thermoelectric materials and narrow gap semiconductors.

[1]This work is supported by DOE Agreements DE-FC52-06NA26274 and DE-FC26-04NT42278. The computation resource (CRAY-XT5) of the NCCS and the CNMS in ORNL are sponsored by DOE.

3:06PM T20.00004 Strong off-stoichiometry and large Grüneisen parameter in $AgSbTe_2$: a first principles study[1]

SERGEY V. BARABASH, VIDVUDS OZOLINS, University of California, Los Angeles, MICHELE D. NIELSEN, JOSEPH P. HEREMANS, The Ohio State University — We use first-principles density-functional theory calculations to study the dynamical and compositional instabilities in $AgSbTe_2$, and compare the theoretical predictions to the results of an experimental investigation. For pure $AgSbTe_2$, some native defects, particularly Ag vacancies, have negative formation energies for a wide range of experimental conditions, thus forming in high concentrations even at low T. This leads to large deviations from the formal stoichiometry, in agreement with experimental results. Substantial deviations of the $AgSbTe_2$ phase field away from the isoplethal Ag_2Te-Sb_2Te_3 section may be expected, potentially explaining the contradictions in the low-temperature regions of the previously published phase diagrams. We estimate the defect concentrations and the resulting intrinsic doping levels under various experimental conditions. Finally, we demonstrate that the stoichiometric $AgSbTe_2$ is at the verge of a dynamical instability: the energies of acoustic phonons near the L point depend strongly on volume, changing sign at nearly the experimental volume. This leads to an unusually large value of the Grüneisen parameter, in agreement with experiment.

[1]Supported by DOE BES EFRC under Award No. DE-SC0001054.

3:18PM T20.00005 Effect of electron correlation on thermoelectric properties of the full-Heusler compound Fe_2VAl[1]

DAT DO, MAL-SOON LEE, S.D. MAHANTI, Department of Physics and Astronomy, Michigan State University — Heusler-type alloys have been studied extensively since they were first discovered by Heusler in 1903. Among those Fe_2VAl became interesting when Nishino *et. al.*[1] suggested that it might be a heavy fermion system. LDA/GGA calculations have shown that Fe_2VAl is a pseudo-gap system with sharp edges in the density of state near the Fermi level. This feature makes it a promising thermoelectric material. Since then electronic properties of nominally pure and doped Fe_2VAl have been studied extensively. However the exact nature of the ground state of this system is still not well understood. Since it contains d-electrons one expects electron correlation effects to be important. We have carried out band structure calculations using GGA+U method with several values of the on-site Coulomb interaction parameter U. Using the obtained band structure, transport coefficients were calculated within Boltzmann approach. Electronic structure and thermoelectric properties were studied for different values of U and compared to available experiments.

[1] Y. Nishino *et. al., Phys. Rev. Lett.* **79** *(10), 1909* (1997).

[1]This work was supported by the US Department of Energy, Office of Basic Energy Sciences as part of an Energy Frontier Research Center.

3:30PM T20.00006 Phase-separated-induced changes in the transport properties of Heusler compounds for thermoelectric applications

TANJA GRAF, MICHAEL SCHWALL, PETER KLAER, HANS-JOACHIM ELMERS, BENJAMIN BALKE, CLAUDIA FELSER, Johannes Gutenberg-University Mainz, Germany — The solid solution $Co_2Mn_{1-x}Ti_xSn$ shows a phase separation into two Heusler compounds, Co_2MnSn and Co_2TiSn. Only at the edges of the composition range a slight admixture of Mn and Ti to the respective other phase is observed. This phase separation leads to a distinct microstructure which can be altered by the composition of the material. Due to the formed phase and grain boundaries, pronounced changes in the magnetic and electronic properties take place with varying composition. The observed reduction of the thermal lattice conductivity is of particular interest for an optimization of Heusler compounds for thermoelectric applications. Thus, the concept of phase separated materials is transferred to Half-Heusler compounds with an improved thermoelectric performance.

3:42PM T20.00007 Strategies to Bulk Half-Heusler Nanocomposites with Simultaneously Enhanced Power Factor and Reduced Thermal Conductivity[1]

PIERRE FERDINAND POUDEU, The Advanced Materials Research Institute and Department of Chemistry, University of New Orleans, New Orleans LA, 70148, USA — Among promising thermoelectric materials for power generation, half-Heusler (HH) phases with general compositions TNiSn and TCoSb (T = Ti, Zr, Hf) have attracted tremendous attention not only because they involve abundant and environmentally friendly elements, but also due to their combination of large Seebeck coefficients with moderately low electrical resistivities. However, the ability to synthesize HH based materials with decent figures of merit (ZT>1) has been jeopardized by their very large thermal conductivities. Strategies to reduce the thermal conductivity of HH phases focusing on mass fluctuation phonon scattering via solid solution alloying or phonon scattering at grain boundaries and interfaces in HH phases with embedded pre-synthesized nanoparticles have failed to generate materials with high figures of merit due to simultaneous reductions in the power factor. Here, we introduce innovative approaches to revolutionary increases in the figure of merit of HH based materials through simultaneous large enhancement of the power factor and drastic reduction in the thermal conductivity. Our strategy is focused on atomic-scale structural engineering of the HH matrix through the confinement of full-Heusler (FH) inclusion phases on the lattice constant length-scale. Emphasis will be placed on the n-type $Zr_{0.25}Hf_{0.75}Ni_{1+x}Sn_{1-y}Pn_y$ and $Ti_{0.5}Zr_{0.5}Ni_{1+x}Sn_{1-y}Pn_y$ as well as the p-type $Ti_{0.5}Zr_{0.5}Co_{1+x}Pn_{1-y}Sn_y$, (Pn = Sb, Bi) nanocomposites. We will discuss the underlying mechanism for the formation of half-Heusler/full-Heusler (HH/FH) nanocomposites with coherent matrix/inclusion interfaces. The role of synthetic and processing methods; and size, dispersion and mole fraction of the FH inclusions on the thermoelectric performance of bulk HH/FH nanocomposites will be assessed by combining transmission electron microscopy studies with thermal and electronic charge transport data.

[1]Financial support from DARPA contract # HR 0011-08-1-0084 is greatly acknowledged. This work made use of the laser flash diffusivity apparatus (Netzsch-LFA457) purchased with funds from the Louisiana Board of Regents (Grant # LEQSF(2008-09)-ENH-TR-58).

4:18PM T20.00008 Thermoelectric Properties of Boron-doped CoSi

BO YU, HUI WANG, Boston College, HONGLI GAO, Zhejiang University, WEISHU LIU, Boston College, XINBING ZHAO, Zhejiang University, GANG CHEN, MIT, ZHIFENG REN, Boston College — Engineering in density of states $D(E)$ has been found effective in improving the transport properties of thermoelectric materials. As one example, intermetallic CoSi, when doped with boron or other suitable elements, exhibits a good combination of high electrical conductivity (σ) and Seebeck coefficients (S) due to possible sharp structures in $D(E)$near Fermi level. However, despite of its high power factor ($S^2\sigma$), the high thermal conductivity (κ) becomes the obstacle for the performance. Here, we present that mechanical alloying and hot press which had been proved successful in many thermoelectric materials, could also reduce the thermal conductivity of boron doped CoSi while keeping its high power factor.

4:30PM T20.00009 The Electrical Contact for Higher Manganese Silicide Thermoelectric Material[1]

XINGHUA SHI, ZAHRA ZAMANIPOUR, DARYOOSH VASHAEE, Oklahoma State University — The Electrical Contact for Higher Manganese Silicide Thermoelectric Material Xinghua Shi, Zahra Zamanipour, Daryoosh Vashaee Several electrical contact materials for Higher Manganese Silicide (HMS) are introduced. HMS is useful thermoelectric material for medium to high temperature applications. We have investigated several materials including Co, Ni, Cr, Ti, Mo, MnSi, MoSi2, and TiSi2 in search of the best contact material to HMS. The low electrical resistivity and reliability of the contact are two important elements to make a high efficient TE device. Moreover, the contact must maintain its chemical, mechanical, thermal, and electrical properties over a broad range of temperature (20C-700C). The investigated elemental metals failed to make reliable contact in terms of mechanical and chemical stability at high temperature. In contrast, the investigated metal silicides showed superior stability over extended operation at high temperature. The thermal stability and strong mechanical bonding of TiSi2 C54 phase and MnSi were specially observed. Their ohmic contact resistance was also within the range of interest over the whole range of temperature (10^{-5}-$10^{-4}\Omega cm^2$).

[1]This work was supported by AFOSR High Temperature Materials and NSF under contract CBET0933763

4:42PM T20.00010 High Thermoelectric Power Factor in $CoSi_{1-x}B_x$ Alloys[1] , HUI SUN, DONALD MORELLI, Michigan State University — $CoSi_{1-x}B_x$ alloys with x ranging from 0 to 0.1 have been prepared by an arc melting and annealing procedure. X-ray diffraction studies suggest the occurrence of minor CoB phase when $x \geq 0.05$. The thermoelectric (TE) properties were measured from 80 to 300K. The samples with $x \leq 0.02$ showed much lower electrical resistivity than CoSi. The Seebeck coefficient was negative for all samples over the investigated temperature range, indicating dominant transport by electrons in this temperature range. A high TE power factor (70 $\mu W/K^2cm$ at room temperature) was obtained in $CoSi_{0.98}B_{0.02}$, which we ascribe to the appropriate tuning of the Fermi level near the pseudogap in the density of states. In optimized samples the dimensionless figure of merit is in excess of 0.13 due to this enhanced power factor. We will also report on our efforts to further increase the figure of merit by thermal conductivity reduction methods.

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

4:54PM T20.00011 Thermoelectric properties of FeSi and Related Alloys: Evidence for Strong Electron-Phonon Coupling , BRIAN SALES, OLIVIER DELAIRE, MICHAEL MCGUIRE, ANDREW MAY, Oak Ridge National Laboratory — The effects of various transition metal dopants on the electrical and thermal transport properties of $Fe_{1-x}M_xSi$ alloys (M= Co, Ir, Os) are reported. The thermoelectric figure of merit ZT is improved from 0.007 at 60 K for pure FeSi to ZT = 0.08 at 100 K for 4% Ir doping. A comparison of the thermal conductivity data among Os, Ir and Co doped alloys indicates strong electron-phonon coupling in this compound. The common approximation of dividing the total thermal conductivity into electronic and lattice components ($\kappa_{Total} = \kappa_{electronic} + \kappa_{lattice}$) fails spectacularly for these alloys. The effects of nanostructuring on thermoelectric properties of $Fe_{0.96}Ir_{0.04}Si$ alloys are also reported. The thermal conductivity can be lowered by about 50% with little or no effect on the electrical resistivity or Seebeck coefficient. This results in $ZT_{max} = 0.125$ at 100 K, still about a factor of five too low for solid-state refrigeration applications. Research sponsored by the Materials Science and Engineering Division, Office of Basic Energy Sciences, U.S. DOE.

5:06PM T20.00012 Electron-phonon coupling in FeSi thermoelectrics: inelastic neutron scattering and first-principles simulations[1] , OLIVIER DELAIRE, JIE MA, BRIAN SALES, PAUL KENT, MATTHEW STONE, KAROL MARTY, MATTHEW LUCAS, DOUGLAS ABERNATHY, DAVID MANDRUS, ORNL TEAM — FeSi is a promising thermoelectric material for refrigeration applications, with a Seebeck coefficient over 500μV/K at 40K. FeSi is a narrow band-gap semiconductor at low temperature (B20 structure), and undergoes a semiconductor-to-metal transition around room temperature. Using inelastic neutron scattering, phonons were measured on both single crystals and powders as a function of composition and temperature. We report a strong coupling between the phonons and the semiconductor-to-metal transition, upon increasing temperature and carrier concentration. Using first-principles electronic structure calculations and ab-initio molecular dynamics, we show that the band gap and the sharp features around the band edges are strongly affected by the thermal disordering induced by phonon excitations. We also report on the effect of heavy impurities (Ir, Os) on the phonons.

[1]O.D. acknowledges funding from US DOE, Office of Basic Energy Sciences as part of an Energy Frontier Research Center, DOE DE-SC0001299.

5:18PM T20.00013 Carrier concentration optimization and electrical and thermal transport properties of the defect manganese silicide $MnSi_\delta (\delta \sim 1.74)$* , V. PONNAMBALAM, GLORIA LEHR, D.T. MORELLI, Dept. of Chemical Engineering and Materials Science, Michigan State University — Defect manganese silicide $MnSi_\delta$ ($\delta \sim 1.74$) is known for unusually low thermal conductivity. In addition, it also exhibits promising thermoelectric properties. We have substituted $MnSi_\delta$ with various elements to optimize the carrier concentration. Electrical and thermal transport properties of the resulting alloys have been studied over a temperature (T) range of 80-300 K. Both resistivity and Seebeck coefficient vary with substitution. Hall measurements suggest that the carrier concentration indeed varies in these alloys. Interestingly, thermal conductivity either remains constant or weakly increases with T in the temperature range 80- 300 K, eventually reaching values $\sim$ 3 W/m K at 300 K. The results will be presented and discussed. *This work was supported as part of the Center for Revolutionary Materials for Solid State Energy Conversion, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001054.

Wednesday, March 23, 2011 2:30PM - 5:30PM –
Session T21 DCOMP: Classical and Quantum Monte Carlo D161

2:30PM T21.00001 Steps beyond the fixed-phase approximation in diffusion Monte Carlo[1] , FERNANDO REBOREDO, Oak Ridge National Laboratory — The self-healing diffusion Monte Carlo algorithm (SHDMC) [Reboredo, Hood and Kent, Phys. Rev. B **79**, 195117 (2009); Reboredo, *ibid.* **80**, 125110 (2009)] is extended to study the ground and excited states of magnetic and periodic systems. The method converges to exact eigenstates as the statistical data collected increases if the wave function is sufficiently flexible. A recursive optimization algorithm is derived from the time evolution of the mixed probability density, which is given by an ensemble of electronic configurations (walkers) with complex weight. This complex weight allows the amplitude of the fixed-node wave function to move away from the trial wave function phase. This novel approach is both a generalization of SHDMC and the fixed-phase approximation [Ortiz, Ceperley and Martin, Phys Rev. Lett. **71**, 2777 (1993)]. The algorithm is demonstrated to converge to nearly exact solutions of model systems with periodic boundary conditions or applied magnetic fields for the ground state and low energy excitations. The computational cost is proportional to the number of independent degrees of freedom of the phase.

[1]Sponsored by the Materials Sciences & Engineering Division of the Office of Basic Energy Sciences U.S. Department of Energy.

2:42PM T21.00002 Understanding framework flexibility of periodic structures by Monte Carlo simulation , AN GHYSELS, University of California - Berkeley, VERONIQUE VAN SPEYBROECK, MICHEL WAROQUIER, Center for Molecular Modeling, BEREND SMIT, University of California - Berkeley — Metal Organic Frameworks (MOFs) are a new class of porous materials synthesized from metal clusters connected by organic linkers. Most crystalline solids are fairly rigid, and undergo small changes in volume when stress is applied. Although most MOFs are rigid, some have an unexpectedly high flexibility, and swell under pressure, temperature or adsorption changes. A well-known structure showing volume changes of over 50% is MIL-53. A better understanding of the process will allow to design materials with improved properties for carbon capture, i.e. the framework captures CO2 from fuel gasses. In this presentation, we explore framework flexibility effects induced by gas adsorption using Monte Carlo techniques. For instance, when MIL-53 is brought into contact with a gas at increasing pressure, the framework's pores constrict, while at even higher pressures, the pores return to their original geometry. To study this phenomenon, it is essential to incorporate framework flexibility into the Monte Carlo free energy calculation.

2:54PM T21.00003 Quantum Monte Carlo studies of solvated systems , KATHLEEN SCHWARZ, Cornell University, Department of Chemistry, KENDRA LETCHWORTH WEAVER, T.A. ARIAS, Cornell University, Department of Physics, RICHARD G. HENNIG, Cornell University, Department of Materials Science and Engineering — Solvation qualitatively alters the energetics of diverse processes from protein folding to reactions on catalytic surfaces. An explicit description of the solvent in quantum-mechanical calculations requires both a large number of electrons and exploration of a large number of configurations in the phase space of the solvent. These problems can be circumvented by including the effects of solvent through a rigorous classical density-functional description of the liquid environment, thereby yielding free energies and thermodynamic averages directly, while eliminating the need for explicit consideration of the solvent electrons. We have implemented and tested this approach within the CASINO Quantum Monte Carlo code. Our method is suitable for calculations in any basis within CASINO, including b-spline and plane wave trial wavefunctions, and is equally applicable to molecules, surfaces, and crystals. For our preliminary test calculations, we use a simplified description of the solvent in terms of an isodensity continuum dielectric solvation approach, though the method is fully compatible with more reliable descriptions of the solvent we shall employ in the future.

3:06PM T21.00004 Fast evaluation of multideterminant wavefunctions in quantum Monte Carlo[1] , MIGUEL A. MORALES, LLNL, BRYAN K. CLARK, Princeton, JEREMY MCMINIS, JEONGNIM KIM, UIUC, GUSTAVO SCUSERIA, Rice Univ. — Quantum Monte Carlo (QMC) methods such as variational and diffusion Monte Carlo depend heavily on the quality of the trial wave function. Although Slater-Jastrow wave functions are the most commonly used variational ansatz, more sophisticated wave functions are critical to ascertaining new physics. One such wave function is the multislater- Jastrow wave function which consists of a Jastrow function multiplied by the sum of slater determinants. In this talk we describe a method for working with these wave functions in QMC codes that is easy to implement, efficient, and easily parallelized. The algorithm computes the multi determinant ratios of a series of particle hole excitations in time $O(n^2)+O(n_s n)+O(n_e)$ where n, n_s and n_e are the number of particles, single particle excitations, and total number of excitations, respectively. This is accomplished by producing a (relatively) compact table that contains all the information required to read off the excitation ratios. In addition we describe how to compute the gradients and laplacians of these multi determinant terms.

[1]This work was performed under the auspices of: the US DOE by LLNL under Contract DE-AC52-07NA27344, the US DOE under Contract DOE-DE-FG05-08OR23336 and by NSF under No.0904572.

3:18PM T21.00005 ABSTRACT WITHDRAWN –

3:30PM T21.00006 Wave Function Optimization in QMCPACK[1] , JEREMY MCMINIS, University of Illinois and NCSA, MIGUEL MORALES, LLNL, JEONGNIM KIM, DAVID CEPERLEY, University of Illinois and NCSA — Wave function optimization is essential for both the accuracy and efficiency of diffusion, reptation, and variational quantum Monte Carlo (QMC). In this talk we outline the wave function optimization strategy used in the QMC software package QMCPACK developed at the University of Illinois. We use an extension of the linear optimization method originally developed by Umrigar et. al.[1] to optimize parameters in Slater-Jastrow, multi-determinant Slater-Jastrow, and Backflow-Jastrow trial wave functions. The efficiency and accuracy of this method is presented for bulk Silicon, Jellium, and the Nitrogen dimer.

[1] Umrigar et al. PRL 98, 110201 (2007)

[1]This work was supported by the U.S. Department of Energy (DOE) under Contract No. DOE-DE-FG05-08OR23336 and by the National Science Foundation under No. 0904572.

3:42PM T21.00007 Testing of He-core pseudopotentials for 3d elements in quantum Monte Carlo , MINYI ZHU, LUBOS MITAS, North Carolina State University — We construct He-core pseudopotentials for several elements in the 3rd row such as for V, Cr, Mn, Fe and Zn, with the goal of using these in high-accuracy quantum Monte Carlo (QMC) calculations. We study the accuracy of constructed pseudopotentials on MnO molecular states with different spin polarizations. We compare these results also with Density Functional Theory and Hartree-Fock approaches since we previously found noticeable differences between Ne-core pseudopotential and relativistic all-electron calculations in high-spin vs. low-spin state comparisons. The result indicates that these discrepancies stem from method biases related to the presence of core states, as we conjectured earlier. Additionally, we also discuss the computational cost of the He-core pseudopotentials in QMC calculations.

3:54PM T21.00008 Spin-orbit interaction in quantum Monte Carlo , LUBOS MITAS, North Carolina State University, RENE DERIAN, Institute of Physics, Slovak Academy of Sciences, SHI GUO, North Carolina State University — For spinless Hamiltonians (ie, no explicit spin operators), real space quantum Monte Carlo (QMC) methods such as variational and fixed-node diffusion Monte Carlo are well established. In these cases the electron spins and their components commute with the Hamiltonian and therefore are conserved quantities. This implies that spins can be fixed as given by the symmetry of a considered state and one solves only for the spatial part of the corresponding wave function. Indeed, this is a common practice in electronic structure QMC and also in most quantum chemical calculations. However, many systems require treating spins as quantum dynamical variables. We will present progress of our studies in this direction both in variational and diffusion Monte Carlo for heavy atoms with spin-orbit operators. One possibility is to use possibilities offered by various formulations of Hubbard-Stratonovitch transformation as realized in QMC for nuclear systems. We explore also other options both in variational and diffusion Monte Carlo framework. In particular, we define new representation for spinors which enable to formulate the diffusion Monte Carlo along the lines of fixed-phase approximation. We compare the results for the considered approaches also from the point of computational efficiency.

4:06PM T21.00009 A quantum Monte Carlo study of molecular systems with heavy elements , SHI GUO, KEVIN RASCH, LUBOS MITAS, North Carolina State University, ENRIQUE BATISTA, RICHARD MARTIN, Los Alamos National laboratory — We use quantum Monte Carlo method to study the bis-cyclopentadienyl Hafnium dichloride molecule Cp_2HfCl_2. There are two Cl dissociation channels for Cp_2HfCl_2: one is to break into neutral fragments, the other one into charged fragments. We employ the Stuttgart pseudopotential to represent the Hf atom and optimized Slater-Jastrow trial wave function at the variational Monte Carlo level. The calculations of the dissociation energies are carried out by the fixed-node diffusion Monte Carlo. We observe that for the heavy elements the low valence density in the core region can generate large energy fluctuations and we address this by improvements of the correlation factor. Alternatively, we construct Hf pseudopotentials with different core sizes and test for the accuracy of such pseudopotential Hamiltonians. We compare the QMC results also with DFT calculations with hybrid functionals.

4:18PM T21.00010 Fixed-Node Errors in Diffusion Monte Carlo Study of Li Molecular and Solid Systems , KEVIN RASCH, LUBOS MITAS, North Carolina State University — We study the fixed-node bias in the Diffusion Monte Carlo calculations of Li systems such as Li dimer, Li clusters, and Li body-centered cubic crystal at the equilibrium lattice constant. The calculations include both core and valence electrons in order to avoid any possible impact by pseudopotentials. We examine the fixed-node errors for different types of orbitals and wave-function forms. We use estimations of exact total energies from alternative approaches such as correlated basis set methods or from experiment. The results suggest that for Li systems it is possible to construct accurate wave-functions which recover correlation energy at 97-99 % of correlation energy in the full many-body framework.

4:30PM T21.00011 Comparison of the Angular Dependence of Monte Carlo Particle Transport Modeling Software , JEFF CHANCELLOR, National Space Biomedical Research Institute, STEPHEN GUETERSLOH, Texas A&M University — Modeling nuclear interactions is relevant to cancer radiotherapy, space mission dosimetry and the use of heavy ion research beams. In heavy ion radiotherapy, fragmentation of the primary ions has the unwanted effect of reducing dose localization, contributing to a non-negligible dose outside the volume of tissue being treated. Fragmentation in spaceship walls, hardware and human tissue can lead to large uncertainties in estimates of radiation risk inside the crew habitat. Radiation protection mandates very conservative dose estimations, and reduction of uncertainties is critical to avoid limitations on allowed mission duration and maximize shielding design. Though fragment production as a function of scattering angle has not been well characterized, experimental simulation with Monte Carlo particle transport models have shown good agreement with data obtained from on-axis detectors with large acceptance angles. However, agreement worsens with decreasing acceptance angle, attributable in part to incorrect transverse momentum assumptions in the models. We will show there is an unacceptable angular discrepancy in modeling off-axis fragments produced by inelastic nuclear interaction of the primary ion. The results will be compared to published measurements of 400 MeV/nucleon carbon beams interacting in C, CH2, Al, Cu, Sn, and Pb targets.

4:42PM T21.00012 A Quantum Monte Carlo study of Hydrogen Adsorption on Carbon and Transition Metal Systems[1] , TODD D. BEAUDET, University of Illinois at Urbana-Champaign, Presently U. S. Army Research Laboratory, JEONGNIM KIM, RICHARD M. MARTIN, University of Illinois at Urbana-Champaign — We present a quantum Monte Carlo study of many molecular structures of Ti-ethylene with up to 5 H_2 molecules. These structures have been of recent interest due to energetics favorable for reversibly storing hydrogen.[2] Diffusion Monte Carlo is employed with the fixed node approximation and pseudopotentials that have been tested for H_2 adsorbed on benzene and calculations on TiH_2 molecules.[3] Many low energy configurations were studied by calculation of ground and excited states energy surfaces. The formation energies are comparable to other work[4] and indicate that at least 3 hydrogen molecules can be adsorbed with energies in the range considered relevant for practical hydrogen storage.

[1]NSF grants DMR-0325939 and DMR-0404853 and U.S. Army A6062 UMC00005071-3.

[2]E. Durgun *et al.*, Phys. Rev. Lett. **97**, 226102 (2006).

[3]T. D. Beaudet, Doctoral Dissertation, University of Illinois at Urbana-Champaign (2010).

[4]Y. Y. Sun *et al.*, Phys. Rev. B **82**, 073401 (2010).

4:54PM T21.00013 Release-Node quantum Monte Carlo studies for molecules[1] , NORM TUBMAN, Northwestern University, JONATHAN DUBOIS, RANDOLPH HOOD, BERNI ALDER, Lawrence Livermore National Lab — Release-Node quantum Monte Carlo (RN-QMC) is a method that calculates unbiased ground-state energies of fermionic systems. However, while RN-QMC has been successfully applied to the homogeneous electron gas with more than one hundred electrons, obtaining converged results for molecular systems has proven to be problematic for all but the smallest systems. A promising route to extending the method's success to a wider class of physically interesting Hamiltonians lies in the application of projection techniques such as Maximum Entropy (MaxEnt) which, in principle, allows for extrapolation to the converged ground-state energy. Direct application of MaxEnt to higher Z elements is, however, not entirely straightforward. We propose strategies for optimizing MaxEnt analysis of short time RN-QMC data and demonstrate their effectiveness in obtaining ground state energies for the first row dimers. Attention is given to the determination of statistical errors in the resulting extrapolations as well as an attempt to characterize the minimum decay time required for unbiased results.

[1]Prepared by LLNL under Contract DE-AC52-07NA27344

5:06PM T21.00014 Melting transition of Lennard-Jones particles in two dimensions , KEOLA WIERSCHEM, Nanyang Technological University, EFSTRATIOS MANOUSAKIS, Florida State University and University of Athens — The melting transition of Lennard-Jones particles in two dimensions is investigated along a single isochore using classical Monte Carlo methods. A finite-size scaling analysis is conducted for the second moments of the translational and bond-orientational order parameters, and their critical exponents are determined. The behavior of these exponents is consistent with the predictions of the two-stage Kosterlitz-Thouless-Halperin-Nelson-Young (KTHNY) theory of melting in two dimensions. The translational and bond-orientational correlation lengths are also studied, with evidence of a divergence in the bond-orientational correlation length while the translational correlation length remains finite. This provides further support for the KTHNY melting scenario, although we cannot rule out possible phase co-existence due to a first order phase transition.

5:18PM T21.00015 Micro-canonical Monte Carlo study of spin wave excitations in 2D XY model[1] , SMITA OTA[2], Institute of Mathematics and Applications, Bhubaneswar 751022 — We have carried out micro-canonical Monte Carlo simulation of 2D XY model in a 30x30 lattice using periodic boundary conditions. In this micro-canonical Monte Carlo simulation, the energy is the input quantity and the temperature of the system is obtained from the simulations. Spin waves and bound vortex excitations dominate in the 2D XY model below the topological vortex unbinding transition. We have studied the spin waves from the energy distribution of an individual spin in the 2D XY model. The most probable spin wave energy corresponds to the maximum in the energy distribution. The probability of the spin wave excitation is found to be reduce exponentially, by an order of magnitude as the temperature increases to the topological transition.

[1]The author acknowledges finantial support from DST, New Delhi, India.

[2]Oral presentation

Wednesday, March 23, 2011 2:30PM - 5:30PM –
Session T22 DCMP: Correlated Electrons and Magnetic Phase Transitions D163

2:30PM T22.00001 Quantum spin metal state on a decorated honeycomb lattice , KONSTANTIN TIKHONOV, Texas A&M Univ., MIKHAIL FEIGEL'MAN, Landau ITP — We present a modification of exactly solvable spin-(1/2) Kitaev model on the decorated honeycomb lattice, with a ground state of "spin metal" type. The model is diagonalized in terms of Majorana fermions; the latter form a 2D gapless state with a Fermi-circle those size depends on the ratio of exchange couplings. Low-temperature heat capacity $C(T)$ and dynamic spin susceptibility $\chi(\omega, T)$ are calculated in the case of small Fermi-circle. Whereas $C(T) \sim T$ at low temperatures as it is expected for a Fermi-liquid, spin excitations are gapful and $\chi(\omega, T)$ demonstrate unusual behavior with a power-law peak near the resonance frequency. The corresponding exponent as well as the peak shape are calculated.

2:42PM T22.00002 Quantum Order by Disorder Driven Phase Reconstruction at Itinerant Electron Quantum Critical Points , UNA KARAHASANOVIC, ANDREW GREEN, University of St Andrews, GARETH CONDUIT, Weizmann Institute of Science — Phase reconstruction at itinerant electron quantum critical points is driven by quantum fluctuations lowering the energy of certain deformations of the Fermi surface through second and higher order perturbation theory, i.e. quantum order by disorder. This approach was previously shown to predict a fluctuation-driven spatially modulated phase near to the ferromagnet to paramagnet quantum critical point [1]; a phase that had previously been predicted from diagrammatic evaluation of non-analytic corrections to Moriya-Hertz-Millis theory. We extend our analysis to include several other phases which may be stabilized at the ferromagnetic quantum critical point, including nematic order and superconductivity. The itinerant quantum critical point is unstable to the formation of multiple phases.

[1] G. J. Conduit, A. G. Green and B. D. Simons, Phys. Rev. Lett. **103**, 207201 (2009)

2:54PM T22.00003 Fixed Spin Moment Study of Quantum Critical Fe_3Mo_3N , BRIAN NEAL, WARREN E. PICKETT, University of California Davis — Quantum critical behavior and weak magnetism occurs in a handful of intermetallic transition metal compounds, with a recent example being Fe_3Mo_3N with the geometrically frustrated *stella quadrangula* lattice. Neutron scattering reveals antiferromagnetic ordering, but a 14 T magnetic field induces a ferromagnetic state as does substitution of 5% Co on the Fe site [1]. We present the energetics of a transition between these states with density functional based fixed spin moment studies. Our (mean field) ground state occurs with nearly equal Fe1 and Fe2 moments of 1.8 μ_B. As the total moment is reduced, a crossover occurs until at zero total moment the Fe1 moment is -1.1 μ_B (antialigned with the strong Fe2 moment). We use these results to construct scenarios for discussing the observations.

[1] T. Waki et al., J. Phys. Soc. Japan **79**, 043701 (2010).

3:06PM T22.00004 Stability of Quantum Critical Points in the Presence of Competing Orders , JIAN-HUANG SHE, JAN ZAANEN, Leiden University, ALAN BISHOP, ALEXANDER BALATSKY, Los Alamos National Laboratory — We investigate the stability of Quantum Critical Points (QCPs) in the presence of two competing phases. These phases near QCPs are assumed to be either classical or quantum and assumed to repulsively interact via square- square interaction. We find that for any dynamical exponents and for any dimensionality strong enough interaction renders QCPs unstable, and drive transitions to become first order. We propose that this instability and the onset of first order transition leads to spatially inhomogeneous states in practical materials near putative QCPs.

3:18PM T22.00005 Field-Induced Orbital Antiferromagnetism in Mott Insulators , K.A. AL-HASSANIEH, C.D. BATISTA, Los Alamos National Laboratory, G. ORTIZ, Indiana University, Bloomington, L.N. BULAEVSKII, Los Alamos National Laboratory — We report on a new electromagnetic phenomenon that emerges in Mott insulators. The phenomenon manifests as antiferromagnetic ordering due to orbital electric currents which are spontaneously generated from the coupling between spin currents and an external homogenous magnetic field. This novel spin-charge-current effect provides the mechanism to measure the so-far elusive spin currents by means of unpolarized neutron scattering, nuclear magnetic resonance or muon spectroscopy. We illustrate this mechanism by solving a half-filled Hubbard model on a frustrated ladder.

3:30PM T22.00006 Global phase diagram of heavy fermions and the Kondo destroyed quantum critical points of Anderson models with a transverse field , JEDEDIAH PIXLEY, Rice University, STEFAN KIRCHNER, Max Planck Institute for the physics of complex systems, QIMIAO SI, Rice University — Recent studies in quantum critical heavy fermion metals have pointed towards a global phase diagram [1]. The zero-temperature phase diagram involves a combination of phases, featuring Kondo screening/breakdown and antiferromagnetic order/disorder as the quantum fluctuations of the local moments are tuned relative to their effective interaction with the spins of the conduction electrons. In the case of Ising-anisotropic Kondo lattice systems, the fluctuations among the local moments can be generated by coupling them to a transverse magnetic field. With these effects in mind, we study the Kondo-destroyed quantum critical behavior of the Anderson impurity model in the presence of a bosonic bath or a transverse field. We extend our recent studies of the low-temperature quantum critical behavior [2,3] based on the continuous time quantum Monte Carlo, and obtain the dynamical scaling functions of the local spin susceptibility and single-electron Green's function.

[1] Q. Si and F. Steglich, Science 329, 1161 (2010).
[2] M. T. Glossop, S. Kirchner, J. H. Pixley and Q. Si, arXiv:0912.4521 to be published (2009).
[3] J. H. Pixley, S. Kirchner and Q.Si, arXiv:1010.3024 to be published (2010).

3:42PM T22.00007 Electron paring instabilities in 8-site Betts lattice: exact result[1] , KUN FANG, GAYANATH FERNANDO, University of Connecticut, ARMEN KOCHARIAN, California State University, Los Angeles — We use numerical methods (exact diagonalization and Lanczos method) to study single-orbital and multi-orbital Hubbard models (off half filling). The whole lattice is divided into identical 8-site square clusters immersed in a thermal bath. The electron pairing instabilities, order parameters and quantum critical points are evaluated by monitoring the charge and spin gaps in a wide range of parameters including the on-site interaction U. Calculations show level crossing behaviors at zero and finite temperature. The corresponding pairing instabilities are remarkably similar to electronic inhomogeneities observed in correlated systems such as the high temperature superconductors and Fe pnictides. The next nearest hopping is also introduced. We find that it can shift quantum crossover point and gap magnitude, but for reasonable hopping amplitudes, it will not eliminate characteristics of electron paring instabilities.

[1]The authors acknowledge the computing facilities provided by the Center for Functional Nanomaterials, Brookhaven National Laboratory, which is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH1088

3:54PM T22.00008 Functional RG for the Single Impurity Anderson Model , MICHAEL KINZA, RWTH Aachen University, CARSTEN HONERKAMP, RWTH Aachen Universtity, JUTTA ORTLOFF, Wuerzburg University — We present a functional Renormalization Group (fRG) approach to the Single Impurity Anderson Model at finite temperatures. Starting with the exact spectral function and interaction vertex of a small system ("core") containing a correlated site, we switch on the hybridization with a non-interacting bath in the RG-flow and calculate spectra of the correlated site. Different truncations of the RG-flow-equations and choices of the core are compared and discussed. Furthermore we calculate the linear conductance as function of temperature and interaction strength.

4:06PM T22.00009 Mesoscopic Anderson Box: Connecting Weak to Strong Coupling , DONG E. LIU, Duke University, SEBASTIEN BURDIN, Univ. of Bordeaux I, France, HAROLD U. BARANGER, Duke University, DENIS ULLMO, Univ. Paris Sud, France — Both the weakly coupled and strong coupling Anderson impurity problem are characterized by a Fermi-liquid theory with weakly interacting quasiparticles. In an Anderson box, mesoscopic fluctuations of the effective single particle properties will be large. We study how the statistical fluctuations in these two problems are connected. We use random matrix theory and the slave boson mean field approximation (SBMF, at low temperature) to address this question, obtaining the following results. First, for a resonant level model such as results from the SBMF approximation, we find the joint distribution of energy levels with and without the resonant level present. Second, if only energy levels within the Kondo resonance are considered, the distribution of perturbed levels collapse to one universal form for both GOE and GUE for all values of the coupling V. Finally, a purely Fermi liquid method is developed for calculating the perturbed levels within the Kondo resonance. Comparing the levels that result to those of the SBMF, we find remarkable agreement.

4:18PM T22.00010 Superconducting pairing of interacting electrons: implications from the two-impurity Anderson model[1] , LIJUN ZHU, JIAN-XIN ZHU, Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — We study the non-local superconducting pairing of two interacting Anderson impurities, which has an instability near the quantum critical point from the competition between the Kondo effect and an antiferromagnetic inter-impurity spin exchange interaction. As revealed by the dynamics over the whole energy range, the superconducting pairing fluctuations acquire considerable strength from an energy scale much higher than the characteristic spin fluctuation scale while the low energy behaviors follow those of the staggered spin susceptibility. We argue that the superconducting pairing might not need the spin fluctuations as the glue, but rather originated from the effective Coulomb interaction. On the other hand, critical spin fluctuations in the vicinity of quantum criticality are also crucial to a superconducting pairing instability, by preventing a Fermi liquid fixed point being reached to keep the superconducting pairing fluctuations finite at low energies. A superconducting order, to reduce the accumulated entropy carried by the critical degrees of freedom, may arise favorably from this instability.

[1]This work is supported by the U.S. DOE through the LANL/LDRD program.

4:30PM T22.00011 Pressure Tuning of the Shastry-Sutherland Quantum Phase Transition , S. HARAVIFARD, Argonne National Laboratory, University of Chicago, A. BANERJEE, T.F. ROSENBAUM, University of Chicago, G. SRAJER, J.C. LANG, Y. FENG, Argonne National Laboratory, B.D. GAULIN, H.A. DABKOWSKA, McMaster University — SrCu2(BO3)2 is a quasi-2D quantum spin system known to possess a collective singlet ground state. It serves as an experimental realization of the Shastry-Sutherland model for interacting S=1/2 dimers. The ratio of the intra and inter-dimer exchange in this compound is close to a quantum critical point, where the ground state transforms from a gapped, non-magnetic state to a gapless long-range ordered antiferromagnetic state as a function of the ratio of the strength of the magnetic interactions. We use synchrotron x-ray diffraction in a diamond anvil cell to investigate the pressure-driven quantum phase transition in high-quality single crystals of SrCu2(BO3). We will present the evolution of both the magnetic and structural properties up to pressures of 5 GPa.

4:42PM T22.00012 Quantum phase transitions in generalized J-Q models , ARNAB SEN, ANDERS SANDVIK, Boston University — The "J-Q" model is an extension of the Heisenberg model which contains multi-spin interactions that suppress Néel order and lead to a valence-bond-solid (VBS) ground state. It is free from quantum Monte Carlo (QMC) sign problems. There is now good evidence from QMC studies for a continuous Néel–VBS transition with non-trivial features like a large anomalous exponent η and an emergent U(1) VBS symmetry at the quantum-critical point in this model. We study various generalizations of the J-Q model, with both SU(2) and U(1) symmetric interactions, to further elucidate unusual aspects of the Néel-VBS transition. In the SU(2) case, we construct a model which stabilizes a staggered VBS instead of the columnar pattern obtained in previous studies. This type of VBS does not harbor an emergent U(1) symmetry near the transition. We find that the transition is strongly first-order, unlike in the original J-Q model. This illustrates the importance of the emergent U(1) symmetry for the possibly exotic transition in the standard J-Q model. We also investigate a new U(1)-symmetric generalization of the J-Q model to explore such unconventional transitions in the easy plane case.

4:54PM T22.00013 Criticality of compact and noncompact $(1+1)D$ quantum dissipative Z_4-models , EINAR STIANSEN, IVER SPERSTAD, ASLE SUDBO, Norwegian University of Science and Technology — We study two versions of a $(1+1)D$ Z_4-symmetric model with Ohmic bond dissipation. In one version the phase variable is restricted to the interval $[0, 2\pi\rangle$, while the domain is unrestricted in the other. The compact model features a completely ordered phase with a broken Z_4-symmetry and a disordered phase, separated by a critical line. The non-compact model features three phases. In addition to the two phases exhibited by the compact model, there is also an intermediate phase, characterized by isotropic power-law phase correlations. We calculate the dynamical critical exponent z along the critical lines of both models to see if the compactness of the variable is relevant to the critical scaling between space and imaginary time. We find $z \approx 1$ for the single phase transition in the compact model as well as for both transitions in the non- compact model.

5:06PM T22.00014 Kondo and spin-Peierls phases and Berry phase effects in Heisenberg-Kondo chain[1] , PALLAB GOSWAMI, QIMIAO SI, Rice University — Recent theoretical and experimental results on heavy fermion systems have motivated a global phase diagram, as a function of the Kondo coupling and the strength of quantum fluctuations of the local moments. Correspondingly, there has been growing interest in understanding the phase transition from a small Fermi surface antiferromagnet to large or small Fermi surface paramagnets with or without Kondo screening respectively. Because a perturbative nonlinear sigma model analysis only accesses the small Fermi surface antiferromagnetic phase, the transition into the paramagnetic phases must involve non-perturbative effects. We consider here the effect of the instanton configurations of the nonlinear sigma model and the associated Berry's phase for the Kondo singlet formation, and for concreteness focus on the one dimensional Heisenberg Kondo lattice model. Using semiclassical nonlinear sigma model and bosonization techniques both at and away from half-filling, we demonstrate how the competition between the Kondo singlet and spin Peierls phases are manifested through the effects of such a Berry phase. Based on these results we comment upon similar effects that may be realized in higher dimensional Kondo lattice models.

[1]NSF

5:18PM T22.00015 Complex Critical Exponents in Diluted Systems of Quantum Rotors[1] , RAFAEL FERNANDES, JÖRG SCHMALIAN, Ames Laboratory and Iowa State University — In this work, we investigate the effects of the Berry phase $2\pi\rho$ on the critical properties of XY quantum-rotors that undergo a percolation transition. This model describes a variety of randomly-diluted quantum systems, such as interacting bosons coupled to a particle reservoir, quantum planar antiferromagnets under a perpendicular magnetic field, and Josephson-junction arrays with an external bias-voltage. Focusing on the quantum critical point at the percolation threshold, we find that, for rational ρ, one recovers the power-law behavior with the same critical exponents as in the case with no Berry phase. However, for irrational ρ, the low-energy excitations change completely and are given by emergent spinless fermions with fractal spectrum. As a result, critical properties that cannot be described by the usual Ginzburg-Landau-Wilson theory of phase transitions emerge, such as complex critical exponents, log-periodic oscillations, and dynamically-broken scale invariance.

[1]Research supported by the U.S. DOE, Office of BES, Materials Science and Engineering Division.

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T23 DMP: Focus Session: Search for New Superconductors III: Reduced Dimensionality

D165

2:30PM T23.00001 Understanding anisotropy to develop superconducting design principles , FILIP RONNING, Los Alamos National Laboratory — Superconductivity is often found in families of compounds which share a common building block (e.g. CuO_2 planes in cuprates, FeAs planes in pnictides, and $CeIn_3$ planes in a subset of heavy fermion superconductors). This fact provides a rationale to search for new superconductors, and subsequently a means to try and understand the origin of superconductivity by examining trends in superconducting behavior within a family of superconductors which hopefully transcends any one particular family of compounds. The notion of common building blocks has led us to the recent discovery of superconductivity at 2.1 K in $CePt_2In_7$, coexisting magnetism and superconductivity in $PuCoIn_5$, and a correlated paramagnet in $PuPt_2In_7$. I will discuss our attempts to understand the role of reduced dimensionality and increased bandwidth within the "115" class of heavy fermion superconductors by examining trends in the charge and spin degrees of freedom that are correlated with superconductivity. In this way, we aim to lay the foundation for a modern, microscopic version of Matthias' rules for unconventional superconductivity from which superconducting design principles can be developed. In collaboration with Eric Bauer, Jianxin Zhu, Paul Tobash, Moaz Altarawneh, HB Rhee, Hironori Sakai, Kris Gofryk, Neil Harrison, and Joe Thompson.

3:06PM T23.00002 $PuCoIn_5$: A New Magnetic Superconductor , ERIC D. BAUER, J.N. MITCHELL, P.H. TOBASH, F. RONNING, J.-X. ZHU, B.L. SCOTT, J.D. THOMPSON, Los Alamos National Laboratory — There is renewed interest in actinide research following the discovery of superconductivity at T_c=18.5 K in $PuCoGa_5$ and at T_c=8.7 K in $PuRhGa_5$. These materials appear to be unconventional superconductors with a moderate effective mass enhancement and are similar to the more well characterized $CeMIn_5$ (M=Co, Rh, Ir) superconductors. We have discovered a new member of this "115" family of superconductors, $PuCoIn_5$. This material superconducts at T_c=2.7 K and exhibits another phase transition at T_N=15 K, likely due to antiferromagnetic order. The Sommerfeld coefficient γ = 200 mJ/mol K^2 and the large initial slope of the upper critical field indicate a large enhancement of the effective mass. The physical properties of $PuCoIn_5$ will be discussed.

3:18PM T23.00003 Search for Superconductivity in Carbon Nanotubes Doped by Boron Ion Implantation , NICHOLAS CORNELL, ALEX KUTSENOV, AUSTIN HOWARD, NATHANIEL MAYO, EDUARD GALSTAYAN, WEI KAN CHU, HERBERT FREYHARDT, ANVAR ZAKHIDOV, XUEMEI WANG, UNIVERSITY OF TEXAS AT DALLAS TEAM, UNIVERSITY OF HOUSTON TEAM — The boron doping of single wall carbon nanotubes(CNT) by laser ablation synthesis has been reported to create superconducting B-CNTs with Tc's ranging from 12-19 Kelvin, depending on CNT inter-tube connection strength. We attempt to create boron doped multiwall CNT by ion implantation doping. Ion doping of boron(B) was performed at 60keV and 20keV, and low temperature transport combined with SQUID and ESR/LFMA was used in searching for SC. We have found that R(T) strongly depends on the metallic contact geometry. With thin film contacts on CNT sheets the R(T) shows no SC signatures, while when an Ag or Au paste penetrates the highly porous network of B doped multiwall CNT then R(T) drops and curvature changes are observed resembling SC transitions with Tc depending on B concentration and metallic electrode distances. We discuss these results in terms of possible SC in hybride "metal-CNT" system in which metal was predicted to supress phase fluctuation in one dimensional CNT network [1].

[1] Erez Berg, Dror Orgad, and Steven A. Kivelson, Phys. Rev. B 78, 094509(2008)

3:30PM T23.00004 Low Field Microwave Absorption Studies of Carbon Nanotubes Doped by Chemical and Ion Implantation Techniques , AUSTIN HOWARD, ALEXANDER KUZNETSOV, NICHOLAS CORNELL, MYRON SALAMON, The University of Texas at Dallas, EDUARD GALSTAYAN, WEI KAN CHU, HERBERT FREYHARDT, The University of Houston, RAY BAUGHMAN, The University of Texas at Dallas, JUNJI HARUYAMA, JASON REPPERT, APPARAO RAO, Clemson University, ANVAR ZAKHIDOV, The University of Texas at Dallas — The motivation of this study is to develop a highly sensitive method of microwave absorption in low magnetic fields (LFMA), combined with SQUID magnetometry and resistivity, for searching for superconducting phases in in-situ doped nanomaterials; either chemically (by alkali metals or metalloids) or through Boron ion implantation. These methods have been applied to both MWNTs grown by CVD, as well as SWNTs which have been separated into metallic and semiconducting chiralities. Regardless of the doping technique or element, we have found a much higher rate of doping in the semiconducting SWNTs. Additionally, in the Boron doped SWNTs, we see two transitions at $\sim$8 K and $\sim$30 K, but the nature of the transition is not clear at the moment: it depends on the type of measurement. While SQUID and resistivity indicate a superconducting type transition, LFMA/ESR reveals that there is a clear magnetic transition at 30 K. Resolution of these differing results will be discussed.

3:42PM T23.00005 Electric Field Induced Superconductivity in Layered Materials , J.T. YE, Department of Applied Physics, The University of Tokyo, M.F. CRACIUN, S. RUSSO, Centre for Graphene Science, University of Exeter, M.F. MORPURGO, DPMC and GAP, Université de Genéve, Y. KASAHARA, H.T. YUAN, H. SHIMOTANI, Y. IWASA, Department of Applied Physics, The University of Tokyo — Using electric double layer (EDL) gating, large amount of carriers can be accumulated on a broad range of materials, which provides new opportunities in effectively manipulating their electronic properties in complementary with the chemical doping. In searching for novel transport phenomena, layered materials are advantageous because atomically flat surface can be easily fabricated using the graphene techniques. We used layered material: ZrNCl and graphite to act as the channel of EDL transistors. For both ZrNCl and graphene, we achieved high carrier density up to 10^{14} cm^{-2}, electrostatically. For graphene, we studied the high carrier density transport for graphene of 1-3 layers. Transport properties at the high carrier density exhibit clear layer dependence governed by the intrinsic band structures of graphene and its multi-layers. For ZrNCl EDL transistor, we observed metallic states at gate voltage higher than 3.5 V followed by gate-induced superconductivity after metal-insulator transition when the transistor was cooled down to about 15 K.

3:54PM T23.00006 Electric Double Layer Charging on Graphene[1] , FENG CHEN, BING LV, YUYI XUE, C.W. CHU[2], Dept. of Physics and Texas Center for Superconductivity, University of Houston, Houston, TX 77204-5002, HOWARD WANG, Dept. of Mechanical Engineering, Binghamton University, Binghamton, NY 13902-6000 — Electric Double Layer (EDL) charging as a new charging method has attracted wide interests recently. We have employed this method to graphene and obtained an estimated surface charge density of 4×10^{15} electrons/cm^2. The resistance dropped significantly upon charging and the physical properties under various charging conditions were studied. We will present these along with results of the EDL charging on other superconducting candidates.

[1]Work supported in part by AFOSR, DoE, CONTACT, the T. L. L. Temple Foundation, the John J. and Rebecca Moores Endowment and the State of Texas through TCSUH

[2]Also at: Lawrence Berkeley National Laboratory

4:06PM T23.00007 Search for new superconductors in the La-Si-C system[1] , JOSE DE LA VENTA, ALI C. BASARAN, University of California, San Diego, TED GRANT, ANTONIO JEFFERSON S. MACHADO, ZACHARY FISK, University of California, Irvine, IVAN K. SCHULLER, University of California, San Diego — We have searched for the presence of superconductivity in the La-Si-C system in bulk and thin film samples. This system has some of the common features that are present in high T_C superconducting materials. It is a multi-element compound and also incorporates a light element, Carbon. Furthermore, one of the binary phases, La_5Si_3 exhibits a tetragonal layered structure. This system exhibits the presence of a possible new superconducting compound with T_C's ranging from 6.1 K to 8.5 K. In the binary La-Si system there are five inter-metallic phases. Among these phases, those that exhibit superconductivity are: $LaSi_2$ with T_C of 2.3 K, La_3Si_2 with a T_C of 2.1 K and La_5Si_3 with a T_C of 1.6 K. A careful analysis of several physical properties (SQUID, Modulated Microwave Absorption) and x-ray powder diffraction, (using Rietveld refinement) shows that superconductivity in this system could be ascribed to intermediate binary (La_2C_3) and single (La-β) phases of the system.

[1]This study was supported by an AFOSR MURI "Search For New Superconductors For Energy And Power Applications."

4:18PM T23.00008 Superconducting properties of quasi-one dimensional graphene , GEORGE KARAKONSTANTAKIS, STEVE KIVELSON, Stanford University — We study quasi-one dimensional graphene (polyacene) two leg ladders modeled by repulsive U Hubbard model using DMRG. The strong repulsive interactions along with the high density of states at the Fermi energy enhance the conducting properties of the ladder (which is a conductor) and give rise to enhancement of the pairing energy scales, having to do with the superconducting properties of the ladder. The presence of phonons in this system has been known to give rise to Peierls ans superconducting instabilities as well.

4:30PM T23.00009 Unusual Superconductivity in the Homologous Series $(Cu_{0.75}Mo_{0.25})Sr_2(Ce,Y)_sCu_2O_{5+2s+\delta}$, OMAR CHMAISSEM, Northern Illinois University and Argonne National Laboratory, Illinois, USA, INGA GRIGORAVICIUTE, MAARIT KARPPINEN, HISAO YAMAUCHI, Aalto University School of Science and Technology, Aalto, Finland and Tokyo Institute of Technology, Yokohama, Japan, MASSIMO MAREZIO, CRETA/CNRS, Grenoble, France — The structures and bulk superconductivity (>30% Meissner volume fraction) of the first four members of the high-T_c series $(Cu_{0.75}Mo_{0.25})Sr_2(Ce,Y)_sCu_2O_{5+2s+\delta}$have been successfully determined. Partial Mo substitution for Cu in the square-chains enhances T_c to 87 K (for s= 1) and leads to significant oxygen loading capabilities well beyond the levels achieved in typical $YSr_2Cu_3O_{6+\delta}$, $YBa_2Cu_3O_{6+\delta}$, and other similar cuprates. Higher members of the series have their adjacent superconducting CuO_2 layers separated by increasingly thicker fluorite-like $(Ce,Y)_2O_2$ insulating blocks. Insertion of two or more of these blocks must drastically affect the CuO_2 interlayer coupling and causes T_c to immediately drop and saturate at ∼57 K (s = 2-4). The infinite chains of Cu-centered squares in YBCO change to alternate chains of mixed Cu squares and Cu and Mo octahedra. Neutron diffraction confirms the formation of reservoir blocks with a new structure and stoichiometry and of a surprisingly large Cu oxidation state of ∼2.5+, suggesting the possibility of an unusual superconducting pairing mechanism.

4:42PM T23.00010 Electrical Transport Properties of Boron-Based Nanostructures[1] , JOEL D. CHUDOW, DANIEL F. SANTAVICCA, LUIGI FRUNZIO, DANIEL E. PROBER, Dept. of Applied Physics, Yale University, MICHAEL ROOKS, Yale Institute for Nanoscience and Quantum Engineering, Yale University, ESWARAMOORTHI IYYAMPERUMAL, GAYATRI KESKAR, FANG FANG, LISA PFEFFERLE, Dept. of Chemical Engineering, Yale University — Many metal boride materials exhibit interesting electrical properties. Bulk MgB_2 has a superconducting transition temperature of 39 K. Boron-based nanostructures are predicted to possess special properties superior to those of other one-dimensional nanomaterials. Recent progress in material fabrication has enabled the successful synthesis of boron-based nanomaterials [J. Phys. Chem. C 113, 17661 (2009)]. Magnetization measurements of magnesium-boride nanostructures show evidence of a diamagnetic transition at high temperature, about 80 K. We describe electrical transport measurements of individual single nanowires composed of these and related materials.

[1]This work supported by AFOSR and NSF-DMR.

4:54PM T23.00011 Structure and electronic properties of the $La_4Ni_3O_8$, KONSTANTIN LOKSHIN, TAKESHI EGAMI, University of Tennessee — The Ni^{1+}/Ni^{2+} states of nickelates have the identical ($3d^9/3d^8$) electronic configuration as Cu^{2+}/Cu^{3+} in the high temperature superconducting cuprates, and are expected to show interesting properties. However, $La_4Ni_3O_8$, has infinite NiO_2 layers with Ni valence 1.33 and demonstrate a magnetic transition at 105 K, which has not been explained unambiguously yet. Here we report X-rays and Neutron diffraction evidences clarifying the nature of the transition. The observed structural changes around 105 K suggest that the magnetic transision in $La_4Ni_3O_8$ originates from Yahn Teller effect that accompanies with high spin – low spin transition. Thus, at low temperature the structural motive, electronic configuration and the spin state of Ni^{1+}/Ni^{2+} nickelates are identical to Cu^{2+}/Cu^{3+} cuprates.

5:06PM T23.00012 Transport and Spectroscopy Studies of Ultrathin Doped Nickelate Films , YARON SEGAL, JOSEPH NGAI, DIVINE KUMAH, ANKIT DISA, JAMES REINER, JARRET MOYER, Yale University Applied Physics, DARIO ARENA, Brookhaven National Lab, FRED WALKER, CHARLES AHN, Yale University Applied Physics — The notion of a rational, first-principles based design of a novel superconducting material has intrigued physicists for decades. Recently it was suggested that by enforcing a two- dimensional confinement and tensile strain on $LaNiO_3$ films, their electronic structure can be made sufficiently similar to that of the Mott-Hubbard system in the cuprates, possibly inducing an antiferromagnetic insulator-superconductor transition [PRL 100, 016404]. We adopt this approach through the synthesis of ultrathin $La_xNd_{1-x}NiO_3$ and hole-doped $La_xBa_{1-x}NiO_3$, $Nd_xBa_{1-x}NiO_3$ films using molecular beam epitaxy. High structural quality is demonstrated by RHEED oscillations and synchrotron x-ray diffraction. Transport measurement show a transition from metallic behavior to localization for films less than 8 uc thick. Tuning of the La/Nd ratio allows the film to be driven into the antiferromagnetic insulating regime. Surprisingly, Ba incorporation increases the localization in the films, which is in contrast to the metallicity-promoting effect of hole doping in bulk nickelates. X-ray absorption measurements allow us to follow the evolution of the Ni and O orbitals and relate it to the observed transport properties.

5:18PM T23.00013 Superconductivity at 7.7 K in new hexagonal bronze Hg_xReO_3 , KENYA OHGUSHI, University of Tokyo, JST-TRIP, AYAKO YAMAMOTO, RIKEN, JST-TRIP, YOKO KIUCHI, CHANDREYEE GANGULI, University of Tokyo, KAZUYUKI MATSUBAYASHI, YOSHIYA UWATOKO, University of Tokyo, JST-TRIP, HIDENORI TAKAGI, RIKEN, University of Tokyo, JST-TRIP — We have successfully synthesized a new rhenium-based hexagonal bronze material, Hg_xReO_3, which exhibits superconductivity with the transition temperature $T_c = 7.7$ K at ambient pressure and 11.1 K at 4 GPa. This compound is a superconductor with the highest T_c among hexagonal bronzes. Moreover, it presents the novel crystallographic feature that $(Hg_2)^{2+}$ polycations, in contrast to monatomic cations in known hexagonal bronzes, are incorporated into open channels. There is evidence that conducting electrons tightly couple with Hg-related phonons. Our results inspire detailed studies on the role of the rattling phonon in the occurrence of superconductivity in the hexagonal bronzes.

Wednesday, March 23, 2011 2:30PM - 5:06PM –

Session T24 DCOMP: Focus Session: Quantum Transport Simulations and Computational Electronics – Disorder D167

2:30PM T24.00001 Recent progress in computational electronics: disorder effects in nonequilibrium quantum transport[1]

, HONG GUO, McGill University — Realistic nanoelectronic devices inevitably have some disorder which affect device operation. Unintentional impurities sit at unpredictable locations and any predicted quantum transport property should be averaged over the impurity configurations. Impurity atoms are also intentionally doped into device material where the average is also necessary. One may generate many impurity configurations, calculate all and average the results. Such a brute force approach is not practical for first principles analysis as it is computationally too costly. I shall present the theory of nonequilibrium vertex correction (NVC) [1] where the configurational average is analytically done resulting to a NVC self-energy contributing to the nonequilibrium density matrix. NVC accounts for multiple impurity scattering at nonequilibrium. By integrating NVC with the density functional theory (DFT) and Keldysh nonequilibrium Green's functions (NEGF), nonequilibrium quantum transport in nanoelectronic systems having atomistic disorder can be carried out. By further integrating a recently proposed semi-local exchange potential that accurately determines band gaps [2], semiconductor nanoelectronics can now be analyzed from atomic first principles. Several examples will be presented including disorder scattering in Fe/MgO/Fe magnetic tunnel junction, electronic structure of $In_xGa_{1-x}N$ with varying concentrations x for solar cells, and quantum transport properties of doped Si membrane.

[1] Youqi Ke, Ke Xia and Hong Guo, Phys. Rev. Lett. 100, 166805 (2008); *ibid* (in print, 2010).
[2] Fabien Tran and Peter Blaha, Phys. Rev. Lett. 102, 226401 (2009).

[1]Work in collaboration with Youqi Ke and Ke Xia.

3:06PM T24.00002 Seebeck Coefficients in Nanoscale Junctions: Effects of Electron-Vibration Scattering and Local Heating[1]

, BAILEY C. HSU, Department of Electrophysics, National Chiao Tung University, Taiwan, YU-SHEN LIU, College of Physics and Engineering, Changshu Institute of Technology, China, SHEN HSIEN LIN, Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan. Department of Applied Chemistry, National Chiao Tung University, Taiwan, YU-CHANG CHEN, Department of Electrophysics, National Chiao Tung University, Taiwan — We report first-principles calculations of inelastic Seebeck coefficients in an aluminum monatomic junction. We compare the elastic and inelastic Seebeck coefficients with and without local heating. In the low temperature regime, the signature of normal modes in the profiles of the inelastic Seebeck effects is salient. The inelastic Seebeck effects are enhanced by the normal modes, and further magnified by local heating. In the high temperature regime, the inelastic Seebeck effects are weakly suppressed due to the quasi-ballistic transport.

[1]This work is supported under Grants NSC 97-2112-M-009-011-MY3 and NSFC 10947130.

3:18PM T24.00003 Critical current noise in rough Josephson junctions[1]

, PIERRE-LUC DALLAIRE-DEMERS, FRANK WILHELM, University of Waterloo — While dissipationless, Josephson junctions as elements in superconducting nanocircuits are plagued by intrinsic noise mechanisms that will limit the coherence time of future high-precision quantum devices. Important sources of noise may arise from the non-cristallinity and disorder of the oxide layer sandwiched between the two superconducting leads. This work presents a microscopic calculation of the spectral density of noise of a rough superconducting tunnel junction. As for disordered conductors, a Josephson junction is modeled as a set of pinholes with a universal bimodal distribution of transmission eigenvalues that add their noise power incoherently. Each of these pinholes is treated as a ballistic point contact with an intrinsic thin barrier that modulates the transmission coefficient. The noise spectrum is computed using the quasiclassical Green's function method for superconductivity. This formalism allows us to investigate high and low transmission limits at finite temperature for any relevant frequency. As suggested by experiments, low transmission pinholes are expected to generate shot noise while fast switching between the subgap states of high transmission channels should create a strong non-poissonian low-frequency noise yet to be measured.

[1]This work is supported by IARPA and NSERC.

3:30PM T24.00004 Computing Transport coefficients from the Microscopic Response Method[1]

, MINGLIANG ZHANG, DAVID A. DRABOLD, Department of Physics and Astronomy, Ohio University, Athens, Ohio 45701 — If an external perturbation to a system may be expressed as additional terms in the Hamiltonian, the microscopic response is determined by the the wave function of the system. To obtain the macroscopic response, an ensemble average can be carried out at the final stage. With the help of a systematic diagrammatic expansion, one is able to consistently compute the corresponding transport coefficient. If the spatial fluctuation of the carrier distribution is small, the microscopic response method reduces to the usual Kubo-Greenwood formula (KGF). We illustrate with the conductivity and Hall mobility of amorphous semiconductors. Because the direction of the Lorentz force is determined by the line connecting the initial and final localized states, the sign of Hall mobility in a-Si:H can be anomalous. The method is being implemented in an *ab initio* code, and it is applicable to any temperature. Thus it significantly improves upon the usual method which averages KGF over a trajectory of classical molecular dynamics.

M.-L. Zhang and D. A. Drabold, Phys. Rev. Lett. **105**, 186602 (2010); Eur. Phys. J. B. **77**, 7-23, (2010); arXiv: 1008.1067.

[1]This work is supported by Army Research Office under MURI W91NF-06-2-0026.

3:42PM T24.00005 Counting Statistics in Nanoscale Junctions from First Principles

, YU-CHANG CHEN, YU-SHEN LIU, Deparment of Electrophysics, National Chiao Tung University — We present first-principle calculations for moments of the current up to the third-order atomic-scale junctions. The quantum correlations of the current calculated in terms of wave functions obtained self-consistently within the static density functional theory are also demonstrated herein. Relationships between the conductance, the second, and the third moment of the current for carbon atom chains of various lengths bridging two metal electrodes in the linear and nonlinear regimes are investigated. The conductance, the second-, and the third-order Fano factors exhibit odd-even oscillation with the number of carbon atoms. The third-order Fano factor is positively correlates with conductance.

3:54PM T24.00006 The Escape Problem in a Classical Field Theory With Two Coupled Fields and its Application to Monovalent Metallic Nanowires

, LAN GONG, Department of Physics, New York University, DANIEL STEIN, Department of Physics and Courant Institute of Mathematical Science, New York University — We introduced and analyzed a system of two coupled partial differential equations with external noise. The equations are constructed to model transitions of monovalent metallic nanowires with non- axisymmetric intermediate or end states, but also have more general applicability. They provide a rare example of a system for which an exact solution of nonuniform stationary states can be found. We have also explored the escape dynamics numerically, using the String Method, a relaxational technique. We find two kinds of transitions in activation behavior as we tune different parameters in our model, such as the interval length on which the fields are defined, and the bending coefficients of the fields. We discuss how these results apply to real nanowires.

4:06PM T24.00007 Non-linear canonical transformations and Kondo physics

, JOHAN NILSSON, University of Gothenburg — We study the Kondo problem and the Kondo lattice using non-linear canonical transformations starting from the underlying Anderson model, generalizing the work of Ostlund in PRB 76, 153101 (2007). One such transformation, which is suitable to describe Fermi-liquid physics, provides an adiabatic connection between the quasi-particles of the interacting model and the electron- and hole-excitations in the non-interacting system as a function of the interaction parameter. We will also discuss other more unconventional transformations.

4:18PM T24.00008 Spatial correlations in chaotic nanoscale systems with spin-orbit coupling , ANH NGO, Department of Physics, and Nanoscale & Quantum Phenomena Institute, Ohio University, 45701 USA, EUGENE KIM, Department of Physics, University of Windsor, Windsor, Ontario, Canada N9B 3P4, SERGIO ULLOA, Department of Physics, and Nanoscale & Quantum Phenomena Institute, Ohio University, 45701 USA — We investigate the properties of wave functions in chaotic nanostructures with spin-orbit (SO) interactions, focusing, in particular, on the evolution of the wave function statistics as the SO interaction is varied. We compare results obtained via random matrix theory for one- and two-point distribution functions with numerical results obtained from microscopic calculations on a stadium billiard, both with and without magnetic fields. We discuss how SO interactions weaken correlations in the system, as it evolves from the gaussian orthogonal (GOE) to the symplectic ensemble (GSE). In the presence of magnetic fields, a weak SO coupling decorrelates the two spin components, resulting in decoupled gaussian unitary ensembles (dGUE). We discuss experimental consequences of these (weakened) correlations, particularly for spin-dependent phenomena.

4:30PM T24.00009 Test of Lattice Constant with Correction from Zero-Point Energy , PAN HAO, YUAN FAN, JOHN PERDEW — In Born-Oppenheimer system, the total energy doesn't include the kinetic energy of the nucleus. The zero point energy of the crystal can influence the lattice constant found by minimizing the total energy. The zero point anharmonic expansion (ZPAE) can be estimated in the Debye model. We can also use a direct way to get the zero point energy by calculating the phonon frequency using density-functional perturbation theory. Some solids were tested using different functionals to get the total energy and using DFPT to get the zero-point energy. We also expanded the vibration frequency as the compression ratio, which can give us the trends of the zero-point energy. For those different correction ways, the phonon frequency correction should be the most precise method in theory. The Debye model gives a reasonable approximation in most of those solids, but for Diamond structure and the Zinc-Blende structures, the Debye model may overestimate the correction. The expansion frequency way also overestimates the corrections compared to the phonon frequency correction.

4:42PM T24.00010 ABSTRACT HAS BEEN MOVED TO W12.00014 –

4:54PM T24.00011 ABSTRACT HAS BEEN MOVED TO T34.00016 –

Wednesday, March 23, 2011 2:30PM - 5:06PM –

Session T25 DCMP: Superconductivity: Theory, Mainly Vortices D166

2:30PM T25.00001 Microscopic investigation of vortex-vortex interaction in conventional and unconventional superconductors[1] , MASARU KATO, YUHEI NIWA, Department of Mathematical Sciences, Osaka Prefecture University — Recently, we have investigated the vortex structures in nano-sized superconductors. We found the interference of vortex bound states around multiple vortices. And their interaction is affected by such quasi-particle interference. Vortex structures becomes different from which phenomenological theory predicts [1]. Therefore we clarify how such quasi-particle structure changes the vortex-vortex interaction. In order for this, we investigate the quasi-particle structures around a pair of vortices, using the Bogoliubov-de Gennes equation in the elliptical coordinates, where two vortices sit at two foci We expand quasi-particle wave functions by the (modified) Mathieu function. From the numerical results, we discuss the distance dependence of interference of the quasi-particle bound states and free energies. We will extend our method to unconventional superconductors.

[1] H. Suematsu, T. Ishida, T. Koyama, M. Machida, M. Kato, J. Phys. Soc. Jpn. 79, no.12 (2010) in press.

[1]This work is partly supported by "The Faculty Innovation Research Project" of Osaka Prefecture University.

2:42PM T25.00002 Type-1.5 superconductivity in multiband systems: the effects of interband couplings[1] , EGOR BABAEV, UMass Amherst and KTH Stockholm, JOHAN CARLSTROM, KTH Stockholm, MARTIN SPEIGHT, University of Leeds — Two-component superconductors can posses a "type-1.5" state which falls outside the usual type-I/type-II dichotomy. In this regime two vortices attract one another at long range but repel at shorter ranges. Multiple vortices thus should form clusters in cases where their interaction could be approximately described by a superposition of such nonmonotonic two-body forces and one can define a negative interface energy inside a cluster and at the same there one can define a positive interface energy associated with the cluster's boundary. We describe the appearance of type-1.5 regimes in the case of two bands with various kinds of substantial interband couplings such as Josephson coupling, mixed gradient coupling and density-density interactions. We show that in these cases the system supports type-1.5 superconductivity with fundamental length scales being associated with the mass of the gauge field and two masses of normal modes represented by mixed combinations of the density fields. Talk based on arXiv:1009.2196 and Phys. Rev. Lett. 105, 067003 (2010)

[1]supported by NSF CAREER Award DMR-0955902, Knut and Alice Wallenberg Foundation through the Royal Swedish Academy of Sciences, Swedish Research Council and UK EPSRC

2:54PM T25.00003 Proposed Aharonov-Casher interferometry of non-Abelian vortices in chiral p-wave superconductors[1] , EYTAN GROSFELD, BABAK SERADJEH, SMITHA VISHVESHWARA, University of Illinois at Urbana-Champaign — We propose a two-path vortex interferometry experiment based on the Aharonov- Casher effect for detecting the non-Abelian nature of vortices in a chiral p-wave superconductor. The effect is based on observing vortex interference patterns upon enclosing a finite charge of externally controllable magnitude within the interference path. We predict that when the interfering vortices enclose an odd number of identical vortices in their path, the interference pattern disappears only for non-Abelian vortices. When pairing involves two distinct spin species, we derive the mutual statistics between half quantum and full quantum vortices and show that, remarkably, our predictions still hold for the situation of a full quantum vortex enclosing a half quantum vortex in its path. We discuss the experimentally relevant conditions under which these effects can be observed.

[1]Work supported by ICMT at UIUC, NSERC of Canada, CAS fellowship at UIUC, and the U.S. Department of Energy.

3:06PM T25.00004 Microscopic theory of vortex interaction in two-band superconductors and type-1.5 superconductivity[1] , MIHAIL SILAEV, Institute for physics of microstructures RAS and Royal Institute of Technology, EGOR BABAEV, Royal Institute of Technology and UMass Amherst — In the framework of self-consistent microscopic theory we study the structure and interaction of vortices in two-gap superconductor taking into account the interband Josephson coupling. The asymptotical behavior of order parameter densities and magnetic field is studied analytically within the microscopic theory at low temperature. At higher temperatures, results consistent with Ginzburg-Landau theory are obtained. It is shown that under quite general conditions and in a wide temperature ranges (in particular outside the validity of the Ginzburg-Landau theory) there can exist an additional characteristic length scale of the order parameter density variation which exceeds the London penetration length of magnetic field due to the multi-component nature of superconducting state. Such behavior of order parameter density variation leads to the attractive long-range and repulsive short-range interaction between vortices.

[1]Supported by NSF CAREER Award DMR-0955902, Knut and Alice Wallenberg Foundation through the Royal Swedish Academy of Sciences and Swedish Research Council, "Dynasty" foundation and Russian Foundation for Basic Research.

3:18PM T25.00005 Hairy balls and flux lines in superconductors , MARK LAVER, Paul Scherrer Institut; Risoe DTU; University of Copenhagen, TED FORGAN, School of Physics and Astronomy, University of Birmingham — Many physical phenomena originate from geometrical effects rather than from local physics. For example, the hairy ball theorem — a hairy sphere cannot be combed — is fulfilled by the atmospheric circulation with the existence of stratospheric polar vortices, and the fact that there is always at least one place on Earth where the horizontal wind is still. We examine the consequences of the hairy ball theorem for the flux line lattice (FLL). We find that discontinuities must exist in lattice shape as a function of field direction relative to the crystal. The remarkable ways in which the hairy ball theorem is fulfilled are demonstrated for FLL's in superconducting niobium. We show that extraordinary, unconventional flux line lattice shapes that spontaneously break the underlying crystal symmetry are surprisingly likely across all Type-II superconductors, both conventional and unconventional.

3:30PM T25.00006 Boundary Wess-Zumino-Novikov-Witten model, BCS superconductivity, and Maxwell-Bloch theory[1] , TIGRAN SEDRAKYAN, VICTOR GALITSKI, University of Maryland, College Park — We establish an exact correspondence between the discrete-state pairing Hamiltonian (Richardson model) and the Wess-Zumino-Novikov-Witten (WZNW) model modified by an additional boundary operator. We solve this boundary WZNW model exactly and from this solution re-derive the Richardson equations of the pairing Hamiltonian. As an example of practical applications of the boundary WZNW model we use the obtained results to derive solution to the Maxwell Bloch theory of a two-level laser with damping and pumping. We use the results to calculate various observable characteristics of a laser: (i) the complex electrical field amplitude, (ii) the polarization of the laser medium, (iii) the population inversion. We discuss the relation of our results to recent experimental data.

[1]This work is financially supported by IARPA

3:42PM T25.00007 Geometric phases of d-wave vortices in a model of lattice fermions[1] , ZHENYU ZHOU, ALEXANDER SEIDEL, Washington University in St. Louis, OSKAR VAFEK, Florida State University — We study the local and topological features of Berry phases associated with the adiabatic transport of vortices in a d-wave superconductor of lattice fermions. At half filling, where the local Berry curvature must vanish due to symmetries, the phase associated with the exchange of two vortices is found to vanish as well, implying that vortices behave as bosons. Away from half filling, and in the limit where the magnetic length is large compared to the lattice constant, the local Berry curvature gives rise to an intricate flux pattern within the large magnetic unit cell. This renders the Berry phase associated with an exchange of two vortices highly path dependent. However, it is shown that "statistical" fluxes attached to the vortex positions are still absent. Despite the complicated profile of the Berry curvature away from half filling, we show that the average flux density associated with this curvature is tied to the average particle density. This is familiar from dual theories of bosonic systems, even though in the present case, the underlying particles are fermions.

[1]This research was supported by NSF under Grant No. DMR-0907793.

3:54PM T25.00008 Quasiparticle scattering from vortices in d-wave superconductors: Superflow and Berry phase contributions , ADAM C. DURST, SRIRAM GANESHAN, MANAS KULKARNI, Stony Brook University — In the vortex state of a d-wave superconductor, massless Dirac quasiparticles are scattered from magnetic vortices via a combination of two basic mechanisms: effective potential scattering due to the superflow swirling about the vortices and Aharonov-Bohm scattering due to the Berry phase acquired by a quasiparticle upon circling a vortex. First, we consider the superflow contribution by calculating the differential cross section for a quasiparticle scattering from the effective non-central potential of a single vortex. Next, we consider the Berry phase contribution, which results in branch cuts between neighboring vortices across which the quasiparticle wave function changes sign. Here, the simplest problem that captures the physics is that of scattering from a single finite branch cut that stretches between two vortices. Elliptical coordinates are natural for this two-center problem and we proceed by separating the massless Dirac equation in elliptical coordinates. The separated equations take the form of the Whittaker-Hill equations, which we solve to obtain radial and angular eigenfunctions. With these eigenfunctions in hand, we construct the scattering cross section via partial wave analysis. We discuss the scattering effect of each mechanism, superflow and Berry phase, leaving the important issue of interference between the two mechanisms to future work.

4:06PM T25.00009 Ground states of multi-band type-I and type-1.5 superconductors and interlaced type-I/type-II layered superconducting structures in external magnetic field[1] , JULIEN GARAUD, UMass Amherst, JOHAN CARLSTROM, KTH Stockholm, EGOR BABAEV, University of Massachusetts Amherst and KTH Stockholm — We report a numerical study of magnetic field-induced structures in multiband/multi-component superconductors and type-I/type-II multilayers. The magnetic ground state in these different regimes shows very rich structure formation. In particular we report vortex cluster formation in the cases of strong interband Josephson coupling. The results in particular can be applied to layered structures manufactured from interlaced layers of type-I and type-II superconductors yielding effectively the type-1.5 superconducting behavior with tunable intercomponent couplings.

[1]Supported by NSF CAREER Award DMR-0955902, Knut and Alice Wallenberg Foundation through the Royal Swedish Academy of Sciences and Swedish Research Council.

4:18PM T25.00010 Properties of vortex clusters and intercluster interaction in type-II and type-1.5 two-band superconductors and type-I/type-II superconducting bilayers[1] , JOHAN CARLSTROM, KTH Stockholm, JULIEN GARAUD, UMass Amherst, EGOR BABAEV, University of Massachusetts Amherst and KTH Stockholm — We discuss magnetic flux-carrying vortex states in multiband type-II and type-1.5 superconductors and interlaced type-I/type-II superconducting multilayers. Especially we focus on the case where there is a substantial disparity in characteristic variations of superfluid densities in bands or superconducting layers. We discuss the properties of vortex clusters in the type-1.5 regime both in the cases of strong and weak interband Josephson coupling, including interaction between vortex clusters with different numbers of vortices.

[1]Supported by NSF CAREER Award DMR-0955902, Knut and Alice Wallenberg Foundation through the Royal Swedish Academy of Sciences andSwedish Research Council.

4:30PM T25.00011 Novel time-dependent Ginzburg-Landau simulation of extreme type-II superconductors with a focus on the Nernst signal and its fluctuations , SANGWOO CHUNG, University of Cincinnati, PAATA KAKASHVILI, NORDITA, Sweden, CARLOS BOLECH, University of Cincinnati — Recently, different transport coefficients have been measured in High-T_c superconductors to pinpoint the nature of the pseudogap phase. In particular, the thermoelectric coefficients received a considerable attention both theoretically and experimentally. We numerically simulate the Nernst effect in extreme type-II superconductors using the time-dependent Ginzburg-Landau equations. We report the sign reversal of the thermoelectric coefficient, α_{xy}, at temperatures close to the mean-field transition temperature $T_c^{MF}(H)$, which qualitatively agrees with recent experiments on high-T_c materials. We also discuss the noise power spectrum of α_{xy}, which shows $1/f^{\beta}$ behavior. Based on this observation, we propose an experiment to determine different regimes of vortex dynamics by measuring the noise correlations of the Nernst signal.

4:42PM T25.00012 Temperature dependence of the superheating field in type-II superconductors , MARK TRANSTRUM, LASSP, Cornell University, GIANLUIGI CATELANI, JAMES SETHNA — The expulsion of an applied magnetic field is a hallmark characteristic of superconductivity. For a sufficiently large external field, the superconducting state transitions to a normal metal (type-I) or a flux-lattice state (type-II) at a field H_{c1}. The superconducting state is metastable and persists up to a field above H_{c1}, the so-called superheating field. We numerically solve the semi-classical equations of Eilenberger for the anomalous Green's functions, order parameter, and vector potential for a clean superconductor in an external magnetic field. We use a linear stability analysis to explore the local stability of the free energy to two-dimensional fluctuations, mapping the stability onto an eigenvalue problem of a linear operator. We systematically calculate the dependence of the superheating field on both temperature and the Ginzburg-Landau parameter κ. We compare our results with the analogous calculation for Ginzburg-Landau theory, which is valid only near the critical temperature, and to experimental measurements.

4:54PM T25.00013 Molecular dynamic simulation on the rule of the defect size on critical current at low temperature[1] , ABDALLA OBEIDAT, HADEEL ABULAHIM, Jordan University of Science and Technology — Molecular dynamics have been used to study the effect of the pinning center sizes on the critical current density of driven vortex lattices interacting with periodic arrays of pinning sites in two dimensions. In our study, we assumed that the radii of the pinning centers are much larger than the coherence length of the vortices. The critical current density has been studied at different temperatures for several values of pinning strengths. The overdamped equation of vortex motion has been solved taking into account the vortex-vortex repulsion, the thermal force, the attractive vortex-pinning interaction, and the driving Lorentz force. We found that the critical current density is independent of pinning size at low temperatures.

[1]We would like to thank the Jordan University of Science and Technology for the financial support.

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T26 DMP DCOMP: Focus Session: Iron Based Superconductors – Magnetic Properties & Phase Diagrams D162/164

2:30PM T26.00001 Magnetic and Structural Phase Diagram of $Ba_{1-x}K_xFe_2As_2$, SEVDA AVCI, DUCK-YOUNG CHUNG, STEPHAN ROSENKRANZ, JOHN-PAUL CASTELLAN, RAY OSBORN, Materials Science Divison, Argonne National Laboratory, Illinois, USA, OMAR CHMAISSEM, Northern Illinois University and Argonne National Laboratory, Illinois, USA, MERCOURI KANATZIDIS, Northwestern University, Illinois, USA, EUGENE GOREMYCHKIN, AZIZ DAOUD-ALADINE, ISIS, Rutherford Appleton Laboratory, UK — It is well known that the partial substitution of Ba by K in $Ba_{1-x}K_xFe_2As_2$ causes a steep suppression of both the antiferromagnetic and tetragonal-orthorhombic transitions, leading to the onset of superconductivity over a large substitution range peaking at 38 K for x = 0.4. We report high resolution neutron powder diffraction results, which show that the magnetic and structural transitions are coincident over the entire phase diagram, in contrast to $Ba(Fe_{1-x},Co_x)_2As_2$. Volume discontinuities show that the combined transitions are first-order. The superconducting phase diagram has been refined with greater precision and a narrow region of phase coexistence have been delineated.

2:42PM T26.00002 Coexistence of Superconductivity and Magnetism in $EuFe_2(As_{0.7}P_{0.3})_2$, A.A. ACZEL, Oak Ridge National Lab, T.J. WILLIAMS, McMaster University, T. GOKO, F.L. NING, Y.J. UEMURA, C. ARGUELLO, Columbia University, W. YU, G.F. CHEN, Renmin University of China, G.M. LUKE, McMaster University — We have performed resistivity, magnetization, and μSR studies on single crystalline $EuFe_2(As_{0.7}P_{0.3})_2$. These measurements provide clear evidence for bulk superconductivity in this system, with the sample resistance dropping to zero around 12 K. This work has also revealed ferromagnetic ordering of the S = 7/2 Eu^{2+} moments along the c-axis ($T_{curie} \sim 19$ K). Finally, our μSR results indicate that the Eu magnetism is very homogeneous and occupies the full-volume fraction, pointing to real-space coexistence of magnetism and superconductivity in this material.

2:54PM T26.00003 Physical and magnetic properties of $Ba(Fe_{1-x}Mn_x)_2As_2$ single crystals[1] , ALEXANDER THALER, SHENG RAN, ALFRED KRACHER, WARREN STRASZHEIM, JIAQIANG YAN, SERGEY BUD'KO, PAUL CANFIELD, Iowa State University/Ames Lab — Single crystals of $Ba(Fe_{1-x}Mn_x)_2As_2$, $0 < x < 1$, have been grown and characterized by structural, magnetic and transport measurements. These measurements show that the structural/magnetic phase transition found in pure $BaFe_2As_2$ at 134 K is suppressed monotonically by Mn doping up to a critical concentration, $x \approx 0.10$. For $x > 0.10$, a similar transition is observed which broadens and trends upward in temperature with increasing doping level. Superconductivity is not observed at any doping level for $T > 1.85K$. Phase diagrams of temperature versus doping level based on electrical transport and magnetization measurements will be presented and compared to those of the $Ba(Fe_{1-x}TM_x)_2As_2$ (TM=Cr, Co, Ni, Cu) series.

[1]Work at the Ames Laboratory was supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

3:06PM T26.00004 The magnetic form factor of SrFe2As2 , WILLIAM RATCLIFF, P.A. KIENZLE, J.W. LYNN, NIST Center for Neutron Research, S. LI, Beijing National Laboratory, Institute of Physics for Condensed Matter Physics, Chinese Academy of Sciences, Beijing China, P. DAI, Department of Physics and Astronomy, University of Tennessee, Knoxville, TN; Neutron Scattering Science Dvision, Oak Ridge National Laboratory, G.F. CHEN, N.L. WANG, Beijing National Laboratory, Institute of Physics for Condensed Matter Physics, Chinese Academy of Sciences, Beijing China — The Fe-pnictide based superconductors have recently been the subject of great interest. In this talk, we discuss recent neutron diffraction measurements of the magnetic form factor of SrFe2As2. These measurements reveal that while the form factor is primarily isotropic, a maximum entropy reconstruction reveals that there is evidence of hybridization between the Fe and As orbitals.

3:18PM T26.00005 Temperature-pressure-composition phase diagram for $Ba(Fe_{1-x}Ru_x)_2As_2$ ($x \leq 0.285$ and $P \leq 84$kbar) , S.K. KIM, Iowa State University and Ames Lab, M.S. TORIKACHVILI, Iowa State University, Ames Lab. and San Diego State University, A. THALER, E.C. COLOMBIER, S.L. BUD'KO, P.C. CANFIELD, Iowa State University and Ames Lab. — $BaFe_2As_2$ shows a structural/magnetic (SM) phase transition near T_{SM}=134K, which is suppressed upon partial substitutions at the Ba (K), Fe (Cr, Mn, Co, Ni, Cu, Ru, Rh, Pd, Ir) or As (P) sites, and also by adding pressure (P), most times leading to the emergence of superconductivity (SC) at low T. Here, we report on the P-dependence of the electrical resistivity in under- to near-optimally doped $Ba(Fe_{1-x}Ru_x)_2As_2$ ($0 \leq x \leq 0.285$) for $P \leq 84$kbar. Pressure suppresses the SM transition at a rate that increases with Ru content, e.g. for x=0.092, 0.161, and 0.210, dT_{SM}/dP ~-0.2, -0.4, and -0.6K/kbar, respectively. Although the x=0.092 and x=0.161 compositions are not SC at P=0, SC is seen when T_{SM} is sufficiently reduced by P. For x=0.161, T_c at first increases to a maximum near 25K at ~20kbar, after which it decreases at a rate of ~-0.4K/kbar. Likewise, the T_c values for the higher dopings peak ~20kbar and decrease at higher P at similar rates. We find that the application of pressure on $Ba(Fe_{1-x}Ru_x)_2As_2$ enhances T_c beyond that which was achieved with only doping, seen before in $Ba(Fe_{1-x}Co_x)_2As_2$. – Supported by U.S. DOE (DE-AC02-07CH11358), AFOSR-MURI (FA9550-09-1-0603), and NSF (DMR-0805335).

3:30PM T26.00006 Phase diagram of superconductivity and antiferromagnetism in single crystals of Sr(Fe1-xCox)2As2 and Sr1-yEuy (Fe0.88Co0.12)2As2[1] , RONGWEI HU, SERGEY BUD'KO, PAUL CANFIELD, Iowa State University — We report magnetic susceptibility, resistivity and heat capacity measurements on single crystals of $Sr(Fe_{1-x}Co_x)_2As_2$ and $Sr_{1-x}Eu_x(Fe_{0.88}Co_{0.12})_2As_2$ series. The optimal Co concentration for superconductivity in $Sr(Fe_{1-x}Co_x)_2As_2$ is determined to be $x = 0.117$. Based on this we grew members of the $Sr_{1-y}Eu_y$ series to examine the effects of well defined local moment scattering on the superconducting state. We show the evolution of superconductivity and development of antiferromagnetism across the whole doping range. The suppression of superconductivity within Abrikosov-Gor'kov's theory and de Gennes scaling as well as the antiferromagnetic transition temperature will be discussed.

[1]Work supported by AFOSR-MURI grant #FA9550-09-1-0603.

3:42PM T26.00007 Lattice distortion and magnetic quantum phase transition in $CeFeAs_{1-x}P_xO$, CLARINA DELA CRUZ, Neutron Scattering Science Division, Oak Ridge National Laboratory — With the advent of Fe-based superconductivity initially discovered in the prototypical electron doped Fe-pnictide LaFeAsOxF1$-x$, came a surge of renewed interest in high temperature superconductivity. The discovery of ubiquitous antiferromagnetic (AFM) order in the parent compounds of iron arsenide superconductors has brought attention to the understanding of the interplay between magnetism and high-transition temperature (high-Tc) superconductivity in these materials. Although superconductivity in iron arsenides arises from charge carrier doping of their semimetal parent compounds, the resulting electronic phase diagrams are dramatically materials dependent, ranging from first-order-like AFM to superconductivity phase transition for LaFeAsO1-xFx, to the gradual suppression of the AFM order before superconductivity for CeFeAsO1-xFx, and finally to the co-existing AFM order with superconductivity in SmFeAsO1-xFx. A feature of the parent compounds is the structural distortion that occurs in the vicinity of the onset of long range magnetic order of the Fe-spins. In the RFeAsO(R=rare earth) family, the magneto-structural transition is suppressed in favor of superconductivity upon doping charge carriers into the system, which alters the system electronically and crystallographically as well. To understand the lattice effect on the suppression of the AFM ground state itself by quantum fluctuations, it is important to isoelectronically tune the crystal lattice structure without the influence of charge carrier doping and superconductivity. Here we use neutron scattering to show that replacing the larger arsenic with smaller phosphorus in CeFeAs1-xPxO simultaneously suppresses the AF order and orthorhombic distortion near x= 0.4, providing evidence for a magnetic quantum critical point. Furthermore, we find that the pnictogen height in iron arsenide is an important controlling parameter for their electronic and magnetic properties, and may play an important role in electron pairing and superconductivity. Preliminary work on systematic phosphorous doping in LaFeAs1-xPxO was also done to possibly identify characteristic changes in the lattice that may be correlated with the phosphorous doping induced superconductivity in the La system and in turn give insights as to the absence of superconductivity in the Ce system.

4:18PM T26.00008 Rare earth substitution in AFe2As2 single crystals[1] , SHANTA SAHA, NICHOLAS BUTCH, TYLER DRYE, JEFF MCGILL, JOHNPIERRE PAGLIONE, Center for Nano Physics and Advanced Materials, Department of Physics, University of Maryland, College Park, MD, PETER ZAVALIJ, Department of Chemistry and Biochemistry, University of Maryland, College Park, MD, JEFFREY LYNN, NIST Center for Neutron Research, Gaithersburg, MD — Synthesis and characterization of aliovalent light rare earth substitutions for alkaline earth atoms are studied in single crystals of FeAs-based compounds with the ThCr2Si2 structure. Electrical resistivity, magnetic susceptibility and structural parameters determined via x-ray and neutron scattering techniques are investigated as a function of chemical pressure and charge doping induced by substitution. Measured physical properties are compared to the effects of external applied pressure on CaFe2As2, known to induce a collapse of the tetragonal unit cell.

[1]This work was supported by AFOSR MURI Grant FA9550-09-1-0603.

4:30PM T26.00009 Magneto-elastic Coupling in Single-crystal CeFeAsO[1] , H.-F. LI, J.-Q. YAN, J.W. KIM, R.W. MCCALLUM, T.A. LOGRASSO, D. VAKNIN, AMES LABORATORY, U.S. DOE, AMES, IOWA 50011, USA TEAM, DEPARTMENT OF PHYSICS AND ASTRONOMY, IOWA STATE UNIVERSITY, AMES, IOWA 50011, USA TEAM, ADVANCED PHOTON SOURCE, ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS 60439, USA TEAM, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING, IOWA STATE UNIVERSITY, AMES, IOWA 50011, USA TEAM — Single-crystal synchrotron X-ray diffraction studies of CeFeAsO reveal strong anisotropy in the charge correlation lengths along or perpendicular to the in-plane antiferromagnetic (AFM) wave-vector at low temperatures. The high-resolution setup allows to distinctly monitor each of the twin domains by virtue of a finite misfit angle between them that follows the order parameter. We find that the in-plane correlations, above the orthorhombic (O)-to-tetragonal (T) transition, are shorter than those in each of the domains in the AFM phase, indicating a distribution of the in-plane lattice constants. This strongly suggests that the phase above the structural transition is virtually T with strong O-T fluctuations that are induced by magnetic fluctuations.

[1]Ames Laboratory is supported by the U.S. DOE under Contract No. DE-AC02-07CH11358.

4:42PM T26.00010 Competing magnetic ground states in $Ba(Fe_{1-x}Cr_x)_2As_2$[1] , K. MARTY, M.D. LUMSDEN, A.D. CHRISTIANSON, C. WANG, M. MATSUDA, H. CAO, ORNL, L. VANBEBBER, University of Tennessee, J.L. ZARESTKY, ORNL and Ames Laboratory, D.J. SINGH, A.S. SEFAT, ORNL — Understanding the origin of unconventional superconductivity is a great challenge of condensed matter physics. In the so called 122 family, doping in the conductive layer (i.e. on the Fe site) of the $BaFe_2As_2$ iron pnictide parent compound leads to superconductivity for almost any transition metal, except for Cr and Mn. The absence of superconductivity in these cases remains an unresolved issue. We report here neutron diffraction measurements of $Ba(Fe_{1-x}Cr_x)_2As_2$ for concentrations up to x=0.47. The results show that Cr doping stabilizes magnetism across the phase diagram with a competing magnetic order favoured at high Cr-doping, in contrast to the other superconducting $Ba(Fe_{1-x}TM_x)_2As_2$.

[1]The work at ORNL was supported by the Scientific User Facilities Division, Office of Basic Energy Sciences, US DOE.

4:54PM T26.00011 Superconductivity and magnetism in $Eu_{1-x}K_xFe_2(As_{1-y}P_y)_2$, H.S. JEEVAN, J. MAIWALD, PHILIP GEGENWART, Physikalisches Institut, Georg-August-Universitaet Goettingen, D-37077 Goettingen, Germany, DEEPA KASINATHAN, HELGE ROSNER, MPI CPfS - Dresden — We report detail investigation of superconductivity and magnetism in $EuFe_2As_2$ by doping of K in Eu site and P in As site. In this new class of FeAs-based superconductors, it is found that superconductivity appears close to a magnetic instability, suggesting a possible unconventional pairing mechanism. We have synthesized single crystals of both doped and undoped samples and investigated their physical properties by means of heat capacity, resistivity, magnetization and thermal conductivity measurements. The parent compound shows an antiferromagnetic spin-density-wave (T_{SDW}) at $\approx$ 190K related to the Fe_2As_2 layers and magnetic ordering of Eu^{2+} (T_N) moments at $\approx$ 20K. Upon doping Eu with K >30%, T_{SDW} gets suppressed and superconductivity (SC) appears at $\approx$ 32K and also Eu^{2+} ordering suppressed to the low temperature. On the other hand, P doping to the As site suppresses the SDW transition and results in SC, but Eu ordering remains undisturbed. Further increasing the P doping, Eu order transitions from AFM to FM phase which leads to disappearance of SC. We will compare our experimental findings with density functional theory based calculations.

5:06PM T26.00012 Effects of annealing time and temperature on the transition temperature and low temperature state of AFe2As2 materials , SHENG RAN, SERGEY BUD'KO, ALEX THALER, Ames Laboratory U.S. DOE and Department of Physics and Astronomy, Iowa State University, DOMINIC RYAN, Physics Department/McGill University, YUJI FURUKAWA, BEAS ROY, ANDREAS KREYSSIG, ROBERT MCQUEENEY, DANIEL PRATT, ALAN GOLDMAN, PAUL CANFIELD, Ames Laboratory U.S. DOE and Department of Physics and Astronomy, Iowa State University — Over the past couple of years the AFe2As2 (A = Ca, Sr, Ba) family of compounds has become a model system for the study of FeAs-based superconductivity. Superconductivity can be stabilized by hole and electron doping (on A and Fe sites) as well as hydrostatic pressure and isoelectronic substitutions on both the Fe and As sites. In all cases the adequate suppression of the structural / antiferromagnetic phase transition appears to be a necessary condition for the appearance of superconductivity. In this talk we will review the effects of annealing time and temperature on the structural / antiferromagnetic phases of AFe2As2. Transition temperature / time and transition temperature / annealing temperature plots will be presented and discussed.

5:18PM T26.00013 Miscibility gap between $BaMn_2As_2$ and $BaFe_2As_2$[1] , ABHISHEK PANDEY, DAVID C. JOHNSTON, Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011 — $BaMn_2As_2$ and $BaFe_2As_2$ both crystallize at room temperature in the same tetragonal $ThCr_2Si_2$-type structure but with divergent unit cell volumes of 234.12 and 204.38 Å^3, respectively, suggesting that the Mn^{+2} is in a high-spin state while Fe^{+2} is in a low-spin state. The physical properties of the two compounds are therefore also highly divergent; *e.g.*, $BaMn_2As_2$ is an insulating local moment antiferromagnet with a high Néel temperature $T_N = 625$ K whereas $BaFe_2As_2$ is a metallic itinerant antiferromagnet with a much lower $T_N = 137$ K.[2] We have discovered a miscibility gap in the pseudobinary phase diagram between these two isostructural compounds, probably arising from their divergent chemistry. Our investigations of the miscibility gap and of the structural, magnetic, electronic transport and thermal properties of various compositions in this system will be discussed.

[1]Work at the Ames Laboratory was supported by the Department of Energy-Basic Energy Sciences under Contract No. DE-AC02-07CH11358.
[2]D. C. Johnston, Adv. Phys. **59**, 803–1061 (2010).

Wednesday, March 23, 2011 2:30PM - 5:30PM –
Session T27 GQI DAMOP: Open Quantum Systems and Decoherence C155

2:30PM T27.00001 Landau-Zener-Stückelberg interference in the presence of quantum noise[1] , YANG YU, LINGJIE DU, MINJIE WANG, National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, China — We investigated the Landau-Zener-Stückelberg (LZS) interference in strongly driven two-level systems subjected to quantum noise. The transition rate induced by consecutive LZ transitions is obtained, from which LZS interference can be analytically calculated based on rate equation. In the presence of significant frequency dependent noise, the evolving paths of LZS interference is going to be detoured. Therefore, the position of the resonant peaks is shifted and a stationary population inversion in TLS without involving the third qubit state is generated. The LZS interferometry can be used to investigate the noise property hence the decoherence source of the system. In addition, the stationary population inversion may find application in lasing and microwave cooling.

[1]This work was supported by the MOST of China (2011CB922104, 2011CBA00205) and the NSFC (10725415, 91021003).

2:42PM T27.00002 Exact master equations for linearly coupled Bosons or Fermions[1] , SHAO-WEN CHEN, REN-BAO LIU, The Chinese University of Hong Kong — Using the coherent-state representation (P-representation), we derived the exact master equation for a quantum system in an environment, which has linear but otherwise arbitrary couplings. This method works for both Boson and Fermion systems, since the coherent states of Bosons and Fermions have the similar algebra structure. The new derivation reproduces the previous works on photon dynamics in coupled cavities or quantum transport through double quantum dots, but it provides a more general theoretical framework for studying quantum dynamics in photonic, mechanical, and photomechanical systems, and quantum transport in nanostructures.

[1]This work was supported by Hong Kong RGC Project CUHK 402208.

2:54PM T27.00003 Engineering inverse power law decoherence of a qubit , FRANCESCO PETRUCCIONE, FILIPPO GIRALDI, University of KwaZulu-Natal and National Institute for Theoretical Physics, QUANTUM RESEARCH GROUP TEAM — The exact dynamics of a Jaynes-Cummings model for a qubit interacting with a bath of bosons, characterized by a special form of the spectral density, is evaluated analytically. The special reservoirs are sub-ohmic at low frequencies and inverse power law at high frequencies. The exact dynamics of the qubit is described analytically through Fox H-functions. Over estimated long time scales, decoherence results in inverse power laws with powers decreasing continuously to unity, according to the particular choice of the engineered reservoir. If compared to the exponential-like relaxation obtained from the original Jaynes-Cummings model for Lorentzian-type spectral density functions, decoherence is considerably hindered.

3:06PM T27.00004 Decoherence of high-ℓ Rydberg wave packets by collisions and electrical noise , BRENDAN WYKER, S. YE, Rice University, T. MCKINNEY, University of California, Berkeley, F.B. DUNNING, Rice University, S. YOSHIDA, Vienna University of Technology, C.O. REINHOLD, Oak Ridge National Laboratory, J. BURGDÖRFER, Vienna University of Technology — Quantum revivals in very-high-n (n ∼300) high-ℓ Rydberg wave packets generated from parent np states are used to examine decoherence induced by collisions and by the application of "colored" noise from a random pulse generator. In the absence of external perturbations, the high-ℓ wave packets maintain their coherence for periods ~ 1 μs, i.e., for many hundreds of orbits. However, their coherence can be destroyed on sub-microsecond timescales by the presence of even small amounts of electrical noise at a rate that depends markedly on the spectral characteristics of the noise. In contrast, measurements over similar timescales with CO_2 target gas at densities of $\sim 10^{11}$ cm^{-3} provide no evidence of collisional dephasing.

3:18PM T27.00005 Non-Markovian trajectory approach of three-level quantum systems[1] , TING YU, JUN JING, Department of Physics and Engineering Physics, Stevens Institute of Technology, Hoboken, New Jersey 07030, USA — The non-Markovian dynamics of a three-level quantum system coupled to a bosonic environment is a difficult problem due to the lack of an exact dynamic equation such as a master equation. We present for the first time an exact quantum trajectory approach to a dissipative three-level model. We have established a convolutionless stochastic Schrödinger equation called time-local quantum state diffusion (QSD) equation without any approximations, in particular, without Markov approximation. Our exact time-local QSD equation opens a new avenue for exploring quantum dynamics for a higher dimensional quantum system coupled to a non-Markovian environment.

[1]This research is supported by grants from DARPA QuEST HR0011-09-1-0008 and the NSF PHY-0925174.

3:30PM T27.00006 Manipulating decoherence of a single solid-state spin by quantum control of its spin bath environment , GIJS DE LANGE, TOENO VAN DER SAR, MACHIEL BLOK, Kavli Institute of Nanoscience Delft, Delft University of Technology, The Netherlands, ZHIHUI WANG, VIATCHESLAV DOBROVITSKI, Ames Laboratory and Iowa State University, Ames, Iowa 50011, USA, RONALD HANSON, Kavli Institute of Nanoscience Delft, Delft University of Technology, The Netherlands — The coherence of solid-state spins is limited by uncontrolled interactions with their spin environment. High-fidelity single-spin control can be used to prolong the coherence by dynamically decoupling the spin from the environment [see De Lange et al., Science 330, 60 (2010)]. Here, we demonstrate a new approach towards decoherence control based on coherent manipulation of the spin bath environment itself. Our system consists of a single NV center spin in diamond, surrounded by a bath of electronic spins belonging to nitrogen impurities. By driving the bath spins resonantly and using the NV spin as a sensor, we are able to detect all transitions of the bath spins and demonstrate independent quantum control of each of them. This newly gained control opens the door to a number of exciting experiments such as measurement of the spin bath dynamics, manipulation of the spin bath correlation time, decoherence editing, and protection of NV spin coherence by suppressing the dynamics in its spin environment. In this talk we will present our latest results towards these goals.

3:42PM T27.00007 Optical cooling of a 122 kHz mechanical resonator , EVAN JEFFREY, PETRO SONIN, University of Leiden, DUSTIN KLECKNER, BRIAN PEPPER, University of California, Santa Barbara, DIRK BOUWMEESTER, University of Leiden — We demonstrate radiation pressure cooling of a 122-kHz, 60-ng mechanical resonator in an optical cavity. We use a dilution refrigerator to achieve a low base temperature ($<$ 100 mK). The resonators consist of high reflectivity mirrors suspended on a stressed silicon nitride cross resonator. Due to their low frequency, high Q ($>$40000) and high finesse ($>$ 10000) these devices are excellent candidates for demonstrating quantum behavior of macroscopic systems, with the possibility of achieving quantum superpositions, entanglement with external degrees of freedom, and studying exotic decoherence mechanisms.

3:54PM T27.00008 Long-lived Fermionic Fock-space coherence in quantum dots , EDUARDO VAZ, JORDAN KYRIAKIDIS, Dalhousie University — The Fock-space coherence between quantum states with different particle numbers naturally arising in an open quantum system, qualitatively differs from the more common Hilbert-space coherence between states with the same particle number. For a quantum dot with multiple channels available for transport, we have found specific energy and coupling regimes where a long-lived resonance in the fermionic Fock-space coherence of the system is realized, even where no resonances are found either in the population probabilities or Hilbert-space coherence of the system. We discuss how this resonance in the Fock-space coherence remains robust even in the presence of both boson-mediated relaxation and transport through the quantum dot, as well as its physical origin.

4:06PM T27.00009 Excitation induced dephasing from indistinguishability , PETER BRYANT, Physics Department, University of Texas at Austin — In a variety of experiments, Rabi oscillations suffer dephasing that often and perhaps generally depends on the Rabi frequency. This unexpected result has been called excitation induced dephasing. Explanations specific to experiments have been suggested, but here we describe a new approach to the treatment of decoherence and open systems, that allows one to address the indistinguishability of quantum systems. When physical systems are indistinguishable, excitation induced dephasing is a general phenomenon, and a preliminary model shows good agreement with a wide range of experimental results.

4:18PM T27.00010 Noise in a Josephson junction qubit due to two-level-systems coupled to a quantum EM field[1] , VICTOR GALITSKI, SO TAKEI, University of Maryland College Park — We theoretically study loss of the dielectric film located within an LC resonator circuit due to two-level defects (TLDs). We present a fully quantum mechanical treatment of the full system in which the TLDs couple to a quantized harmonic oscillator, which models the resonator, and to quantized bosonic fields that describe the feedline used to pump and probe the resonator. We focus on the forward transmission as a function of the microwave pump frequency, and investigate how the fluctuating defects affect the noise spectrum of the transmitted voltage signal. Our quantum mechanical treatment makes connections to experiments conducted down to energies where a single photon is stored in the resonator.

[1]This work was funded by IARPA.

4:30PM T27.00011 Suppression of Decoherence and Disentanglement in Qubits via the Exchange Interaction[1] , AMRIT DE, DONG ZHOU, ROBERT JOYNT, Department of Physics, University of Wisconsin- Madison, WI-53706 — We show that the decoherence and disentanglement for a pair of interacting qubits can be suppressed by the exchange interaction in the presence of one or more uncorrelated random telegraphic noise sources. The suppression of the dissipative dynamics is more apparent for the maximally entangled Bell states, particularly if the noise is non-Markovian. Hence, the entangled singlet-triplet superposition state of two qubits can be protected by the interaction, while for the triplet-triplet state, it is less effective. This makes the former more suitable for encoding quantum information. Our calculations are done using a recently developed quasi Hamiltonian formalism that is suitable for describing non-unitary temporal dynamics in an open quantum system subjected to classical stochastic noise processes. Exact and approximate solutions are obtained for a number of cases.

[1]This work is supported by the DARPA/MTO QuEST program through a grant from AFOSR.

4:42PM T27.00012 Concatenated Stabilizer Dynamical Decoupling , GERARDO PAZ SILVA, DANIEL LIDAR, University of Southern California — We show how to integrate concatenated dynamical decoupling (CDD) techniques with quantum error correction (QEC) codes: the two main strategies to protect quantum information from the decoherence induced by unwanted interaction with the environment. It has been shown that CDD can be used as a lower level protection layer against decoherence and improves the effective error rate of a physical gate, provided one assumes certain locality conditions (local bath assumption) [Ng, Lidar, Preskill, arXiv:0911.3202]. The typical CDD protocol uses pulses from a group of non-commuting operators to decouple to arbitrary order, in the sense of Magnus expansion, the state one wants to protect from the environment. Here, in the same spirit as [Lidar, Phys. Rev. Lett. 100, 160506 (2008)], we show how to decouple a state encoded in some stabilizer QEC code to arbitrary order by applying pulses from the stabilizer group of the QEC code. We demonstrate the technique for concatenated and non-concatenated QEC codes and show that, in contrast to the CDD case, (i) one can omit the local bath assumption, and (ii) has the freedom of simultaneously introducing evolution for the protected state.

4:54PM T27.00013 Decoherence and entanglement of a pair of coupled qubits , MOHAMMAD SAHRAPOUR, NANCY MAKRI, University of Illinois at Urbana-Champaign — We analyze the quantum dynamics of a pair of qubits coupled via Ising-type coupling under the influence of a common dissipative bath. We present results of simulations for a range of system biases and spin-spin couplings at two values of bath temperature ($\beta = 1, 5$). We also discuss the dynamics of entanglement when starting with fully entangled states and find that for some values of the system parameters, steady-state entanglement is observed. These simulations are carried out via the iterative path integral methodology developed earlier in our group which delivers efficient, numerically exact long time quantum dynamics.

5:06PM T27.00014 Entanglement and Coherence: Differences and Similarities , ROBERT O'CONNELL, Louisiana State University, Physics Dept. — Entanglement and coherence both decay due to environmental (heat bath) effects. Apart from the well-known fact that decoherence occurs exponentially and disentanglement occurs with a sudden death, there are many other differences. Here, we concentrate on the effects of temperature T along in the absence of dissipation. Thus, whereas the effect of T on decoherence increases exponentially with time [1], the effect of T on disentanglement is constant for all times [2], reflecting a fundamental difference between the two phenomena. Also, the possibility of disentanglement at a particular T increases with decreasing initial entanglement. Supported in part by NSF under Grant No. ECCS-0757204.

[1] G. W. Ford and R. F. O'Connell, Phys. Lett. A 286, 87 (2001).
[2] G. W. Ford and R. F. O'Connell, Phys. Scr. 82, 038112 (2010).

5:18PM T27.00015 Quantum signatures of chaos in quantum tomography[1] , CARLOS RIOFRIO, VAIBHAV MADHOK, IVAN DEUTSCH, Center for Quantum Information and Control, University of New Mexico — We study the connection between quantum chaos and information gain in the time series of a measurement record used for quantum tomography. The record that is obtained as a sequence of expectation values of a Hermitian operator evolving under repeated application of the Floquet operator of the quantum kicked top on a large ensemble of identical systems. We find that, in the limit of vanishing noise, the fidelities of reconstruction are independent of the underlying chaos of the Floquet map. In the presence of noise, however, the fidelities on an average increase with the chaoticity of the map. Moreover, the number of time steps required to achieve a given fidelity decreases with the increase in the chaoticity, suggesting a connection between the rate of information gain and classical Lyapunov exponents.

[1]NSF PHY-0903692

Wednesday, March 23, 2011 2:30PM - 5:30PM –
Session T28 DCMP: Graphene: Optical and Transport Properties C156

2:30PM T28.00001 Selection rule for Raman spectroscopy at graphene edge , KEN-ICHI SASAKI, KATSUNORI WAKABAYASHI, National Institute for Materials Science, TOSHIAKI ENOKI, Department of Chemistry, Tokyo Institute of Technology — The optical matrix element may depend on position in graphene since an electronic wave function is position dependent. In particular, the matrix element near the edges of graphene can differ greatly from that in the bulk. We are pursuing our studies on this point in relation to Raman spectroscopy. We found a selection rule for the G band near the edges of graphene: the intensity is enhanced when the polarization of incident laser is parallel (perpendicular) to the armchair (zigzag) edge [1]. This asymmetry between the armchair and zigzag edges is useful in identifying the orientation of the edge of graphene. Some application of the selection rule is mentioned. We have extended our study to the polarization dependences of the D and 2D (G') bands [2]. The D and 2D bands have different selection rules at bulk and edge. At bulk, the 2D band intensity is maximum when the polarization of the scattered light is parallel to that of incident light, whereas the D band intensity does not have a polarization dependence. At edge, the 2D and D bands exhibit a selection rule similar to that of the G band.

[1] Sasaki et al., J. Phys. Soc. Jpn. 79, 044603 (2010).
[2] Sasaki et al., Phys. Rev. B 82, 205407 (2010).

2:42PM T28.00002 Photoconductive response study on a dual-gated bilayer graphene , M.-H. KIM, J. YAN, G.S. JENKINS, A.B. SUSHKOV, D.C. SCHMADEL, M.S. FUHRER, J. MELNGAILIS, H.D. DREW, Department of Physics, University of Maryland, College Park — A continuously tunable bandgap as high as 100 meV is produced in a gated bilayer graphene (BLG) by applying an electric field perpendicular to the layers (J. Yan, Nano Lett. 2010). The bandgap and the Fermi energy of BLG are tuned by top and bottom gate potentials. We measure the infrared photoconductive response from the dual-gated BLG from far infrared 30 cm^{-1} to mid-infrared 5000 cm^{-1} by broadband spectroscopy and with a CO_2 laser near 10.6 μm. We report the photoresponse and the measured band gap as a function of an applied electric field perpendicular to the BLG layers. This work is supported by IARPA grant #W911NF1010443.

2:54PM T28.00003 Ultrafast carrier dynamics in pristine and $FeCl_3$-intercalated bilayer graphene , XINGQUAN ZOU, Nanyang Technological University, Singapore, DA ZHAN, XIAOFENG FAN, DONGWOOK LEE, SARITHA K. NAIR, LI SUN, ZHENHUA NI, ZHIQIANG LUO, LEI LIU, TING YU, ZEXIANG SHEN, ELBERT E.M. CHIA — Ultrafast carrier dynamics of pristine bilayer graphene (BLG) and bilayer graphene intercalated with $FeCl_3$ ($FeCl_3$-G), were studied using time-resolved transient differential reflection ($\Delta R/R$). Compared to BLG, the $FeCl_3$-G data showed an opposite sign of $\Delta R/R$, a slower rise time, and a single (instead of double) exponential relaxation. We attribute these differences in dynamics to the down-shifting of the Fermi level in $FeCl_3$-G, as well as the formation of numerous horizontal bands arising from the d-orbitals of Fe. Our work shows that intercalation can dramatically change the electronic structure of graphene, and its associated carrier dynamics. Appl. Phys. Lett. **97, 141910** (2010)

3:06PM T28.00004 Microwave microscopy of graphene and graphite , VLADIMIR TALANOV, Neoceral LLC Beltsville, MD 20705, CHRISTOPHER DEL BARGA, LEE WICKEY, IRAKLI KALICHAVA, Materials Engineering Department, New Mexico Tech, Socorro NM 87801, EDWARD GONZALES, ERIC SHANER, AARON GIN, Center for Integrated Nanotechnologies and Sandia National Laboratories, Albuquerque, NM 87185, NIKOLAI KALUGIN, Materials Engineering Department, New Mexico Tech, Socorro NM 87801 — Graphene has emerged as a promising material for high speed nano-electronics applications due to the relatively high carrier mobility that can be achieved. To further investigate electronic transport in graphene and reveal its potential for microwave applications [1,2], a near-field scanning microwave microscope with the probe formed by an electrically open end of a 4 GHz half-lambda parallel-strip transmission line resonator has been employed [3]. We find that the microwave response of mono- and few-layer graphene flakes is determined by the local sheet impedance, which is found to be predominantly active. From fitting a quantitative electrodynamic model (relating the probe resonant frequency shift to 2D conductivity of single- and few-layer graphene) to the experimental data we evaluate graphene sheet resistance as a function of thickness. Near-field scanning microwave microscopy can simultaneously image location, geometry, thickness, and distribution of electrical properties of graphene without a need for device fabrication.

3:18PM T28.00005 Laser Scanning Microscopy of Few-Layer Graphene: Optical Reflectivity Contrast[1] , BEHNOOD GHAMSARI, Center for Nanophysics and Advanced Materials, University of Maryland, College Park, ALEXANDER ZHURAVEL, B. Verkin Institute for Low Temperature Physics & Engineering, NAS of Ukraine, DANIEL LENSKI, Intel Corporation, 5200 NE Elam Young Parkway, Hillsboro, OR 97124, MICHAEL FUHRER, STEVEN ANLAGE, Center for Nanophysics and Advanced Materials, University of Maryland, College Park — We report laser scanning microscopy (LSM) of few-layer graphene, where a laser beam is raster scanned over the samples and the local reflectivity of the structure is directly measured through a silicon photodiode. The samples are grown by ambient-pressure chemical vapor deposition on copper foils, and transferred to SiO2/Si substrates, and consist of regions of single- and multi-layer graphene (D. R. Lenski, and M. S. Fuhrer, e-print arXiv: 1011.1683). While the local reflectivity of the structure depends on the thickness of the graphene layer, the LSM data is used to construct a two-dimensional reflectivity image of the sample which, in turn, enables identifying the local distribution of different graphene multilayers and local microscopic properties of the graphene sample.

[1]This work is supported by Department of Energy/High Energy Physics through grant number DESC0004950 and ONR through the Maryland AppEl, Task D10, through grant number N000140911190.

3:30PM T28.00006 Terahertz Imaging and Spectroscopy of Large-Area Single-Layer Graphene[1] , ETHAN MINOT, JOE TOMAINO, ANDREW JAMESON, JOSHUA KEVEK, MICHAEL PAUL, Oregon State University, AREND VAN DER ZANDE, ROBERT BARTON, PAUL MCEUEN, Cornell University, YUN-SHIK LEE, Oregon State University — The high electron mobility of graphene points to potential for high-speed electronic and opto-electronic devices operating at terahertz (THz) switching rates. Therefore, there is great interest in probing the electronic properties of large-area graphene at ultrafast time scales. We have demonstrated THz imaging and spectroscopy of a 15x15-mm^2 single-layer graphene film using broadband THz pulses. The THz images clearly map out the THz carrier dynamics of the graphene-on-Si sample, allowing us to measure sheet conductivity with sub-mm resolution without fabricating electrodes. The THz carrier dynamics are dominated by intraband transitions and the THz-induced electron motion is characterized by a flat spectral response. A theoretical analysis based on the Fresnel coefficients for a metallic thin film shows that the local sheet conductivity varies across the sample from 1.7 – 2.4 x 10^{-3} Ohm^{-1} (sheet resistance 420 - 590 Ohm/sq).

[1]This work was partially supported by Oregon Nanoscience and Microtechnologies Institute

3:42PM T28.00007 Aromatic molecule-like fluorescence from Graphene Oxide , CHARUDATTA GALANDE, Rice University, ADITYA MOHITE, Los Alamos National Laboratory, ANTON NAUMOV, WEI GAO, LIJIE CI, ANAKHA AJAYAN, HUI GAO, Rice University, ANCHAL SRIVASTAVA, Banaras Hindu University, R. BRUCE WEISMAN, PULICKEL M. AJAYAN, Rice University — Graphene Oxide (GO) is a functionalized derivative of graphene, obtained by chemical exfoliation and chemical oxidation of graphite. Recent NMR studies on GO have revealed presence of hydroxyl, epoxy, carbonyl, carboxyl and lactols. Although there have been several studies on electronic and optical properties of GO, the role of functional groups in determining the electronic density of states is still unclear. Here we report pH dependent fluorescence and excitation spectra of GO, with spectroscopic signatures indicating the presence of molecule-like fluorophores in GO. In acidic medium, a single, broad emission peak is observed at ca. 660nm. In contrast, relatively sharp emission at lower wavelengths (480nm-515nm) appears in a short pH range between 7.6 and 8.0, while the broad peak is completely quenched in basic conditions. The fluorescence and excitation spectra have pH-dependence strikingly similar to several aromatic carboxylic acids. The observed spectral features are proposed to arise from quasi-molecular fluorophores, similar to polycyclic aromatic compounds that are formed by the electronic coupling of carboxylic acid groups with nearby carbon atoms of the graphene.

3:54PM T28.00008 Broadband spatial self-phase modulation of few-layer graphene sheet in solution , RUI WU, YINGLI ZHANG, FEI BIAN, SHICHAO YAN, RUI WANG, WENLONG WANG, XUEDONG BAI, XINGHUA LU, JIMIN ZHAO, Institute of Physics, Chinese Academy of Sciences — Spatial self-phase modulation (SPM) was found for a suspension of few-layer graphene flakes. Multiple concentric conical diffraction rings was observed as a 532nm cw laser beam passes through the nearly transparent suspension, of which self-focusing occurred. The dependence of ring numbers and ring diameters on the laser intensity was recorded, from which we obtained the third order optical nonlinearity $n_2$of the sample. In our case n_2=10^{-9} m^2/W, which is the one of the largest among the reported carbon materials including carbon nanotubes and C_{60} samples. We also found that the intensity threshold for observing the diffraction rings is as low as about $0.6W/cm^2$, which is the smallest compared with most of the reported sample having spatial SPM, including nematic liquid crystals. Furthermore we found that both 267nm and 800nm ultrashort laser pulses can also easily generate spatial SPM. This large and broadband optical nonlinearity is a manifestation of the few-layer graphene's conical-shaped band structure, which is true for a relatively large energy scale.

4:06PM T28.00009 Optical transitions between Landau levels: AA-stacked bilayer graphene[1] , YEN-HUNG HO, Physics, National Sun Yat-Sen University, Taiwan, RONG-BIN CHEN, Center of General Education, National Kaohsiung Marine University, Taiwan, JHAO-YING WU, YU-HUANG CHIU, MING-FA LIN, Physics, National Cheng Kung University, Taiwan — The magneto-absorption spectra are calculated for the AA- stacked bilayer graphene. Two groups of Landau levels with different symmetry in wave function are found to coexist in the low energy region. The optical transitions between the two groups give rise to two kinds of absorption peaks. The wave- function distribution can clearly characterize individual Landau levels, and further determine the optical selection rules and absorption rates. The AA bilayer has quite different spectral features compared to the AB bilayer and monolayer, as a result from the interlayer interactions and stacking symmetry. Only a single absorption survives below certain critical frequency, while other peaks are paired together and sequentially emerged above this critical energy. With a continuous change in field strength, the excitation channels are switched, associated with the abrupt changes in their frequency.

[1]NSC 99-2112-M-110-009 and NSC 98-2112-M-006-013-MY4

4:18PM T28.00010 High temperature Graphene-based Quantum Hall Effect Infrared photodetector[1]

, NIKOLAI G. KALUGIN, New Mexico Tech, LEI JING, WENZHONG BAO, UC-Riverside, LEE WICKEY, CHRISTOPHER DEL BARGA, MEKAN OVEZMYRADOV, New Mexico Tech, ERIC A. SHANER, SNL, CHUN NING LAU, NEW MEXICO TECH TEAM, UC-RIVERSIDE TEAM, SNL COLLABORATION — We demonstrate successful operation of quantum Hall effect (QHE) graphene-based detectors at 70K, a temperature achievable using simple pumped liquid Nitrogen cryostats, and in magnetic field of 7.35T. Because of graphene's unique band structure, the first few Landau levels are well-separated energetically, thus allowing observation and manipulation of QHE at unprecedentedly high temperatures [1]. Our results overcome the obstacle of low operating temperature of traditional semiconductor systems-based QHE photodetectors [2], and open the door for wide arrays of applications.

[1] K.S. Novoselov *et al*. *Science* **315**, 1379 (2007).
[2] N. G. Kalugin *et.al*. *Phys.Rev.B* 66, 085308 (2002).

[1]We acknowledge support from NSF (proj. #0926056, #0925988); DOE CINT grants #U2008A061, #RA2009B066. Sandia is a multiprogram laboratory operated by Sandia Corp., a Lockheed Martin Comp., for US DOE NNSA (contract DE-AC04 94AL85000).

4:30PM T28.00011 Phonon scattering in intrinsic graphene using tight-binding Bloch waves[1]

, NISHANT SULE, IRENA KNEZEVIC, University of Wisconsin - Madison — The overall interest in graphene as a material for devices has led to tremendous advances in the understanding of transport in graphene. However, there are still questions about the intrinsic limit to electron mobility. Recent experiments have demonstrated mobility greater than 10^7 cm^2/Vs at temperatures close to 50 K, exceeding previous theoretical predictions of the limit for intrinsic mobility. Here, we present a simple model for phonon scattering rates in intrinsic graphene using tight-binding Bloch wave functions for electrons. The tight binding approximation produces an accurate band structure near the Dirac points, as opposed to the nearly free electron model; thus, it is reasonable to assume that the electron wave functions are localized near the atomic centers. These tight-binding Bloch wave functions are calculated by linear combination of the carbon p_z orbitals. We show that the scattering matrix is anisotropic and the small overlap of the Bloch functions results in scattering rates that are lower in comparison to those calculated by assuming plane-wave wave functions. Electron mobility calculated in the relaxation time approximation is compared for scattering rates with Bloch functions and as well as plane waves.

[1]This work is supported by University of Wisconsin MRSEC, NSF award DMR-0520527.

4:42PM T28.00012 Chirality-dependent phonon-limited resistivity in graphenes[1]

, HONGKI MIN, EUYHEON HWANG, SANKAR DAS SARMA, Condensed Matter Theory Center, Department of Physics, University of Maryland — We develop a theory for the temperature and density dependence of phonon-limited resistivity $\rho(T)$ in bilayer and multilayer graphene, and compare with the corresponding monolayer result. For the unscreened case, we find $\rho \approx CT$ with $C \propto v_{\rm F}^{-2}$ in the high-temperature limit, and $\rho \approx AT^4$ with $A \propto v_{\rm F}^{-2} k_{\rm F}^{-3}$ in the low-temperature Bloch-Grüneisen limit, where $v_{\rm F}$ and $k_{\rm F}$ are Fermi velocity and Fermi wavevector, respectively. If screening effects are taken into account, $\rho \approx CT$ in the high-temperature limit with a renormalized C which is a function of the screening length, and $\rho \approx AT^6$ in the low-temperature limit with $A \propto k_{\rm F}^{-5}$ but independent of $v_{\rm F}$. These relations hold in general with $v_{\rm F}$ and a chiral factor in C determined by the specific chiral band structure for a given density.

Reference: Hongki Min, E. H. Hwang, and S. Das Sarma, arXiv:1011.0741 (unpublished).

[1]The work is supported by the NRI-SWAN, US-ONR and CNAM.

4:54PM T28.00013 Boundary properties between monolayer and bilayer graphene and valley filter

, TAKESHI NAKANISHI, AIST, MIKITO KOSHINO, Tohoku Univ., TSUNEYA ANDO, Tokyo Inst. Tech. — Graphene consists of a two-dimensional hexagonal crystal of carbon atoms, in which electron dynamics is governed by the Dirac equation. The purpose of this paper is to study the boundary between monolayer and bilayer graphenes and show a valley polarization in transmission probability through the boundary [1]. We consider the boundary of monolayer and bilayer graphene, in which lower layer in bilayer graphene is continuously connected to the monolayer graphene and upper layer is terminated along a straight edge having zigzag or armchair structures. Boundary conditions between monolayer and bilayer graphene are derived in an effective-mass scheme. The transmission probability vanishes at the Dirac point and increases roughly in proportional to the electron density. The transmission probability varies strongly as a function of the incident angle and its maximum appears at an angle deviating from the vertical direction. This asymmetry is opposite between the K and K' points, showing that strong valley polarization can be induced across the interface of monolayer and bilayer graphenes.

[1] T. Nakanishi et al., PRB 82 (2010) 125428.

5:06PM T28.00014 Anomalous tunneling of dressed Dirac electrons through potential barrier[1]

, ANDRII IUROV, Graduate Center, CUNY; Hunter College, CUNY, OLEKSIY ROSLYAK, GODFREY GUMBS, Hunter College, CUNY — It has been shown that when a potential barrier is placed on a layer of graphene, electrons incident on the barrier head-on can be transmitted without any reflection, regardless of how high the barrier is made to become. This anomalous scattering has also been investigated in the case of bilayer graphene. The energy gap between the valence and conduction bands for bilayer graphene leads to perfect reflection for head-on collisions for all barrier heights. We report on results for reflection and transmission coefficients for dressed Dirac electrons when circularly polarized light is applied to graphene and an energy gap in the energy bands is opened up. Since this gap depends on the frequency and intensity, we investigate how the electron and hole scattering off a fixed barrier is modified by varying the energy gap produced by light. We also present results for the transmission for the perpendicular incidentce. Both numerical and analytical results are obtained.

[1]This work was supported by contract # FA 9453-07-C-0207 of AFRL.

5:18PM T28.00015 In-gap transport in random-gap grapheme: metallic and insulating phases

, VAGHARSH MKHITARYAN, MIKHAIL RAIKH, Department of Physics and Astronomy, University of Utah, Salt Lake City, UT 84112, USA — 1D- like counter-propagating states at a gap center of graphene with random gap constitute two chiral networks. In the absence of intervalley scattering, transport over each network is either metallic or insulating, depending on the gap randomness. We demonstrate that properties of both phases as well as transitions between them are accurately captured within a simple real-space renormalization group approach. The most striking feature of this network transport is that it can be metallic even when the neighboring plaquettes are weakly coupled. We show that randomness in local gap signs reflected in randomness in signs of local transmission coefficients, gives rise to resonant transmission of the RG superblock. Delocalization occurs by proliferation of these resonances to larger scales. As the disorder exceeds a critical value, the RG flow towards insulator switches to a flow towards metallic fixed point. Evolution of the conductance distribution to metallic fixed point is synchronized with evolution of transmission coefficient signs, so that delocalization is accompanied with sign percolation.

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T29 GQI: Focus Session: Superconducting Qubits - Coherence and Materials I

2:30PM T29.00001 Feedback suppression of the low-frequency noise in qubits by the low-frequency quantum measurements , QIANG DENG, DMITRI AVERIN, Department of Physics and Astronomy, SUNY, Stony Brook — The problem of the low-frequency noise has dominated the development of the solid-state qubits. Up to now, the main approach to solve this was to employ the qubit structures with the basis states having the same values of the main qubit coordinate (e.g., electric charge or magnetic flux) that are, as a result, not decohered by the noise. The goal of this work is to suggest an alternative approach based on direct suppression of the low-frequency noise in a qubit through the measurement/feedback loop. Continuous quantum measurement required for this loop should also be "low-frequency" so that it does not affect the quantum dynamics of the qubit. We calculate the minimal noise induced in the qubit by such a feedback loop when the measurement is the quantum-limited.

2:42PM T29.00002 Tunable quantum beam splitters for quantum manipulation of a hybrid tripartite qubit system[1] , G.Z. SUN, J. CHEN, P.H. WU, Research Institute of Superconductor Electronics, School of Electronic Science and Engineering, Nanjing University, X.D. WEN, Y. YU, Department of Physics, Nanjing University, Nanjing 210093, China, B. MAO, S.Y. HAN, Department of Physics and Astronomy, University of Kansas, Lawrence, KS 66045, USA — We demonstrated coherent control of quantum states in a tripartite system consisting of a superconducting qubit and two microscopic two-level states (TLS). An initially prepared qubit state was swept through qubit-TLS avoided crossings in the energy-level spectrum. The avoided crossings act as tunable quantum beam splitters of wave function. In an analogy to optics, the transmission coefficient of the beam splitters can be varied from zero to unity or any value in between by adjusting the rate of energy sweep. When performed within the decoherence time, consecutive crossings through the beam splitters lead to coherent quantum oscillations between the quantum states of the tripartite qubit-TLS system. This Landau-Zener-Stueckelberg interference controlled by the sweeping rate provides an alternative means to manipulate multiple qubits and demonstrates macroscopic quantum coherence.

[1]Supported by NCET, NSFC, the MOST of China (2011CB922104), NSF (DMR-0325551), and DMEA (H94003-04-D-0004-0149).

2:54PM T29.00003 Surface and Interface Defects in Linear and Nonlinear Superconducting Resonators , STEVEN WEBER, KATER MURCH, UC Berkeley, ALLISON DOVE, University of Illinois Urbana-Champaign, GUSTAF OLSON, gustafolson@gmail.com, ZACK YOSCOVITS, University of Illinois Urbana-Champaign, R. VIJAY, ELI LEVENSON-FALK, UC Berkeley, JAMES ECKSTEIN, University of Illinois Urbana-Champaign, IRFAN SIDDIQI, UC Berkeley — We report on progress to identify and mitigate noise mechanisms in both linear superconducting resonators and devices embedded with Josephson junctions. Defects, either microscopic fluctuators or remnant residue layers associated with nanofabrication, can exist on metal surfaces, at the metal-dielectric interface, within the dielectric, or within the Josephson junctions themselves. We have investigated the quality factor and phase noise of lumped element and distributed element resonators at low temperature and photon number- the operating regime of superconducting qubits. In particular, we compare the performance of poly-crystalline and epitaxial films, silicon and sapphire substrates, and weak link and tunnel type Josephson junctions.

3:06PM T29.00004 Quantum model for superconducting resonator loss via a two-level system , MISHKATUL BHATTACHARYA, K. OSBORN, A. MIZEL, Laboratory for Physical Sciences, University of Maryland, College Park, MD 20740 — Clarifying the mechanisms of dissipation in superconducting resonators is crucial for advancing superconducting quantum computation. The models currently employed to study dielectric loss due to two level charge fluctuators have been based largely on a classical treatment of the problem. In contrast, we carry out a quantum mechanical investigation using a dissipative Jaynes-Cummings model in which the resonator is coupled to a two-level system that is in turn coupled to a bath. We present an analysis of the dynamics of energy decay in the system, comparing its predictions to those of well-known classical models, which agree with our results in the limit of high oscillator excitation.

3:18PM T29.00005 Possible interactions between two-level system defects in SiNx films , SERGIY GLADCHENKO, MOE KHALIL, Laboratory for Physical Sciences, MD, C.J. LOBB, F.C. WELLSTOOD, University of Maryland, Department of Physics, KEVIN D. OSBORN, Laboratory for Physical Sciences, MD — Low-temperature properties of PECVD SiNx dielectric films are measured within the capacitor of superconducting LC resonators. Experiments are made at temperatures from 30 to 300 mK, and at storage energies from 1 to 10^6 photons in a resonant cavity. While the power and temperature dependence of the loss agrees with two-level system (TLS) theory above 60 mK, below this temperature we observe significant deviations. In this regime we observe a reduction in loss upon lowering dielectric temperature, in direct contrast with the independent TLS model of defects within our film. This new phenomena may indicate interactions between two-level systems. We can also spectroscopically resolve the loss from dominant defects in our capacitors, which have a volume of $\sim$2000 μm^3.

3:30PM T29.00006 A study of glassy behavior in amorphous dielectrics using GHz frequency superconducting resonators , MOE KHALIL, M.J.A. STOUTIMORE, University of Maryland and Laboratory for Physical Sciences, AARON HOLDER, CHARLES MUSGRAVE, University of Colorado, C.J. LOBB, F.C. WELLSTOOD, University of Maryland, K.D. OSBORN, Laboratory for Physical Sciences — It has been shown that the dielectric constant of certain glassy materials can be changed with a dc electric field bias. Here we extend those studies to higher frequencies where both the real and imaginary part of the dielectric constant can be studied. We have designed a dc electric-field tunable LC resonator built from superconducting thin-film aluminum to test this effect in SiN_x at GHz frequencies. We will report progress on measuring these devices down to single photon storage energies at temperatures of approximately 30 mK, where the dynamics are dominated by the tunneling of two-level defects.

3:42PM T29.00007 Microwave loss of novel epitaxial superconductor-insulator-superconductor (SIS) trilayers , U. PATEL, Department of Physics, University of Wisconsin, Madison, Wisconsin 53706, USA, K.H. CHO, Department of Materials Science and Engineering, University of Wisconsin, Madison, Wisconsin 53706, USA, L. MAURER, S. SENDELBACH, D. HOVER, Department of Physics, University of Wisconsin, Madison, Wisconsin 53706, USA, C.B. EOM, Department of Materials Science and Engineering, University of Wisconsin, Madison, Wisconsin 53706, USA, R. MCDERMOTT, Department of Physics, University of Wisconsin, Madison, Wisconsin 53706, USA — The performance of superconducting phase qubits is currently limited by spurious coupling of the qubit to two-level state (TLS) defects in the amorphous dielectric materials of the circuits. Thus, it is highly desirable to develop defect free epitaxial dielectric materials for improved junction barriers and capacitor dielectrics. We have characterized the dielectric loss of several candidate SIS trilayers including Re/MgO/Al and Re/$LaAlO_3$/Al grown on c-sapphire substrates. We describe our multiplexed microstrip resonator device layout and present data on the intrinsic quality factors of the MBE-grown dielectrics.

3:54PM T29.00008 Growth of epitaxial superconductor/dielectric heterostructures using a sputtering PLD hybrid system with in-situ RHEED , KWANG HWAN CHO, JACOB PODKAMINER, CHAD FOLKMAN, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison — One of limiting factors in superconducting qubits is decoherence caused by microscopic defects in dielectric layer such as nanocrystalline regions and grain boundaries in a shunted capacitor. We have grown epitaxial Re thin films on a c-plane sapphire substrate using RF magnetron sputtering, then transferred *ex-situ* to a pulsed laser deposition (PLD) system where dielectrics thin film layer is deposited. One drawback of this fabrication approach is the necessity to expose the sample to air when the sample is transferred to different deposition chambers. In order to avoid these drawbacks, we have employed a hybrid PLD-sputtering deposition that will allow us to grow the oxide dielectric/Re heterostructures in an *in-situ* environment without breaking vacuum. The system is also equipped with a reflection high energy electron diffraction (RHEED) which will allow us to perform *in-situ* characterization of the structure and growth dynamics. We will discuss our strategy of epitaxial growth of various single crystal dielectrics on superconducting thin films in this system and their structural and electrical properties of the heterostructures

4:06PM T29.00009 Barrier defect analysis using Josephson junction resonators[1] , M.J.A. STOUTIMORE, BAHMAN SARABI, MOE KHALIL, University of Maryland and Laboratory for Physical Sciences, C.J. LOBB, University of Maryland, K.D. OSBORN, Laboratory for Physical Sciences — We have designed Josephson junction (JJ) resonators by adding an Al/AlO_x/Al Josephson junction in parallel with a coplanar sapphire capacitor and an inductor so that the total loss will be dominated by the junction barrier. JJ resonators couple to individual defects in the junction barrier, causing splittings in the spectroscopy of the resonator when it is excited near single-photon energies, similar to phase and other qubits. Measurements are performed in a dilution refrigerator at 30mK with a drive frequency of approximately 7GHz. By applying a dc flux bias, we can tune the resonance frequency by as much as 1GHz. Analysis of the frequency of splittings as a function of junction area and barrier growth process provides a method for determining the source of the defects. We will use these devices to study amorphous aluminum oxide barriers and will report our progress towards studying novel barrier dielectrics.

[1]This research was supported by the Intelligence Advanced Research Projects Activity through the U.S. Army Research Office award No. W911NF-09-1-0351.

4:18PM T29.00010 Losses in Josephson junction resonators , MARTIN WEIDES, National Institute for Standards and Technology, Boulder, JIANSONG GAO, JEFFREY KLINE, MICHAEL VISSERS, DAVID WISBEY, DAVID PAPPAS — Josephson junctions for superconducting circuits such as SQUIDs and qubits are conventionally based on Al-AlO_x-Al multilayer technology, which was shown to have a low quality factor and two-level-fluctuators in the dielectric AlO_x as limiting decoherence source. By replacing the amorphous Al-rich tunnel oxide with nearly stoichiometric Al_2O_3 we aim to increase the qubit coherence times by reducing the number of dangling bonds in the Josephson tunnel junction. In this talk a test platform for loss determination in high-Q tunnel oxides based on junction resonators will be presented. We will show alternative tunnel junctions based on high temperature grown tunnel oxides.

4:30PM T29.00011 Growth and Properties of Epitaxial Dielectrics/Superconducting Thin Film Heterostructures , CHANG-BEOM EOM, University of Wisconsin-Madison, KWANG-HWAN CHO, JACOB PODKAMINER, CHAD FOLKMAN — Our objective is the growth of epitaxial dielectrics on crystalline superconducting underlayers to improve the performance of superconducting Qbits. A major challenge is heteroepitaxial growth of single crystal dielectric layers with high crystalline quality and atomically sharp interfaces between the dielectric and superconducting electrodes. First, we have grown high quality epitaxial rhenium (Re) thin films on c-plane sapphire substrates by DC magnetron sputtering. The full width at half maximum (FWHM) of Re 0002 rocking curve is less than 0.5 degrees. The RMS surface roughness determined by AFM is less than 1 nm. We have also grown epitaxially various dielectric thin films on top of the single crystal Re bottom electrode by pulsed laser deposition with in situ high pressure reflection high energy electron diffraction (RHEED). In this talk, we will discuss our strategy of epitaxial growth of various single crystal dielectrics on superconducting thin films and their structural and electrical properties of the heterostructures.

4:42PM T29.00012 Microwave Response of Superconducting Resonant Circuits based on 3D Aluminum Nanobridge Josephson Junctions , ELI LEVENSON-FALK, R. VIJAY, KATER MURCH, IRFAN SIDDIQI, QNL, UC Berkeley — Metallic weak links are attractive candidates for low loss superconducting circuits as they offer a route to realize Josephson junctions without the need for an amorphous tunnel barrier-a potential source of both low and high frequency noise. We discuss microwave measurements of high quality factor resonators incorporating both single nanobridges and nanobridge-based SQUIDs. Our results indicate low loss and strong nonlinearity, suggesting the future utility of these devices in qubit and amplifier circuits. Our data are in quantitative agreement with numerically computed nanobridge current-phase relations and dc transport measurements. We show preliminary results on nanobridge-based qubits and parametric amplifiers.

4:54PM T29.00013 Josephson junctions formed from superconducting nanowires[1] , B. XIAO, H.Y. CHEN, I. NSANZINEZA, C. SONG, B.L.T. PLOURDE, Syracuse University — We are investigating the possibility of forming Josephson junctions from thin-film superconducting nanowires. The Josephson coupling through such a constriction can provide the necessary nonlinearity, for example, for forming a qubit, while avoiding the influence of defects in the amorphous tunnel barriers used in conventional Josephson junctions that can contribute to qubit decoherence. We have developed a fabrication process based on high-resolution electron-beam lithography with a negative-tone resist combined with ion-beam etching to pattern nanowires from 10 nm-thick, sputter-deposited, amorphous MoGe thin films. We have studied nanowires with widths between 20 - 100 nm and lengths between 50 - 200 nm. A Nb wiring layer provides electrical connections to the nanowires. Low-temperature transport measurements allow us to study the nanowire critical current and the influence of microwave irradiation on the current-voltage characteristics.

[1]Work supported by IARPA

5:06PM T29.00014 Via fabrication process for epitaxial superconducting qubits , JEFFREY KLINE, FABIO DA SILVA, MICHAEL VISSERS, DAVID WISBEY, MARTIN WEIDES, DAVID PAPPAS, NIST — Reducing the density of spurious two level systems (TLS) in the dielectric layers of superconducting qubits has been shown to improve performance. We aim to reduce TLS density in the Josephson junction tunnel barrier through the use of epitaxial materials. The investigation of some new material systems using a trilayer process wherein the base electrode, tunnel barrier, and top electrode are grown and subsequently patterned is problematic due to sidewall damage during the mesa etch. We apply the via fabrication process wherein the base electrode and wiring insulator layers are grown and patterned prior to tunnel barrier growth. The via process is compatible with a different set of electrode materials than the trilayer process and allows us to investigate the suitability of these materials for qubit applications. We present room temperature and low temperature data for Re/Al_2O_3/Re Josephson junctions fabricated using the via process.

5:18PM T29.00015 Introduction of a DC Bias into a High-Q Superconducting Microwave Cavity , FEI CHEN, JULIANG LI, M.P. BLENCOWE, A.J. RIMBERG, Dartmouth College, ADAM SIROIS, University of Colorado, Boulder, RAYMOND SIMMONDS, National Institute of Standards and Technology, Boulder — The circuit quantum electrodynamics (QED) architecture has been demonstrated to allow study of cavity QED physics in a high-Q on-chip microwave cavity[1]. Here we develop a technique to apply a DC current or voltage bias to nanostructures embedded in the microwave cavity without significantly degrading the Q at high frequencies. Experimental results show good agreement with theoretical predictions. New highly non-linear fully quantum mechanical devices can be developed by embedding Josephson junction devices such as single electron transistors (SETs) in the high-Q microwave cavity. The interplay between the SET and the microwave cavity offers an interesting system for studying nonlinear quantum dynamics and the quantum-to-classical transition. Recent experimental results will be discussed.

[1] A. Wallraff et al, Nature, 431, 162 (2004).

Wednesday, March 23, 2011 2:30PM - 5:18PM –

Session T30 DCMP: Materials: Synthesis, Growth and Processing (Bulk & Films) C147/154

2:30PM T30.00001 ABSTRACT WITHDRAWN –

2:42PM T30.00002 UHV-Compatible Aerosol-Molecule Beam Deposition Source for Organic Electronic Films[1] , LEVAN TSKIPURI, QIAN SHAO, JANICE REUTT-ROBEY, University of Maryland — The rapidly advancing technologies of flexible electronics and organic photovoltaics have triggered strong interest in new methods for electronic materials deposition from the solution phase. Materials deposition based upon direct aerosol flow offers advantages both for fundamental studies of film growth and analysis and for industrial preparation of high-performance materials. We describe an aerosol deposition source based upon a spray-jet molecular beam technique. The source produces a supersonic molecular beam of solutes (such as C_{60}PCBM ([6,6]-phenyl-C_{61}-butyric acid methyl ester) or graphene flakes) in $\sim$10 μ solvent droplets entrained in a nitrogen carrier gas. The twice-differentially pumped source is then mated to a UHV-STM system, for fundamental studies. The source has been used to generate films of C_{60}PCBM, CNT's, and graphene/PPV composites on SiO_2 and mica substrates. The spray-jet deposition provides much greater control of the growth kinetics, relative to conventional spin-coating, permitting films to be grown with submonolayer control, as we demonstrate in the growth of C_{60}PCBM films.

[1]This work has been supported by the UMD MRSEC (DMR 0520471) and NSF Surface and Analytical Chemistry (CHE0750203).

2:54PM T30.00003 Preparation and Characterization of α-Fe_2O_3 Nanoparticles by a Solution-Phase Auto-Combustion Method , MARC DOYLE, Drexel University, MICHAEL LATTANZI, BRIAN KELLY, KARL UNRUH, University of Delaware — The effects of the reaction conditions on the structural and magnetic properties of α-Fe_2O_3 nanoparticles prepared from the combustion products of Fe(III)-nitrate/citric acid/NaOH solutions have been systematically studied in order to gain insights that might be useful in the preparation of more complex oxides from other solution-phase auto-combustion precursors. This work has focused on the effects of the initial solution pH and fuel/oxidant ratio. In particular, precursor powders have been prepared from solutions with pH values between 1 and 12 and with fuel/oxidant ratios between 0.5 and 1.5. Increasing the solution pH and/or the fuel/oxidant ratio lead to significantly less dense and more porous precursor powders due to the greater amount of gaseous reaction products produced under these conditions. X-ray diffraction measurements indicated that under these reaction conditions a higher annealing temperature was required to obtain a phase pure α-Fe_2O_3 product.

3:06PM T30.00004 Synthesis, Microstructure and Bulk Properties of Complex Nasicon-Type Ceramics[1] , KRISTINA LIPINSKA, OLIVER HEMMERS, JULIEN ROMANN, Harry Reid Center for Environmental Studies, University of Nevada Las Vegas, NV, USA, STANISLAV SINOGEIKIN, Geophysical Lab, Carnegie Institution of Washington, Washington, DC, USA, PATRICIA KALITA, HiPSEC & Dept.of Physics, University of Nevada Las Vegas, Las Vegas, NV, USA, SHEKAR BALAGOPAL, ANTHONY NICKENS, CERAMATEC Inc. Salt Lake City, UT, USA — Fast ion-conductors from the NASICON family ($Na_{1+x}Zr_2Si_xP_{3-x}O_{12}$) have been the subject of extensive research due to their use in electrochemical devices such as batteries, fuel cells, thermoelectric generators and chemical sensors A fabrication challenge for these materials is to maintain long term chemical and physical stability in harsh environments We apply a multi-technique approach to show how partial substitutions with tetravalent and pentavalent cations produce NASICONs with specific morphology and modify the primary to secondary crystalline phase ratios. We use in situ synchrotron x-ray diffraction to investigate pressure-induced structural modifications and compressibility.

[1]DOE award DE-FG36-06GO86036. Use of HPCAT: DOE-BES, DOE-NNSA (CDAC), NSF, DODTACOM, W.M. Keck Found. Use of APS: DOE-BES, W-31-109-ENG-38.

3:18PM T30.00005 Crystal structure and multiferroic properties of the $0.7(BaTiO_3) - 0.3(Bi_{0.45}Dy_{0.55}FeO_3)$ ceramic composite , RICARDO MARTINEZ, NORA ORTEGA, ASHOK KUMAR, RATNAKAR PALAI, RAM S. KATIYAR, University of Puerto Rico — Magnetoelectric multiferroics are a novel class of next generation multifunctional materials. Intensive research is being pursued towards the development of new room temperature multiferroics with strong magnetoelectric (ME) coupling. $BaTiO_3$(BT) is well known ferroelectric and $Bi_{0.45}Dy_{0.55}FeO_3$(BDFO) is multiferroic in nature with weak ferroelectric properties. We have synthesized lead free ceramic composite consisting of 0.7BT–0.3BDFO (BT-BDFO) by conventional solid state. X-ray diffraction and Raman analysis revealed two sets of peaks which belong to BT and BDFO suggesting that the individual phases are retained in the composite ceramic, no additional peaks were observed. The presence of ferromagnetic and ferroelectric hysteresis loops at room temperature (M_s=14.3 emu/cm^3, M_r=1.7 emu/cm^3, P_r=3.6 μC/cm^2 and E_c=1.7 kV/cm) showed multiferroic nature of the BT-BDFO ceramic. Although the polarization and magnetization values obtained were lower compared with pure $BaTiO_3$and BDFO respectively, magneto-dielectric measurements reveled a shifting of the dielectric constant peak from 2 MHz to 4 MHz with increase of magnetic field from 0 T to 2 T.

3:30PM T30.00006 Cation Ordering within the Perovskite Block of a Six-layer Ruddlesden-Popper Oxide from Layer-by-layer Growth , LEI YAN, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, H.J. NIU, M.J. ROSSEINSKY, Department of Chemistry, University of Liverpool, Liverpool, L697ZD, UK — The $(AO)(ABO_3)_n$ Ruddlesden-Popper structure is an archetypal complex oxide consisting of two distinct structural units, an (AO) rock salt layer separating an n-octahedra thick perovskite block. Conventional high-temperature oxide synthesis methods cannot access members with $n > 3$, but low temperature layer-by-layer thin film methods allow the preparation of materials with thicker perovskite blocks, exploiting high surface mobility and lattice matching with the substrate. This presentation describes the growth of an $n = 6$ member $CaO/(ABO_3)_n$ (ABO_3: $CaMnO_3$, $La_{0.67}Ca_{0.33}MnO_3$ or $Ca_{0.85}Sm_{0.15}MnO_3$) epitaxial single crystal films on the (001) $SrTiO_3$ substrates by pulsed laser deposition with the assistance of a reflection high energy electron diffraction (RHEED).

3:42PM T30.00007 Morphological Transformation of Copper Catalysts within Helically Coiled Carbon Nanofibers[1]

, LIFENG DONG, Missouri State University, LIYAN YU, QIAN ZHANG, Qingdao University of Science and Technology — With tailoring synthesis parameters, different carbon nanostructures including carbon nanotubes, carbon nanofibers, and graphene, can be synthesized using copper (Cu) as catalysts and acetylene as carbon source. Some remarkable progress has been made in synthesis techniques; however, pioneering breakthroughs have not been made yet in terms of growth mechanism, especially interactions between catalyst particles and acetylene molecules. In this study, the growth mechanism of helically coiled carbon nanofibers and morphological changes of Cu catalysts were investigated using a number of electron microscopy and microanalysis techniques, such as scanning electron microscopy (SEM), transmission electron microscopy (TEM), scanning transmission electron microscopy (STEM), and electron energy loss spectroscopy (EELS). Following the synthesis, single-crystal Cu particles deformed to small nanoparticles of cuprous oxide (Cu2O) due to internal strain, and Cu2O nanoparticles migrated within carbon nanofibers.

[1]This work was supported by Missouri State University, American Chemical Society Petroleum Research Fund, Research Corporation for Science Advancement, National Science Foundation, and Taishan Scholar Overseas Distinguished Professorship program.

3:54PM T30.00008 ABSTRACT WITHDRAWN –

4:06PM T30.00009 Templated Electrodeposition of Highly Porous Nanostructured Materials[1]

, HAN-CHANG YANG, STEPHANIE LIM, JIABIN LIU, QIAN WU, X.M. CHENG, Bryn Mawr College — The fabrication of nanoporous materials has been of great interest for applications such as biosensors, photonic materials and energy storage. Compared to many other methods, the templated electrodeposition method is low cost, fast, and compatible with large-scale production. In this work, we developed a templated electrochemical deposition technique for fabricating highly ordered and highly porous nanostructured materials. The fabrication involves the following steps: self-assembly of monodispersed polystyrene spheres, electrochemical deposition of the desired materials, and sphere removal by a dissolution process. Deposition of Au and Ni layered metallic nanoporous structures were studied using different electrolytes at appropriate potentials. The pore size of the materials was tuned by using different sizes of template polystyrene spheres ranging from 50nm to 1000nm. Scanning electron microscopy images confirmed the highly ordered 3-dimensional hexagonal closed pack (hcp) structures in the samples. The templated electrochemical deposition technique provides a promising alternative approach to preparing highly porous anode materials for battery applications.

[1]Work supported by Bryn Mawr K/G fund for faculty research.

4:18PM T30.00010 Entropic inflation of ideal zeolitic frameworks

, VITALIY KAPKO, COLBY DAWSON, MICHAEL TREACY, Arizona State University — Ideal zeolites can be viewed as flexible networks of rigid, corner-sharing tetrahedra. Recent studies have shown that such systems can exist at a range of densities (termed the "flexibility window") without breaking topology or deforming the comprising tetrahedra. They also have shown that densities of real zeolites almost always correspond to the lowest densities within this range. This anomalous behavior is usually attributed to coulombic repulsion between oxygen atoms in framework cavities and channels. In this paper we show that the inflation of ideal zeolites can be driven by entropy. This effect is closely related to displacive phase transitions often observed in zeolites and related materials like quartz, which cannot be explained by potential energy minimization alone. We show that periodicity and high symmetry in ideal zeolites is a result of entropy maximization. An estimation of entropy using a harmonic oscillator model with a realistic force field is given.

4:30PM T30.00011 Topological defects in model nanoporous carbon: population, structural characterizations and adsorption properties

, XI MI, JEREMY PALMER, JORGE PIKUNIC, KEITH GUBBINS, YUNFENG SHI — Nanoporous carbon materials have drawn substantial research interests because of their unique capabilities to mediate the mass-transport, uptake through adsorptions and catalyze chemical reactions of the guest species. All aforementioned properties depend sensitively on the structural characteristics of the nanoporous carbon, including hybridization state of carbon, presence of functional groups, topology of carbon rings and curvature/connectivity of graphene sheets. Among all these defects, carbon pentagons are of particular interests since they possess 108° C-C-C bond angles which are dramatically different from the 120° angles typical for carbon hexagons and larger carbon rings. However, the pentagon concentration in the bulk has not been determined. Here we use a realistic nanoporous carbon model proposed recently to systematically synthesize a large number of samples with different concentrations of carbon pentagons using molecular simulation methods. We evaluate the different porous structures in terms of their deviations in s(q) from experiments so as to estimate pentagon concentrations. Moreover, the porous structures are related to the adsorption properties through simulated argon adsorption tests.

4:42PM T30.00012 The stability of capillary climbing flows in porous media opposed by gravity force

, B. MARKICEVIC, H.K. NAVAZ, Kettering University — The experimental and numerical data reveal that the capillary climb opposed by gravity force starts as a stable flow for low climbing height, which is followed by unstable flow and multiphase pattern for higher climbing heights. For the stable flow, a sharp interface between the liquid and gas phase exists, which transforms later into a flow front of increasing thickness as climbing progresses. The flow front thickness is calculated from the difference between instantaneous climbing height and maximum stable climbing height. We carry out the analysis of capillary climb flow stability using the capillary and the Bond number, as well as using the generalized Bond number. The critical generalized Bond number defines the condition for which the interface transforms to the flow front. For three distinct porous media consisting of glass beads, and having a thin layer of low permeable material at the bottom of the glass beads columns, the values of critical generalized Bond number and the exponents in the power law of flow front thickness as a function of the generalized Bond number are compared. Furthermore, the flow stability analysis is extended to two additional cases in which a low-permeable layer is removed from the column bottom, and the case of pure capillary flow (without gravity). The corresponding critical generalized Bond numbers and the power law exponents are compared.

4:54PM T30.00013 Soaring to New Heights in Natural Materials[1]

, SARA BODDE, JAMES KIANG, JOANNA MCKITTRICK, University of California, San Diego — Feathers are the most distinguishable feature of all modern Aves. Flight feathers exemplify several materials science phenomena. The most obvious attribute is the branching or hierarchical structure at macroscale to mesoscale. The primary shaft, or rachis from which secondary features project, of the flight feather is a sandwich structured composite. The thin brittle cortex of the rachis and barbules encloses a relatively thick, low-density medullary core or cellular solid. The cortex of the rachis is constructed as a fiber-reinforcement composite, and structural variations along the length of the feather invoke the comparison to functionally graded materials. We have studied microstructure and mechanical properties of the feather rachis in a piecewise fashion, and we will present results of investigations of the mechanical behavior and failure of the composite and parts thereof in tension, compression, and flexure.

[1]Research support: N.S.F. Biomaterials Program (Grant DMR 0510138)

5:06PM T30.00014 Three-dimensional video imaging of drainage and imbibition processes in model porous medium , PRERNA SHARMA, P ASWATHI, ANIT SANE, SHANKAR GHOSH, SABYASACHI BHATTACHARYA, TIFR, Mumbai, India — We report experimental results where we have performed three dimensional video imaging of the displacement of an oil phase by an aqueous phase and vice versa in a model porous medium. The stability of the oil water interface was studied as a function of their viscosity ratios, the wettability of the porous medium and the variation in the pore size distribution. Our experiments captures the pore scale information of the displacement process and its role in determining the long time structure of the interface.

Wednesday, March 23, 2011 2:30PM - 5:30PM –
Session T31 DCMP: Novel Structural Chemistry & Materials C145

2:30PM T31.00001 Theoretical studies of the caged hydrocarbon, octahedrane ($C_{12}H_{12}$, D_{3d})[1] , STEVEN RICHARDSON, Howard University, DANIEL FINKENSTADT, U. S. Naval Academy, MICHAEL MEHL, MARK PEDERSON, Naval Research Laboratory — Polyhedral hydrocarbon cages provide an interesting class of molecules for experimental and theoretical study because of their unique shapes. One such molecule is octahedrane ($C_{12}H_{12}$, D_{3d}) which was first synthesized by Lee *et al.* in 1993.[2] Octahedrane contains two fused three-membered rings and six five-membered rings. Theoretical work by de Meijere *et al.*[3] using density-functional theory (DFT) has shown that octahedrane is more strained than the structurally related molecules decahedrane ($C_{16}H_{16}$, D_{4d}), which has two fused four-membered rings and eight five-membered rings, and dodecahedrane ($C_{20}H_{20}$, I_h), which has two fused-membered rings and ten five- membered rings. In this work we report the first DFT calculations of the infrared and Raman vibrational spectra for octahedrane which will be of importance for future efforts in characterizing this unique caged hydrocarbon.

[1]We are grateful to the ONR for financial support of this work.

[2]C-H Lee, S. Liang, T. Haumann, R. Boese, and A. de Meijere, *Angew. Chem. Int. Ed. Engl.* **1993,** 32, 559.

[3]A. de Meijere, C-H Lee, M. A. Kuznetsov, D. V. Gusev, S. I. Kozhushkov, A. A. Fokin, and P. R. Schreiner, *Chem. Eur. J.* **2005,** 11, 6175.

2:42PM T31.00002 Golcondane (C20H24): Theoretical studies of a novel strained, caged hydrocarbon molecule[1] , DANIEL FINKENSTADT, U.S. Naval Academy, MICHAEL MEHL, MARK PEDERSON, U.S. Naval Research Laboratory, STEVEN RICHARDSON, Howard University — In 1993 Mehta and Reddy reported the synthesis of a new C_{20} polyhedrane, which they named golcondane ($C_{20}H_{24}$, D_{2d}) in honor of the 400^{th} anniversary of the founding of the Indian city of Hyderabad, whose original name was Golconda. Golcondane is a caged, nonacyclic hydrocarbon that has two fused four-membered rings, four fused five-membered rings, and two fused seven-membered rings. Its chemical structure was determined by ^{13}C NMR spectroscopy and unpublished X-ray crystal diffraction studies. Motivated by our previous success in using density-functional theory (DFT) to compute the structural, electronic, and vibrational properties of other hydrocarbons such as cubane, octanitrocubane, the medium-sized diamondoid molecule cyclohexamantane, as well as the novel class of materials known as *sila*-diamondoids, we have used DFT and tight- binding molecular dynamics (TBMD) to compute from first- principles similar properties for golcondane. Our work is especially significant with the lack of other theoretical or experimental studies on this interesting molecule in the published literature.

[1]We are grateful to the ONR for financial support of this work.

2:54PM T31.00003 Spectroscopic identification of bond strain and pi interactions in a series of saturated carbon-cage molecules: adamantane, twistane, octahedrane, and cubane , TREVOR M. WILLEY, J.R.I. LEE, T. VAN BUUREN, LLNL, L. LANDT, TU Berlin, P.R. SCHREINER, A.A. FOKIN, B.A. TKACHENKO, N.A. FOKINA, JLU Giessen, D. BREHMER, SLAC — Novel nanocarbons such as fullerenes, nanotubes, graphene, and nanodiamond reside at the cutting edge of nanoscience and technology. Along with chemical functionalization, geometrical constraints such as extreme curvature or defects in crystallites can modify the electronic properties. This paper presents a fundamental study of how bond strain affects electronic structure in a benchmark series of novel saturated carbon cage compounds. Adamantane, the smallest diamondoid, has carbon atoms commensurate with the diamond lattice. Twistane has the same stoichiometry ($C_{10}H_{16}$), but introduces some bond strain into the cage. Octahedrane ($C_{12}H_{12}$) and cubane (C_8H_8) have increasing strain, culminating in cubane where C-C bonds lie either parallel, or orthogonal to one another. Using gas-phase NEXAFS spectroscopy, we observe the broad C-C σ* splits into two more narrow and intense resonances with increasing strain. Also, LUMO states associated with tertiary C-H σ* broaden and shift to lower energy, and are 3X more intense in cubane than octadedrane. The differences are entirely due to the shape rather than stoichiometry, and indicate, we believe, some π interaction between parallel C-C bonds in the cubane.

3:06PM T31.00004 Spectroscopy and Structure of Diamondoid-Fullerene Hybrid Molecules at the Single-Molecule Level[1] , JASON C. RANDEL, GEORGES NDABASHIMIYE, HARI C. MANOHARAN, Stanford University — Diamondoids—a nanometer-scale form of carbon sharing the sp^3 bonding structure of bulk diamond—are promising new electronic and mechanical device elements and have recently become accessible to experiments. While new fields of research have also sprouted from carbon's sp^2 forms (such as graphene, fullerenes, and carbon nanotubes), materials representing the intersection of sp^2 and sp^3 bonding structures are an exciting new arena for nanoscale science and technology. In this study, we investigate hybrid molecules fusing sp^2 and sp^3 allotropes of carbon (in the form of C_{60} fullerenes and molecular diamondoids, respectively) into one well-defined system. We use low-temperature scanning tunneling microscopy to characterize monolayers and single molecules with sub-molecular resolution. We show the degree to which the electronic properties of the hybrid molecules differ from their single-allotrope components, and highlight the intriguing electronic features that emerge which have no analog in either of the separate molecular constituents.

[1]We thank S. Melinte for aiding measurements, and J. E. P. Dahl, R. M. Carlson, and P. R. Schreiner for materials and synthesis. We acknowledge support from DOE and the Chevron Corporation.

3:18PM T31.00005 The Study of Hypothetical Carbon Allotropes Using Hartree Fock and Density Functional Computational Methods , P.A. ECTON, C.J. MORRIS, J.M. PEREZ, Department of Physics, University of North Texas, S.G. SRIVILLIPUTHUR, Department of Materials Science and Engineering, University of North Texas, G.F. VERBECK, Department of Chemistry, University of North Texas — We have investigated the possibility of hypothetical alternative carbon allotropes using computational methodologies using Gaussian and VASP molecular simulation programs. We investigate the possible existence of carbon based balls, nanotubes and sheets composed of hexagonal rings, cyclobutane rings or pentagonal rings. The possibility of the existence of a hypothetical allotrope is determined by the convergence of the given allotrope under geometric optimization. The theories used to compute such convergence are Hartree-Fock theory and density functional theory. The theoretical Raman spectra of each allotrope can also be computed using Gaussian. The results concerning the reality of the substances under investigation are inconclusive except for a C_{24} ball, which has been shown to converge to graphene and is therefore an unstable molecule.

3:30PM T31.00006 Electron Beam Stimulated Molecular Motions of C_{60}s inside Single-Walled Carbon Nanotubes , KE RAN — Electron beam irradiation stimulated motions of carbon nanostructures from single C_{60} to C_{60}s chain inside single-walled carbon nanotubes (CNTs) were investigated by low voltage and high resolution TEM. Single C_{60}'s jump in a defective zigzag C_{60}s molecular chain inside host CNT was observed. A cluster of C_{60}s inside an isolated partially filled CNT can translate back and forth within the hollow space for several times. Intermediate states of these translations were recorded as well, together with pickup of additional C_{60}s when the moving cluster reached either end of the hollow space. Continuous rotation of a zigzag C_{60} molecular chain inside an overloaded CNT resulted in alternate expansion and contraction of the projected width of the host CNT in the TEM images. The maximum expansion was up to 29%. Potential calculation for the molecular motion was performed based on the van der Waals interaction among C_{60}s and CNT. Activation energies ranging from 0.3 eV to 0.7 eV were estimated. The molecular motion was attributed to momentum transfer during elastic scattering of electrons by the molecules, instead of thermal energy or thermal gradient. Our study demonstrates the potential of driving molecular motion by electron irradiation.

3:42PM T31.00007 First-Principles Calculations of Graphene Nanomesh , WILLIAM OSWALD, ZHIGANG WU, Colorado School of Mines — Graphene has recently attracted intensive attentions owing to its remarkable structural and electronic properties and its significant potential for applications in electronic and optoelectronic devices for size miniaturization and fast electron transportation. However, bulk graphene is a semi-metal with zero bandgap E_g, and opening a sizable E_g is critical for building operational graphene-based transistors. Recently, a new scheme of opening bandgap through punching nanoscale holes in graphene sheet, the graphene nanomesh, was proposed and verified experimentally [1]. However, the mechanism leading to the bandgap opening remains unknown. We have carried out first-principles calculations based on density functional theory (DFT) to study the bandgap opening mechanism and E_g as functions of structural parameters, including the hole size, the hole shape, and the hole-hole distances. Our results suggest that the bandgap opening is a result of quantum confinement at nanomesh necks, while the value of E_g depends not only on the width of nanomesh necks, but also on the chirality of the hole edge. This work was supported by the start-up research funds from Colorado School of Mines.

[1] J. Bai, X. Zhong, S. Jiang, Y. Huang, and X. Duan, Nature Nanotech. **5**, 190 (2010).

3:54PM T31.00008 ABSTRACT WITHDRAWN –

4:06PM T31.00009 Effects of shape and edge-passivation on magnetic moments in graphene nanomesh by first-principles investigation , HONGXIN YANG, MAIRBEK CHSHIEV, SPINTEC, UMR-8191, CEA-INAC/CNRS/UJF-Grenoble 1/Grenoble-INP, Grenoble, France, SPINTEC TEAM — First-principles calculations of electronic and magnetic properties of pure and H-terminated graphene nanomesh (GNM) are presented. We found stable antiferromagnetic and non-magnetic ground state for GNM with balanced zigzag and armchair-type edge structures, respectively. At the same time, a band gap opening in the balanced zigzag edge GNMs which can reach up to 0.40 eV is also found. Interestingly, GNM with unbalanced edge structure shows stable ferrimagnetic state giving rise to a net moment up to 4 Bohr magnetons per unit cell, and the exchange energy between ferrimagnetic state and paramagnetic state is larger than 1 eV per unit cell providing potential for high Curie temperature in this material. Furthermore, we found that the ground states for H-terminated GNM strongly depend on the hole symmetry: large spin polarization ground state is found for GNMs with triangle and pentagon hole shapes, while for GNMs with parallelogram and hexagon shaped holes the ground states are paramagnetic. Finally, we found that the magnetization of the GNM structure is strongly affected by the hole size: the larger hole size attains large moments, while small one may even kill all the moments.

4:18PM T31.00010 Sensing gas molecules using graphitic nanoribbon films and networks , YANBIN AN, JASON L. JOHNSON, ASHKAN BEHNAM, S.J. PEARTON, ANT URAL, University of Florida — We fabricate and study the gas sensing properties of graphitic nanoribbon (GNR) films and networks consisting of multi-layer graphene nanoribbons with an average width of 7 nm. We experimentally demonstrate the high sensitivity of these films and networks for sensing gas molecules at the parts-per-million (ppm) level, in particular hydrogen and ammonia. The sensing response exhibits excellent repeatability and full recovery in air. Furthermore, our results show that functionalization by metal nanoparticles could significantly improve the sensitivity. We characterize the sensing response at various temperatures, gas concentrations, recovery ambients, and film thicknesses. We find that the relative resistance response of the GNR films shows a power-law dependence on the gas concentration, which can be explained by the Freundlich isotherm. The activation energy obtained from the sensing experiments is consistent with the theoretical calculations of the adsorption energies of gas molecules on graphene sheets and nanoribbons. Their simple and low-cost fabrication process and good sensing response open up the possibility of using graphitic nanoribbon films and networks for large-scale sensing applications.

4:30PM T31.00011 Opening of slit-shaped pores from bending of graphene walls[1] , MATTHEW CONNOLLY, University of Missouri-Columbia, CARLOS WEXLER, University of Missouri - Columbia — Graphene has gained particular interest in many areas of research including adsorption. Recent studies have shown deformations in graphene resulting from the pressure of intercalants or edge bonds. In this talk, the opening of slit shaped pores from uniaxial bending of the graphene walls of the pore is examined. The energy functional associated with the deformation from equilibrium shape is minimized to obtain an optimal shape. The minimization is done analytically for a simple model and numerically for various graphene-graphene interaction potentials. The strain induced from bending has been shown to effect the hybridization of carbon bonds within the graphene sheet. The effect of any increase in the number of binding sites due to bending as well as hybridization effects on excess adsorption are studied by Molecular Dynamics simulations.

[1]This material is based upon work supported in part by the Department of Energy under Award Nos. DE-FG02-07ER46411, DE-FG36-08GO18142 and DE-AC02-06CH11357.

4:42PM T31.00012 Magneto-reflectance studies of graphite in intense magnetic field , LI-CHUN TUNG, National High Magnetic Field Laboratory, PAUL CADDEN-ZIMANSKY, Columbia University, JINBO QI, Los Alamos National Laboratory, ZHIGANG JIANG, Georgia Innstitute of Technology, DMITRY SMIRNOV, National High Magnetic Field Laboratory — Magnetic subbands of Kish graphite have been investigated by the magneto-infrared reflectance spectroscopy at 4K up to 31T. Both of the Schrödinger- (K-point) and Dirac-like (H-point) Landau level transitions have been observed. The intense magnetic field resolves the transitions caused by the symmetry breaking of the doubly degenerate E3 band near the charge-neutrality point and the splitting of interband transitions due to electron-hole asymmetry. These transitions were not evident in the recent magneto-transmittance studies at high magnetic fields and are important in understanding electron-hole asymmetry and the opening of the energy gap between electron and hole bands. From the SWMC model, we derived a new formula to describe the magnetic field dispersion of the K-point transitions and a good agreement is achieved with a set of band parameters consistent with the ones reported in the literature.

4:54PM T31.00013 Size-dependence of electronic and optical properties of armchair graphene nanoislands[1] , JONATHAN MOUSSA, JAMES CHELIKOWSKY, UT Austin — Atomicly precise armchair graphene nanoislands (benzenoid polycyclic aromatic hydrocarbons) have been produced by organic synthesis and to-date have attained sizes up to 222 carbon atoms. The electronic and optical properties of these nanoislands are studied using a combination of semi-empirical methods, time-dependent density functional theory, and the GW/Bethe-Salpeter formalism. Comparisons are made with experimental measurements where available. For this class of materials, theory is able to predict the necessary nanoisland sizes required for potential photovoltaic and light-emitting applications. The study of large nanoislands is focused on parallelogram-shaped islands, which should be particularly amenable to synthesis over a wide range of sizes.

[1]Supported by 'Understanding Charge Separation and Transfer at Interfaces in Energy Materials and Devices (EFRC:CST),' an Energy Frontier Research Center funded by the U.S. DOE, Office of Science, Office of Basic Energy Sciences under Award #DE-SC0001091.

5:06PM T31.00014 Modifying Electronic and Magnetic Properties of BCN sheets by Boron Nitride Domain Size and Tensile Strain[1] , CHUN TANG, CHANGFENG CHEN, Department of Physics and Astronomy and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, NV 89154 — Recent experiments have successfully synthesized atomic thin BCN hybrid composites with controllable BN domain concentration. Using first principles calculations, we report the scaling law of electronic and magnetic properties of this novel structures with respect to BN domain size and geometry. We find due to the BN domain induced internal electric field, the magnetic moment can be effectively modified. External tensile strain engineering can also be applied as an efficient tool to modify the electronic and magnetic properties. Our results may have important applications in semiconducting devices.

[1]Work supported by DOE Grant:DE-FC52-06NA26274.

5:18PM T31.00015 Functionalized 2D atomic sheets with new properties , QIANG SUN, JIAN ZHOU, Peking University, QIAN WANG, PURU JENA, Virginia Commonwealth University — Due to the unique atomic structure and novel physical and chemical properties, graphene has sparked tremendous theoretical and experimental efforts to explore other 2D atomic sheets like B-N, Al-N, and Zn-O, where the two components offer much more complexities and flexibilities in surface modifications. Using First principles calculations based on density functional theory, we have systematically studied the semi- and fully-decorated 2D sheets with H and F and Cl. We have found that the electronic structures and magnetic properties can be effectively tuned, and the system can be a direct or an indirect semiconductor or even a half-metal, and the system can be made ferromagnetic, antiferromagnetic, or magnetically degenerate depending upon how the surface is functionalized. Discussions are made for the possible device applications.

Wednesday, March 23, 2011 2:30PM - 5:30PM –
Session T32 FIAP: Semiconducting Devices & Applications C144

2:30PM T32.00001 Tunable nonadiabatic excitation in a single-electron quantum dot , J.D. FLETCHER, MASAYA KATAOKA, P. SEE, S.P. GIBLIN, T.J.B.M. JANSSEN, National Physical Laboratory, Hampton Road, Teddington, Middlesex TW11 0LW, United Kingdom , J.P. GRIFFITHS, G.A.C. JONES, I. FARRER, D.A. RITCHIE, Cavendish Laboratory, University of Cambridge, J J Thomson Avenue, Cambridge CB3 0HE, UK — We report observation of nonadiabatic excitation of single electrons in a quantum dot. We have developed a way of measuring the excitation spectrum of the quantum dot formed in a tunable-barrier single-electron pump. When the confinement potential is deformed at sub-nanosecond timescales, electrons are excited to states with higher back-tunneling rates leading to a measureable reduction in the pumped current. In the presence of a perpendicular magnetic field we have observed that these states follow a Fock-Darwin spectrum. Our experiments demonstrate a simple model system to study nonadiabatic processes of quantum particles.

2:42PM T32.00002 The dynamic quantum dot as an accurate electron pump[1] , STEPHEN GIBLIN, National Physical Laboratory, SAMUEL WRIGHT, University of Cambridge, JONATHAN D. FLETCHER, MASAYA KATAOKA, National Physical Laboratory, MICHAEL PEPPER, University College London, J.T. JANSSEN, National Physical Laboratory, DAVID RITCHIE, CHRISTINE NICOLL, DAVE ANDERSON, GEB JONES, University of Cambridge — We have developed an accurate single electron pump based on a dynamic quantum dot realised in a GaAs two-dimensional electron system. We report an accurate comparison between the pump current and a reference current derived from quantum standards of voltage and resistance: the Josephson effect and quantum Hall effect. We find that, at a clock frequency of several hundred Megahertz, the pump can transfer one electron per clock cycle with an accuracy approaching 10 parts per million. We discuss the significance of this result in relation to the proposed re- definition of the SI base unit Ampere. Theoretical estimations of the pump error rate indicate that an accuracy of one part in a hundred million is attainable, making our type of pump a candidate for a metrological current standard.

[1]We acknowledge support from the European Metrology Research Programme, grant no. 217257.

2:54PM T32.00003 Measurement of Tunneling Conductance of Two-Dimensional Electrons in a Si MOSFET Nanostructure , HONG PAN, MATTHEW HOUSE, MING XIAO, HONGWEN JIANG — The properties of strongly correlated two-dimensional electrons in semiconductor heterostructure continue to be of a fundamental interest of condensed matter physics [1]. A collection of transport studies have revealed a wealthy of interesting effects in the low-electron density limit, particularly in Si MOSFET structures [2]. In this talk, we present an alternative, tunneling conductance measurement of the 2D electrons in a Si MOSFET nanostructure. In our device, a global gate is used to control the 2D electron density. In addition, a set of small gates, as small as 50nm, forms a lateral tunneling barrier for the measurements. We find that there is a strong correlation between the still puzzling metal-insulator transition observed in transport [2] and our tunneling characteristics. The tunneling conductance is studied under different carrier density and in-plane Magnetic field. The project is supported by the NSF under Grant No. DMR-0804794.

[1] B. Spivak, S. V. Kravchenko, S. Kivelson, and X.P.A. Gao, Rev. Mod. Phys. 82, 1743 (2010).
[2] E. Abrahams, S. V. Kravchenko, M. P. Sarachik, Rev. Mod. Phys. 73, 251 (2001)

3:06PM T32.00004 The magnetized quantum wire: a potential candidate to act as an *active* laser medium , MANVIR KUSHWAHA, Rice University — The fundamental issues associated with the magnetoplasmon excitations are investigated in a quantum wire characterized by a confining harmonic potential and subjected to a perpendicular magnetic field. We embark on the charge-density excitations in a two-subband model within the framework of Bohm-Pines' random-phase approximation. Essentially, the focus of our study is the intersubband (magnetoroton) collective excitation which changes the sign of its group velocity twice before merging with the respective single-particle continuum. The computation of the gain coefficient suggests an interesting and important application: the electronic device based on such magnetoroton modes can act as an *active* laser medium. The situation is analogous to the (quasi-two dimensional) superlattices where the crystal can exhibit a negative resistance: it can refrain from consuming energy like a resistor and instead feed energy into an oscillating circuit.

3:18PM T32.00005 Gain-Induced Refractive Index Changes in Resonantly Pumped Optical Pumping Injection Cavity Lasers , LINDA OLAFSEN, LAUREN BAIN, LAUREN ICE, BEN BALL, Baylor University — An optical pumping injection cavity (OPIC) laser contains a type-II W active region enclosed between two GaSb/AlAsSb distributed Bragg reflector mirrors, where the thickness of the etalon cavity surrounded by the mirrors is tuned to the desired pump wavelength. Multiple reflections of the pump photons result in more efficient absorption of the pump beam and consequently higher efficiencies and lower lasing thresholds. An optical parametric oscillator is used to pump the OPIC lasers at resonance, where the threshold pump intensities are minimized and output efficiencies are maximized. The resonant pump wavelength is found to vary quadratically with temperature, not linearly as would be expected from temperature-dependence of the lattice constant and refractive indices. Possible sources of this nonlinearity are lattice heating and gain-induced changes in the refractive indices resulting from the increase of optical pumping intensity with temperature. Through spectral measurements using step-scan Fourier Transform Infrared spectroscopy and multilayer reflectivity modeling, the relative contributions of these possible sources of parabolic temperature dependence of resonant wavelength are investigated.

3:30PM T32.00006 ABSTRACT WITHDRAWN –

3:42PM T32.00007 Mapping of Strain and Induced Polarization in GaMnAs/GaAs nanowires , EDWIN FOHTUNG, Physics Department, University of California San Diego, A. MINKEVICH, A.A. MATYSHEV, M. RIOTTE, D. GRIGORIEV, T. SLOBODSKYY, V. HOLY, O.G. SHPYRKO, T. BAUMBACH — The effects of surface energy and non-localized interactions are the two major physical mechanisms that guarantees size dependent of elastic properties at the nanoscale. With the limit for linear elasticity defined in the vicinity of the lattice parameter for most materials, non-localized interaction can only arise due to the discrete nature of matter and fluctuations in interatomic forces averaged out within the elastic tensors. Using an extended elasticity theory that introduces higher order perturbations to the classical energy density state of a crystalline material, we demonstrate the possibility of mapping the strain and polarization in device nanostructures with the aid of synchrotron radiation coherent diffraction imaging. We provide experimentally confirmed 2D mapping of the strain field and polarization in etched GaMnAs on GaAs periodic wires.

3:54PM T32.00008 Reflectance Spectra of Plasmon Waveguide Interband Cascade Lasers , ROBERT HINKEY, ZHAOBING TIAN, RUI YANG, TETSUYA MISHIMA, MICHAEL SANTOS, University of Oklahoma — Non-invasive reflectivity measurements have been explored as a method for measuring the carrier concentrations of the Si-doped cladding layers of Plasmon-Waveguide Interband Cascade (IC) Lasers. We present measurements and modeling done both on the IC laser structures, as well as highly doped InAs films grown on GaAs substrates that were used to calibrate the Molecular Beam Epitaxy growth. We have found that there is a sharp drop in the signal of the reflectance spectrum for p- polarized light oscillating near the plasma frequency, which falls in the mid-infrared for the cladding layers of the laser structure. This feature in the spectrum is caused by the interaction of the incident light with collective plasmon modes, and is distinct from the plasma edge feature seen in the reflectance spectrum of semi-infinite samples. A similar "plasma absorption" effect has been observed in thin metal films in the ultraviolet. The doping concentration and layer thicknesses of the structure were obtained by fitting a modeled curve to the measured spectrum. We were able to obtain measurements of the cladding layer doping concentrations (in a range from 10^{18} to 10^{19} cm^{-3}) with values that were in good agreement with those found using Hall effect measurements. We will discuss how these results can aid in improving the design of mid-infrared plasmon waveguide lasers.

4:06PM T32.00009 ABSTRACT WITHDRAWN –

4:18PM T32.00010 Electrical and Optical Characterization of α-Silicon Thin Films[1] , KIRAN SHRESTHA, TANWEER MIRZA BEIG, PRADEEP GALI, PRATHYUSHA NUKALA, CHRIS LITTLER, VINCENT LOPES, USHA PHILIPOSE, Dept. of Physics, University of North Texas, NIGEL SHEPHERD, Materials Science and Eng., University of North Texas, A. J. SYLLAIOS, L-3 Communications EOS — We report on progress in the characterization of amorphous silicon thin-films utilized in infrared detectors. Specifically, we have observed changes in the Raman spectra, resistivity, and activation energy in protocrystalline Si films grown by PECVD as substrate temperature, dopant type and concentration, and hydrogen dilution of the reactants are varied. Both n- and p-type films exhibit four Raman spectral peaks [1]. The TO Raman peak becomes better defined and shifts towards the crystalline TO energy for increasing substrate temperature or H dilution, or for decreasing dopant concentration. Hall and resistivity measurements as a function of both magnetic field and temperature on the same material have been conducted to better understand the relationships between specific growth parameters and key electrical properties.

[1] A. J. Syllaios, et al, "Raman Characterization of Protocrystalline Silicon Films", MRS Symp. Proc.Vol.1153, A16-04, 2009.

[1]Supported by ARO grant W911NF-10-1-0410, William W. Clark Program Manager.

4:30PM T32.00011 Single-Crystalline Germanium Nanowire Heterostructure for High-Performance Transistors and Spintronics[1] , JIANSHI TANG, KANG L. WANG, Device Research Laboratory, Department of Electrical Engineering, University of California, Los Angeles, California, 90095, USA, CHIU-YEN WANG, LIH-JUANN CHEN, Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, Taiwan, 30013, Republic of China — The formation of single-crystalline $Ni_2Ge/Ge/Ni_2Ge$ nanowire heterostructure and its field effect characteristics by controlled reaction between a Ge nanowire and Ni contacts were studied. Transmission electron microscopy (TEM) studies reveal a wide temperature range to convert the Ge nanowire to single-crystalline Ni_2Ge by a thermal diffusion process. The *in-situ* reaction examined by TEM shows atomically sharp interfaces for the $Ni_2Ge/Ge/Ni_2Ge$ heterostructure with good epitaxial matches of Ge[-110]//Ni_2Ge[0-11] and Ge(111)//Ni_2Ge(100). Field effect transistors (FETs) built on this nanowire heterostructure show a high-performance p-type FET behavior with an on/off ratio over 10^5 and a field-effect hole mobility of 210 cm^2/Vs. This nanowire heterostructure with atomically sharp interfaces opens an opportunity to achieve high-performance nanowire transistors and explore promising application in spintronics.

[1]The work was supported in part by FCRP-FENA (Functional Engineered Nano Architectonics)

4:42PM T32.00012 Schottky Barrier Heights in low-k dielectric/Cu Interconnects as Determined by X-ray Photoelectron Spectroscopy , MARC FRENCH, MILT JAEHNIG, MARKUS KUHN, BENJAMIN FRENCH, SEAN KING, Intel Corporation — In order to understand the various possible leakage mechanisms in low-k/Cu interconnects, a knowledge of the basic band alignment between Cu and low-k dielectric materials is needed but has gone largely unreported. In this regard, we have utilized X-ray Photoelectron Spectroscopy (XPS) to measure the Schottky Barrier at interfaces of importance to Cu/low-k interconnects. Specifically, we have utilized XPS to determine the Schottky Barrier at the interface between Cu and low-k SiCN capping layers deposited on Cu via Plasma Enhanced Chemical Vapor Deposition (PECVD). We have also utilized XPS to determine the Schottky Barrier at interfaces between Ta barrier layer materials and low-k SiOC:H ILD materials and the valence band alignment at low-k SiCN:H/SiOC:H interfaces. Lastly, the impact of various plasma surface treatments on the band alignment at these interfaces was also investigated. The cumulative results indicate that electron transport along the SiCN:H/SiOC:H may represent the lowest energy barrier path for line-line Schottky emission based leakage.

4:54PM T32.00013 Plasma Process to Simultaneously Clean ILD and CMP Cu Surfaces[1] , XIN LIU, SANDEEP GILL, FU TANG, Arizona State University, SEAN KING, Intel Corp., R.J. NEMANICH, Arizona State University — Low-k inter-layer dielectrics (ILD) with copper interconnects display advantages for reducing energy consumption in silicon technology. However, the processing induced degradation of the ILD low-k properties has become a challenge. In this work, we have employed remote N_2/H_2 plasma processes to simultaneously clean both low-k ILD (k=2.5) and chemical-mechanical polished (CMP) Cu surfaces. FTIR and C-V results indicate that N_2 plasma cleaning processes show low carbon abstraction as well as a relatively small increase in the dielectric constant (k=2.6). A carboxamide layer is formed which apparently inhibits further etching. In contrast, the k value increases to 3.5 after an H_2 plasma treatment. For the CMP-Cu surfaces, an N_2/H_2 plasma process at 380C effectively removes the oxide and carbon contamination. In addition, the affects of plasma-induced UV light has been studied, and the results indicate enhanced carbon depletion in the ILD. Degradation of the low-k properties is attributed to carbon abstraction which is enhanced by the plasma induced UV and hydrophilic character. The results establish a range of N_2/H_2 plasma processes for simultaneous cleaning of CMP Cu and low-k ILD surfaces.

[1]Supported by the Semiconductor Research Corporation.

5:06PM T32.00014 Elastic properties of high porosity low-k thin films measured by Brillouin light scattering , S. BAILEY, R. SOORYAKUMAR, The Ohio State University, S. KING, G. XU, E. MAYS, C. EGE, J. BIELEFELD, Intel Corporation — The continued scale down of material components present increasing challenges to technology development in the semiconductor industry. In particular, with the introduction of more porous materials and air gaps to further reduce permittivity, one significant issue is that low-k dielectrics in interconnects have sufficient mechanical strength. Since nano-indentation methods are questionable at these ultra-small thicknesses there is a need for non-invasive methods to characterize the mechanical properties of such highly compact porous structures. In this talk results of Brillouin scattering to measure elastic constants of thin ($<$ 200 nm) low-k SiOC:H films with porosities up to 35% will be presented. Discrete longitudinal and transverse acoustic standing modes and their transformation to propagating excitations are investigated. The resulting mode dispersions provide for the Poisson's ratio (ν) and Young's modulus (E) and confirm that, for highest porosity, the reduction in dielectric constant does not result in severe degradation in ν and E.

5:18PM T32.00015 Effective Materials Properties of Interconnections in Industrial Microprocessor Designs , MARY LANZEROTTI, Pacific Lutheran University, GIOVANNI FIORENZA, RICK RAND, IBM T J Watson Research Center — This talk presents a methodology to evaluate tradeoffs between technology and design to obtain the highest performance in industrial VLSI designs [1]. It is well known that the most significant circuitry constraint is that signals must arrive on time. Since the design cycle is time-consuming and complex, there is a need to migrate designs to future technology nodes to amortize design cost. However, models do not exist [1] to guide designers in their evaluation of whether migrated designs will operate successfully in a future technology or whether migrated designs will cause chip failure. There is therefore a need to evaluate the impact of design changes on performance. This talk evaluates this impact and describes it as an effective change in material properties of the design interconnections. Model estimates are compared with industrial microprocessor design data [1]. References [1] M. Y. Lanzerotti, G. Fiorenza, R. Rand, "Impact of interconnect length changes on effective materials properties (dielectric constant)," *Proc. Ninth International ACM Workshop on System-Level Interconnect Prediction (SLIP 2007)*, Austin, TX, USA, March 17-18, 2007. Online: http://www.informatik.uni-trier.de/∼ley/db/conf/slip/slip2007.html, current as of 11-16-2010.

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T33 DMP DCOMP: Focus Session: Dielectric, Ferroelectric, and Piezoelectric Oxides: Pb-based and novel materials C143/149

2:30PM T33.00001 Origin of diffuse scattering in relaxor ferroelectrics , P. GANESH, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, TN — High-pressure and variable temperature single crystal synchrotron X-ray measurements combined with first-principles based molecular dynamics simulations study diffuse scattering in the relaxor ferroelectric system PSN (PbSc1/2Nb1/2O3). Constant temperature experiments show pressure induced transition to the relaxor phase at different temperatures characterized by butterfly and rod shaped diffuse scattering around the {h00} and {hh0} Bragg spots, respectively. The simulations [1] reproduce the observed diffuse scattering features as well as their pressure-temperature behavior, and show that they arise from polarization correlations between chemically-ordered regions, which in previous simulations were shown to behave as polar nanoregions. Simulations also exhibit radial diffuse scattering (elongated towards and away from Q=(000)), that persists even in the paraelectric phase, consistent with previous neutron experiments on (PbMg1/3Nb2/3O3) (PMN). DFPT calculations to elucidate origin of Raman peaks in the relaxor phase will also be presented.

[1] P. Ganesh, E. Cockayne, M. Ahart, R. E. Cohen, B. Burton, Russell J. Hemley, Yang Ren, Wange Yang and Z.-G. Ye, Phys. Rev. B **81**, 144102 (2010)

3:06PM T33.00002 Linear dichroism dependence on ferroelectric polarization , SRINIVAS POLISETTY, JINLING ZHOU, MIKEL HOLCOMB, West Virginia University, ANDREAS SCHOLL, Lawrence Berkeley National Laboratory, LANE W. MARTIN, University of Illinois at Urbana-Champaign — X-ray absorption spectroscopy (XAS) and photoemission electron microscopy (PEEM) have been used to determine the magnetic properties of magnetoelectrics, possessing both ferroelectric and magnetic order; however, the additional sensitivity to the ferroelectricity in these films complicates the analysis. Nevertheless, an exclusive knowledge of ferroelectric order is important due to its vital role in manipulating magnetic properties of the magnetoelectrics. To shed light on ferroelectric order and polarization near surface region, we employed mainly PEEM and XAS on ferroelectric $PbZr_{0.2}Ti_{0.8}O_3$ (PZT) film deposited on $LaAlO_3$ substrate. Both out-of-plane and in-plane ferroelectric contributions at Ti $L_{3,2}$ and O-absorption edges have been measured over multiple poled regions on the sample to test various potential mechanisms causing this ferroelectric dichroism, such as surface charge. The ferroelectric order in PZT determined to be systematically evolving as a function of incident x-ray polarization for different rotated angles of the sample revealing a similar angular dependence to that of magnetic samples, allowing a formula for linear dichroism in complex ferroelectrics. This development allows this dynamic approach to be used to study the effect of ferroelectricity on interface coupling in a various materials.

3:18PM T33.00003 Second harmonic generation and high pressure ferroelectricity in $PbTiO_3$(II)[1] , MUHTAR AHART, ALEXANDER F. GONCHAROV, MADDURY SOMAYAZULU, RUSSELL J. HEMLEY, Geophysical Laboratory, Carnegie Institution of Washington — We employed the Raman scattering, x-ray diffraction, and second harmonic generation (SHG) experiments to investigate the behavior of $PbTiO_3$ under pressure up to 100 GPa at 300 K. The experimental results reveal that lead titanate undergoes a second order phase transition from a tetragonal to a cubic at 12 GPa and continuously to a non-cubic structure at 30 GPa. The integral intensity of SHG in the material decreases monotonically with pressure below 12 GPa, and does not depend on pressure above 12 GPa. The results provide no-evidence for high pressure ferroelectricity in $PbTiO_3$ at high pressure and room temperature.

[1]This work is supported by the Carnegie/Department of Energy Alliance Center (CDAC) (DF-FC03N00144).

3:30PM T33.00004 First-principles study to identify heterostructures of (Pb, Sr)TiO_3 with enhanced ferroelectric polarisation , ZHE LIU, Department of Mechanical Engineering, Monash University, Australia — A first-principle cluster expansion method is employed to study the ferroelectric (FE) polarisation properties of $Pb_xSr_{1-x}TiO_3$ perovskite oxide grown on $SrTiO_3$ (001)-substrate. Our results indicate that some heterostructures can significantly enhance polarisation in comparison with the (001) superlattice and the random alloy structures. At $x = 0.5$, an (110) A/B mono-layer superlattice is identified as the structure with the most enhanced polarisation, and at $x = 0.25$, the optimal structure is determined to be a body-centred superstructure. Detailed structural analysis reveals the atomic configurational patterns in the (001) plane that benefit the off-centering of Pb and Sr cations. Explanation is provided in terms of dipole interactions. Our results should apply to other multicomponent FE perovskites as well and they could have a significant impact in the design of FE materials.

3:42PM T33.00005 Interatomic force constants and effective Hamiltonians for structural phase transitions , ANIL KUMAR, KARIN M. RABE, Rutgers University — Expansion of the total energy of a crystal around a high-symmetry reference structure provides information about material properties including the phonon dispersion, responses to applied fields, magnetostructural coupling, and structural transitions. For complex oxides, parameterization of the structural energetics by real-space interatomic force constants (IFCs) provides a computationally convenient and physically transparent way of analyzing these properties. By projection into a subspace containing the relevant degrees of freedom, one can construct an effective Hamiltonian to study properties that are not readily accessible with DFT based calculations, including properties at finite temperature or long length scales. It is well known that first-principles density-functional-theory (DFT) based-calculations can be systematically used to determine real-space IFCs of materials; this is part of several first-principles packages including ABINIT and Quantum Espresso. Here, we discuss a simple and efficient approach for construction of first-principles effective Hamiltonians which uses this computational capability to generate and compute the quadratic inter-cell parameters in a single step. We illustrate the method through the application to systems for which effective Hamiltonians have previously been constructed, and show how this approach facilitates the construction of effective Hamiltonians for new classes of crystal structures.

3:54PM T33.00006 All-atom effective models for first-principles simulations of the temperature-dependent behavior of complex ferroelectric oxides[1] , JORGE INIGUEZ, JACEK C. WOJDEL, ICMAB-CSIC, PATRICK HERMET, PHILIPPE GHOSEZ, University of Liege, ZEILA ZANOLLI, ICMAB-CSIC and University of Liege — Since its introduction in the 90's, the first-principles effective-Hamiltonian method has been successfully used to simulate temperature-driven phenomena in increasingly complex ferroelectrics, from classic compound $BaTiO_3$ to multiferroic $BiFeO_3$. Currently, the emergence of nano-structured materials – e.g., in the form of ultra-thin films or short-period superlattices – poses new challenges to the simulations, and the development of predictive models seems to require a reconsideration of the traditional approach. Of particular interest are cases in which novel interfacial effects determine the behavior, as in the $PbTiO_3$-$SrTiO_3$ superlattices of Bousquet *et al.* [Nature **452**, 7188 (2008)]. In such situations a large number of structural distortions may become active, and it may be difficult to decide which ones need to be included in the model. In order to tackle these difficulties, we are extending the first-principles effective-Hamiltonian method so as to retain a full atomistic description of the material, thus removing the so-called *local mode* approximation. I will describe our new approach and show preliminary results for $PbTiO_3$.

[1]Work funded by the Spanish DGI and the FP7 program of the EU.

4:06PM T33.00007 Prediction of a Low Band Gap Oxide Ferroelectric[1] , DAVID SINGH, ORNL, BO XU, National University of Singapore, VALENTINO R. COOPER, ORNL, YUAN PING FENG, National University of Singapore — We report a first principles study of $Bi_6Ti_4O_{17}$ which is an alternate stacking of ferroelectric $Bi_4Ti_3O_{12}$ (BiT). We the standard PBE GGA functional for the structure and polarization and a recently developed functional that yields accurate band gaps for the electronic structure. We find that this compound is ferroelectric although with a reduced polarization relative to BiT. Importantly, calculations of the electronic structure yield a band gap of approximately 1.4 eV. Therefore, we predict that this stacking is a low band gap oxide ferroelectric.

[1]This work was supported by A*STAR (BX,YPF), the DOE, BES, Materials Sciences and Engineering (DJS,VRC, Ferroelectricity), and the ORNL LDRD Program (DJS, Electronic Structure).

4:18PM T33.00008 Band Gap Engineering via Local Environment in Complex Oxides[1] , TINGTING QI, ILYA GRINBERG, ANDREW RAPPE, University of Pennsylvania — We describe how the electronic structure energy level of the recently-developed highly polar tetragonal perovskite oxides, most prominently $Bi(Zn,Ti)O_3$, can be dramatically changed by a simple rearrangement of the B-cation. Using LDA+Hubbard U, we determine the impact of B-site cation ordering, lattice strain, cation identity, and oxygen octahedral cage tilts on the valence and conduction bands. We find that a combination of ultra-high tetragonality and a careful choice of B-cations can lead to changes of 1-2 eV in the band gap for the same composition, through a change in the B-cation ordering alone. We also find that a layered B-cation ordering exhibits high-mobility 2D hole gas (2DHG) behavior. The lower band gaps of the layered B-cation ordering makes these materials suitable for photovoltaic and photocatalytic applications, due to their good match with the solar spectrum. Our analysis of the crystal structure and the valence and conduction bands shows that these unusual effects can be explained in the framework of crystal field theory and underscores the crucial role that ultra-high tetragonality plays in making the band gap sensitive to the B-cation ordering.

[1]We acknowledge support from ONR, DOE and DOD

4:30PM T33.00009 Modeling the Frequency Dependence of the Complex In-plane Permittivity of Strained Ruddlesden-Popper Series Sr(n+1)Ti(n)O(3n+1) (n = 2, 3, 4, 5, 6) Phases on DyScO3 and GdScO3 , N.D. ORLOFF, National Institute of Standards and Technology, C.-H. LEE, Cornell University, M.D. BIEGALSKI, Oak Ridge National Laboratory, ICHIRO TAKEUCHI, University of Maryland, D.G. SCHLOM, Cornell University, J.C. BOOTH[1] — We explore the in-plane complex relative permittivity as a function of frequency of epitaxial thin-films of the Ruddlesden-Popper series Srn+1TinO3n+1 (n = 2, 3, 4, 5, 6) grown on the rare-earth scandate substrates DyScO3 and GdScO3, which correspond to biaxial tensile strain of approximately 1.1% and 1.7%, respectively. The thin films are 50 nm on DyScO3 and 25 nm thick on GdScO3, to ensure uniform strain throughout the film. We characterize the thin films with a set of optimally designed coplanar waveguides from 45 MHz to 40 GHz and with a set of interdigitated electrodes of varying active lengths from 10 Hz to 100 MHz. We then extract the in-plane complex permittivity from 10 Hz to 40 GHz for these thin films. We report the dependence of the Curie temperature, tunability, and loss tangent on series number and strain at 1 MHz. We also present a frequency-dependent model and the corresponding fit parameters for these thin films as a function of temperature. The model assumes a distribution of domains below the Curie temperature and high frequency relaxation that we attribute to the lowest-order phonon

[1]National Institute of Standards and Technology

4:42PM T33.00010 Study of Temperature-Graded Ferroelectrics Using First-Principle-Based Approaches[1] , QINGTENG ZHANG, INNA PONOMAREVA, University of South Florida — Temperature-graded ferroelectrics have attracted a lot of attention in the recent years owing to their many remarkable properties. Here we develop a microscopic approach based on first-principles effective Hamiltonian to simulate temperature-graded ferroelectrics. Accuracy of such approach is confirmed by comparing our computational results for $(Ba_{0.75}Sr_{0.25})TiO_3$ alloy with available experimental data. Our computations further reveal: 1) strong anisotropy in polarization response: the polarization offset along the temperature gradient is an order of magnitude smaller than in the perpendicular direction; 2) coexistence of different phases (including low-symmetry phases) in chemically homogeneous regions; 3) rotation of polarization in response to temperature gradient in the unclamped samples. These findings could potentially lead to many novel applications such as energy converters, thermally tunable devices and efficient photovoltaics [1].

[1] Q. Zhang *et al*, Phys. Rev. Lett. **105**, 147602 (2010).

[1]This work is supported by DOE grant DE-SC0005245, USF Grant No. R070699.

4:54PM T33.00011 Ferroelectric polarizations of $Pb(Zr_{0.5}Ti_{0.5})O_3$ nanotube array , R. ADHIKARI, HUAXIANG FU, Department of Physics, University of Arkansas, Fayetteville, AR 72701 — Ferroelectric polarization and structural properties are determined for the $Pb(Zr_{0.5}Ti_{0.5})O_3$ (PZT) nanotube array embedded in matrix materials of different polarizability, by means of first-principles derived effective Hamiltonian and finite-temperature Monte Carlo simulations. The polarizability of the matrix is controlled by the on-site κ_2 quantity. We found three drastically different structural phases in PZT nanotubes, depending on the polarizability of the matrix. Microscopic insight for these structural phases will be revealed.

5:06PM T33.00012 Raman scattering studies of the pressure- and temperature-dependent phases of the orbital ordering material $KCuF_3$[1] , SHI YUAN, S. LANCE COOPER, Department of Physics and Frederick Seitz Materials research laboratory, University of Illinois at Urbana-Champaign, Urbana, IL 61801 — We present a study of the temperature- and pressure-dependence of the prototypical orbital ordering system $KCuF_3$ using Raman scattering. Temperature-dependent measurements offer evidence for structural instabilities in $KCuF_3$ at temperatures well below the putative 800K orbital ordering temperature; this evidence includes the observation of anomalous softening of several phonon modes between 50K and 300K and an E_g phonon mode splitting below 50K. The latter indicates a tetragonal-to-orthorhombic structural transition near 50K just preceding the 3D magnetic ordering temperature at $T_N \approx 40$K. Low-temperature, pressure-dependent Raman studies of $KCuF_3$ are also reported to clarify the pressure dependence of the low temperature structural phases in this material.

[1]Work supported by the U.S. Department of Energy under Award No. DE-FG02-07ER46453.

5:18PM T33.00013 Unusually strong Stark effect in electronic ferroelectric $Er_{1-x}Yb_xFe_2O_4$, JIMIN ZHAO, Institute of Physics, Chinese Academy of Sciences, RUI WANG, HUANXIN YANG, JIANQI LI — Strong Stark splitting, which is nearly independent of the R-ions replacement, has been observed through the photoluminescence investigation of electronic ferroelectric $Er_{1-x}Yb_xFe_2O_4$(x=0, 0.8, 0.9, and 0.95). Initially multiple radiative decay channels have been investigated, especially the visible transition $^4F_{9/2} \rightarrow ^4I_{15/2}$, of which a quenching effect has been observed. A series of small non-Raman peaks have been observed superimposed on a broadband photoluminescence spectrum, of which we tentatively assign Stark splitting to be the cause. The splitting of the $^4F_{9/2}$ and $^4I_{15/2}$ levels is found to be 54 meV and 66 meV, respectively. This unusually large Stark splitting at visible range indicates the existence of strong local field originated from the W-layer in the charge-frustrated $ErFe_2O_4$.

Wednesday, March 23, 2011 2:30PM - 5:42PM –

Session T34 DCMP: Optical and Electronic Properties of Nanocrystals and Wires C141

2:30PM T34.00001 Colloidal Quantum Dot Red-Shifting on Textured Metal Surfaces[1] , CHRISTOPHER FERRI, University of California, Merced, School of Natural Sciences, ANTHONY GRIMES, University of California, Merced, School of Engineering, SAYANTANI GHOSH, University of California, Merced, School of Natural Sciences — We have studied the influence of textured metal surfaces on the emission of an ensemble of colloidal CdSe/ZnS core-shell quantum dots (QDs). The texture was generated by sputter coating a thin film of Gold Paladium (AuPd) on a thermoplastic Polydimethylsiloxane (PDMS) sheet. We used two separate protocols to generate two types of surfaces. We constrained some substrates such that they shrunk along only one planar dimension (uniaxial) while some were allowed to shrink along both planar directions (biaxial). The uniaxial substrates forced the metal to buckle along one dimension and the biaxial substrates buckled into a pseudorandom texture. We found that the QDs deposited on the biaxial substrates had a general red shift in the emission wavelength compared to their emission in solution, which also corresponded to a change in the temporal dynamics of the emission. The QDs on the uniaxial substrates showed a change in their temporal dynamics corresponding to plasmonic coupling, but no spectral shift. We hypothesize that the effects observed on the biaxial substrates are caused by the Franz-Keldysh effect.

[1]National Science Foundation

2:42PM T34.00002 Single-molecule spectroscopy study of interfacial charge separation and energy transfer between quantum dots and conjugated polymers , ZHIHUA XU, MIRCEA COTLET, Center for Functional Nanomaterials, Brookhaven National Laboratory — Blends of semiconducting quantum dots (Qdots) and conjugated polymers (CPs) are promising materials for light-emitting diodes or photovoltaic devices. Effective design of optoelectronic devices relies on further understanding of the photophysics in these hybrid materials, including charge separation (CS) and energy transfer (ET). We have studied the photophysics of the blends of two water-soluble conjugated polymers and CdSe/ZnS quantum dots with varying shell thickness, which enable us to control the competitive CS and ET processes by tuning energy-band alignment and interfacial distance. Combining single –molecule spectroscopy with ensemble-based measurements provides deeper understanding of the dynamic interactions at inhomogeneous interfaces.

2:54PM T34.00003 Broadband ultrafast transient absorption of multiple exciton dynamics in lead sulfide nanocrystals , FELICE GESUELE, CHEE WEI WONG, Columbia University, MATTHEW SFEIR, JAMES MISEWICH, Brookhaven National Laboratory, WEONKYU KOH, CHRISTOPHER MURRAY, University of Pennsylvania — Multiple exciton generation (MEG) is under intense investigation as potential third-generation solar photovoltaics with efficiencies beyond the Shockley-Queisser limit. We examine PbS nanocrystals, dispersed and vigorously stirred in TCE solution, by means of supercontinuum femtosecond transient absorption (TA). TA spectra show the presence of first and second order bleaches for the 1Sh-Se and 1Ph-Pe excitonic transition while photoinduced absorption for the 1Sh,e-Ph,e transitions. We found evidence of carrier multiplication (MEG for single absorbed photon) from the analysis of the first and second order bleaches, in the limit of low number of absorbed photons (Nabs$\sim$0.01), for energy three times and four times the Energy gap. The MEG efficiency, derived from the ratio between early-time to long-time TA signal, presents a strongly dispersive behavior with maximum red shifted respect the first absorption peak. Analysis of population dynamics shows that in presence of biexciton, the 1Sh-Se bleach peak is red-shifted indicating a positive binding energy. MEG efficiency estimation will be discussed with regards to spectral integration, correlated higher-order and first excitonic transitions, as well as the nanocrystal morphologies.

3:06PM T34.00004 The effects of controlled charging on photoluminescence of individual "giant" core/shell nanocrystals , CHRISTOPHE GALLAND, YAGNA GHOSH, BHOLA PAL, JENNIFER HOLLINGSWORTH, MILAN SYKORA, VICTOR KLIMOV, HAN HTOON, Los Alamos National Laboratory — We report the first single-nanocrystal photoluminescence (PL) study under controlled charge injection. We investigate so-called "giant" nanocrystal quantum dots (g-NQDs) that comprise a CdSe core and a thick CdS shell. We use solid-state gated devices as well as electrochemical cells for charged injection. When the gate bias or electrochemical potential is tuned, we observe dramatic changes in the PL dynamics that are accompanied by spectral shifts and intensity modulations. Our initial results suggest that negatively charged excitons are at least as bright as neutral excitons in these g-NQDs for which Auger recombination has been shown to be strongly suppressed. Surprisingly, hole injection leads primarily to quenching of the NQD emission, which might explain the appearance of "gray" or "dark" periods in the single-dot PL trajectories.

3:18PM T34.00005 Near-Unity Biexciton Quantum Yields in Individual Giant Nanocrystal Quantum Dots , YOUNG-SHIN PARK, Los Alamos National Lab, ANTON MALKO, University of Texas at Dallas, JAVIER VELA, YONGFEN CHEN, YAGNASENI GHOSH, FLORENCIO GARCIA-SANTAMARIA, JENNIFER HOLLINGSWORTH, VICTOR KLIMOV, HAN HTOON, Los Alamos National Lab — We report quantitative studies of photoluminescence (PL) quantum yields of biexcitons (Q_{BX}) in individual CdSe/CdS core/shell nanocrystal quantum dots (NQDs) as a function of shell thickness. Q_{BX}s measured by two independent techniques show a gradual increase with increasing shell thickness, reaching a near-unity value of $\sim$0.9 for the NQDs with a 19 monolayer-thick shell. These results imply a strong suppression of Auger decay. However, Q_{BX}s show a wide variation among nominally identical NQDs implying a strong dependence of Q_{BX} on subtle structural differences of the core/shell interfaces. Surprisingly, despite a wide variation in Q_{BX}, all thick-shell NQDs exhibit a complete suppression of PL blinking, implying that this non-blinking behavior does not result from the suppression of Auger decay and instead may simply arise from a reduced likelihood of photocharging.

3:30PM T34.00006 Axially localized optical properties of individual nanowires[1] , JUNPING ZHUANG, YAO LIANG, S.K. HARK, The Chinese University of Hong Kong — Nanowires are not always uniform in their properties. Studying the localized optical properties of the nanowires is thus important for their characterization and potential applications. Micro-photoluminescence spectra and fluorescence lifetime along individual ZnSe nanowires were measured and studied using laser scanning confocal microscopy. The nanowires were selected from an array that was synthesized via self catalyzed VLS mode on GaAs substrates. Through fluorescent imaging, the distribution of the deep-level emissions along the nanowires, in which a bright-tip and a dim-tail were observed, is found to be very different from the relatively uniform distribution of the near-band-edge emissions. Using fluorescence lifetime imaging, we found that the fluorescence decay behaviors are very different between the two emission bands and have position dependence. We believe that the unintended Ga diffusion during the growth of the nanowires should be responsible for the observed distributions.

[1]Supported by a grant from the RGC of the HKSAR, China (Project 417507).

3:42PM T34.00007 Polarization dependence of ultrafast dynamics in single Si nanowires , M.A. SEO, S.A. DAYEH, P.C. UPADHYA, S.T. PICRAUX, Los Alamos National Laboratory, USA, J. MARTINEZ, B.S. SWARTZENTRUBER, Sandia National Laboratory, USA, A.J. TAYLOR, R.P. PRASANKUMAR, Los Alamos National Laboratory, USA — Understanding how light interacts with individual nanowires (NWs), particularly depending on its polarization with respect to the NW alignment, is essential for a wide range of applications. We present the first ultrafast time-resolved, polarization-dependent experiments on both single- and ensemble-silicon nanowires using non-degenerate pump-probe spectroscopy to excite and probe carriers above the indirect band gap. Polarization sensitive pump-probe excitation and detection reveal a clear anisotropy in the ultrafast dynamics measured parallel and perpendicular to the long axis of a single nanowire. In addition, the magnitude of the photoinduced change in ensembles of NWs varies for four different sets of pump and probe polarization, without an anisotropy in relaxation time. The comparison of ultrafast dynamics between single and ensemble nanowires provides great insight into the influence of incident light polarization on different absorption and interaction mechanisms. The observed anisotropy in single NWs could enable advanced applications, such as optical switching and polarization sensitive photo detection, on the nanoscale, where directional control and high spatial resolution are much desired

3:54PM T34.00008 Space-and-Time-Resolved Spectroscopy of Single GaN Nanowires , PRASHANTH UPADHYA, Los Alamos National Laboratory, JULIO MARTINEZ, QIMING LI, GEORGE WANG, BRIAN SWARTZENTRUBER, Sandia National Laboratories, ANTOINETTE TAYLOR, ROHIT PRASANKUMAR, Los Alamos National Laboratory — Understanding the carrier relaxation pathways in individual semiconductor nanowires (NWs) is crucial, since the geometry of these nanostructures can significantly influence carrier recombination and trapping. In particular, GaN NWs are promising wide bandgap semiconductors for applications in nanophotonics, but the efficiency and lifetime of GaN-based devices are largely affected by the presence of structural and point defects. In this study we employ wavelength-tunable femtosecond optical pump-probe spectroscopy to study carrier relaxation through the defect states responsible for yellow luminescence in both a single GaN NW and NW ensembles. These are the first ultrafast optical experiments on single group III-V NWs, revealing spatially resolved carrier dynamics along the length of an individual wire.

4:06PM T34.00009 Electronic Structure of PbSe Nanorods , ADAM BARTNIK, Cornell University, ALEXANDER L. EFROS, Naval Research Laboratory, WEON-KYU KOH, University of Pennsylvania, JUN YANG, Cornell University, CHRISTOPHER MURRAY, University of Pennsylvania, FRANK WISE, Cornell University — In spherical lead-salt (PbS and PbSe) nanocrystals, their large dielectric constant and mirror-like band structure significantly weaken the Coulomb interaction, while their large exciton Bohr radii place them at the limit of strong confinement. But in a 1-dimensional structure, the Coulomb interaction can act primarily through the medium, greatly reducing screening. Thus, by controlling their length, the lead-salts can uniquely switch from strong confinement to strong Coulomb binding. To investigate this, we develop a 4-band k-p model of the electronic structure of lead-salt nanorods (NRs), which includes the Coulomb interaction through an effective 1D potential along the NR axis. Perpendicular to the cylindrical axis, confinement dominates and is the major determinant of the location of peaks in the optical spectra. Along the rod axis, the effective Coulomb potential dominates, highly correlating the electron and hole in this direction and enhancing multiparticle interactions, with the observable effect of producing isolated peaks in optical spectra. Predictions of the locations of these enhanced transitions are shown to have good agreement with measured optical spectra of recently synthesized colloidal PbSe NRs.

4:18PM T34.00010 Atomistic calculations of the exciton-biexciton mixing and biexciton lifetime in CdSe nanocrystals[1] , MAREK KORKUSINSKI, OLEKSANDR VOZNYY, PAWEL HAWRYLAK, Institute for Microstructural Sciences, NRC Ottawa, Canada K1A 0R6 — We present an atomistic tight-binding theory of multi-exciton complexes in spherical CdSe nanocrystals. As shown previously [1] the properties of exciton (X) and biexciton (XX) are determined by the shell of four quasi-degenerate states at the top of the valence band, resulting in a band of correlated XX states. This XX fine structure affects the Coulomb mixing of the low-lying XX with excited X states. Here we compare different approaches to computation of the XX ground state lifetime. The Fermi's golden rule accounting only for directly coupled XX and X configurations is compared to configuration-interaction approach where XX and X with energy close to 2Eg are taken into account. We show that the expansion of the basis of single particle configurations used to describe XX leads to a significant increase of the amount of X configurations to which XX can couple. The effect of inclusion of the X configurations coupled to XX indirectly via the intermediate X states is also discussed.

[1] M. Korkusinski, O. Voznyy, and P. Hawrylak, arXiv:1010.0021 (Phys. Rev. B, 82, 2010, in press).

[1]The authors acknowledge funding from NRC-NSERC-BDC Nanotechnology Project.

4:30PM T34.00011 Can nanocrystals be charge-doped using surface adsorbates? , ALEX KUTANA, STEVE ERWIN, Center for Computational Materials Science, Naval Research Laboratory — We study theoretically the possibility that lead selenide nanocrystals can be doped with electrons or holes by charge transfer from molecules (hydrazine, N2H4) adsorbed on their surface. Despite experiments showing that hydrazine adsorption greatly increases the conductivity of PbSe nanocrystal films, our density-functional theory results show no evidence that carriers are directly created by adsorption. Instead, we find that PbSe always remains intrinsic for a variety of hydrazine coverages and PbSe surface orientations. Moreover, analysis of the charge density shows negligible electron transfer from hydrazine to the surface. We tentatively attribute the discrepancy between experiment and theory to extrinsic factors such as surface defects, doping by surface ligands, or dopant activation by hydrazine. For example, we predict that adsorption of acetic acid will create mobile holes in PbSe, and that surface adsorption of lead atoms will result in mobile electrons.

4:42PM T34.00012 Surface states in CdSe nanocrystals with carboxylic acid ligands: an ab initio study[1] , OLEKSANDR VOZNYY, Quantum Theory Group, Institute for Microstructural Sciences, NRC Ottawa, Canada K1A 0R6 — The electronic properties of the realistic Cd-rich CdSe quantum dots with covalently bound (X-type) carboxylic ligands are investigated using density functional theory for the nanocrystal (NC) sizes sufficient to distinguish core and surface states. We find that Cd and Se atoms with only one dangling bond do not create surface traps. The amount of ligands and the crystal shape is dictated by the overall electronic balance of the NC rather than by the surface free energies of particular ligated facets. To achieve this balance more ligands are required than there are "ideal" adsorption sites for them, creating ligand-induced trap states near the valence band maximum. These extra ligands are mobile on surface, resulting in spectral diffusion of the trap levels, providing first atomistic example of diffusion and activated recombination centers models for blinking.

[1]The author acknowledges funding from NRC-NSERC-BDC Nanotechnology Project.

4:54PM T34.00013 First-Principles Calculations of Lattice-Strained Core-Shell Nanocrystals[1] , K.H. KHOO, Institute of High Performance Computing, A*STAR, J.T. ARANTES, Universidade Federal do ABC, JAMES R. CHELIKOWSKY, University of Texas at Austin, G.M. DALPIAN, Universidade Federal do ABC — We have studied the properties of CdS-ZnS and ZnS-CdS core-shell nanocrystals over a range of shell thicknesses using real-space pseudopotential density functional theory. The effect of structural relaxation was shown to be important as it leads to significant changes in the HOMO-LUMO gap and frontier orbital localizations. Also, strains due to lattice mismatch are predicted to be highly localized around the core-shell interface, giving rise to a thin shell regime where both confinement and strain effects are important and a thick shell regime where confinement effects dominate. This has interesting implications for the evolution of the HOMO-LUMO gap with shell thickness.

[1]The work was supported in part by the U. S. Department of Energy, Office of Basic Energy Sciences and Office of Advanced Scientific Computing Research from DE-FG02-06ER15760 on nanostructures and DE-SC000187 on algorithms.

5:06PM T34.00014 First Principles Study of Core-Shell Semiconductor Nanocrystals[1] , IGOR VASILIEV, New Mexico State University — Core-shell nanocrystals composed of two different semiconductors have recently attracted considerable attention. These structures provide enhanced functionality and possess more degrees of freedom than single-component semiconductor nanocrystals and quantum dots. I present the results of *ab initio* density functional calculations for the structures, electronic densities of states, and optical absorption gaps of core-shell nanocrystals composed of group II-VI semiconductors, such as CdSe, CdTe, ZnSe, and ZnTe. The outer surfaces of the nanocrystals are passivated using partially charged hydrogen atoms. The calculations are performed for "traditional" core-shell nanocrystals, in which a core a narrow gap semiconductor is covered with a shell of a wide gap material, and "inverted" core-shell nanocrystals, in which a wide-gap core is enclosed in a narrow-gap shell.

[1]Supported by the Donors of the American Chemical Society Petroleum Research Fund under Grant No. PRF-48556-AC10 and by the U. S. Department of Energy under Grant No. DE-FG36-08GO88008.

5:18PM T34.00015 Jahn-Teller distortion in semiconductor nanocrystals[1] , GUSTAVO M. DALPIAN, ALINE L. SCHOENHALZ, JEVERSON T. ARANTES, Universidade Federal do ABC — Semiconductor nanocrystals or quantum dots can present properties that are very different from their bulk counterparts. Quantum confinement and surface effects play important roles in determining these unusual properties. Here we report a Jahn-Teller distortion in pristine nanocrystals upon the addition of charges. Results will be presented for Si, InAs and CdSe nanocrystals. In order to observe this effect, we have performed calculations using the Density Functional Theory and hybrid functionals. We will discuss the implications of this distortion on the electronic and optical properties of these materials.

[1]Brazilian agencies CAPES, FAPESP and CNPq support this work.

5:30PM T34.00016 Memory, Photoconductivity, and Traps in Semiconducting Nanocrystal Arrays , JESSAMYN FAIRFIELD, LAUREN WILLIS, TALI DADOSH, MARIJA DRNDIC, University of Pennsylvania — Nanoscale devices are extensively studied for their tunable electronic and optical properties, but the influence of impurities and defects is amplified at these length scales and can lead to poorly understood variations in material characteristics. By performing a large ensemble of photoconductivity measurements in nanogaps bridged by core-shell CdSe/ZnS semiconductor nanocrystals, we discover optoelectronic methods for affecting solid-state charge trap populations. We show that the magnitude and temperature dependence of the photocurrent depends on the illumination and electric field history on a few-hour timescale. Subband gap illumination of nanocrystals prior to measurements modifies the photocurrent more than band gap illumination. We introduce a model that unifies previous work and transforms the problem of irreproducibility in nanocrystal electronic properties into a robust photocurrent response due to trap state manipulation. Because traps dominate many physical processes, these findings may lead to improved performance and device tunability for nanoscale applications through the control and optimization of impurities and defects.

Wednesday, March 23, 2011 2:30PM - 5:30PM –
Session T35 DCMP: Metals: Defects and Surfaces C140

2:30PM T35.00001 Orientation effect on dislocation nucleation and related interaction during void growth simulations in Aluminum , AMITAVA MOITRA, MEHUL BHATIA, KIRAN N. SOLANKI, Mississippi State University — Molecular dynamics simulations are performed to understand the void growth for fcc Aluminum. Dislocation nucleation at the void surface and growth of those dislocations in matrix, are studied for seven different crystallographic orientations: [100], [110], [111], [210], [211], [221], and [321]. A significant effect of the loading orientation on dislocation loop nucleation and configuration, and consequently the shape change of voids are found. Calculations related to the interaction of burgers vectors of the nearby leading and trailing dislocations are performed to find the reason why dislocation extremities are attached to the void surface. It has been also shown for a particular orientation that the extremities leave the void surface in order to reduce the interaction energy. Cross slip and triplanar loops are also found during the study of void growth simulations.

2:42PM T35.00002 MD Study of the Nucleation and Growth of Deformation Twins in Polycrystalline Tantalum[1] , LUIS SANDOVAL, DAVID RICHARDS, Condensed Matter and Materials, Lawrence Livermore National Laboratory, Livermore, California 94550, USA — Recovered samples from high strain rate experiments clearly show that twin formation serves as an important plasticity mechanism in Tantalum. Despite years of study however, the nucleation and growth mechanisms of twining are still poorly understood, especially in bcc metals. Twins are typically thought to nucleate at grain boundaries via a cooperative emission of partials after a critical value of shear stress. We have used molecular dynamics (MD) simulation to observe the nucleation and growth of twin domains from grain boundaries and grain boundary junctions in polycrystalline cells, which have been prepared as arrangements of hexagon-columnar grains. Using a Finnis-Sinclair potential, we have examined the role of strain rate, temperature and hydrostatic pressure on the kinetic phenomena, in particular the twinning threshold and twin growth rates. We discuss how kinetic parameters extracted from MD simulations help inform a multiscale strength model for Tantalum that includes both twinning and slip as deformation mechanisms in the regime of high strain rates.

[1]This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 (LLNL-ABS-461533).

2:54PM T35.00003 Large Scale Dislocation Dyniamics Simulation of Precipitation Hardening in Ni-based Superalloys , RENGE LI, ZHIQIANG WANG — The precipitation hardening in Ni-based superalloys, which contain up to 73% volume fraction of γ', has been investigated by large scale 3D dislocation dynamics simulations. Dislocations glide under external stress across a {111} plane of γ/ γ' phase, intersected by cubic γ'precipitates. The critical resolved shear stress (CRSS) has been investigated for different microstructureal parameters: γ'volume fraction, anti-phase boundary (APB) energy and channel width. It is shown that the CRSS depends on the square root of the volume fraction of γ'. The CRSS is linearly proportional to the APB energy. Stuctures with a non-uniform distribution of γ'have CRSS that is 20%-30% smaller than a stucture with unique γ' size corresponding to the average size of the non-uniform disribution of γ'. The fact is that the channel width is not uniform and some channel width is larger than the average channel width of a stucture with a non-uniform distribution of γ', which makes the dislocation line easier to bend. This reveals that the channel width plays more important role than the γ' size. When channel width decreases to about 20nm, CRSS weakly depends on the γ'size and increases dramatically.

3:06PM T35.00004 Thermodynamics of point defects in deformable lattices , ROMAN GROGER, LIBOR SMEJKAL, Institute of Physics of Materials, Academy of Sciences of the Czech Republic, TURAB LOOKMAN, Theoretical Division, Los Alamos National Laboratory, USA — We develop a mean-field model that can be used to study the evolution of microstructure and the density of point defects in irradiated materials. Within this model, the lattice is viewed as an elastic template that is distorted by point defects. The stresses that each defect exerts on its immediate neighborhood in the lattice are represented by its elastic dipole tensor. The lattice responds to these stresses by developing long-range strains that mediate interactions between spatially separated defects. Nonlocal (gradient) elasticity is used to describe the elastic strain energy of the distorted lattice. This gives rise to the gradients of strain in the free energy and ensures an accurate representation of the phonon dispersion curves. In order to demonstrate this model, we consider a cubic lattice with a given density of randomly distributed vacancies and $\langle 100 \rangle$ split interstitials (dumbbells). The occupation of each cell is described by a "spin" with the states {ideal lattice, vacancy, and the three orientations of the $\langle 100 \rangle$ dumbbell}. The evolution of this spin field is obtained by the Monte Carlo (Metropolis) method, with the free energy calculated for each state of the system as described above. Double spin-flip mechanism is adopted to conserve the total mass of the system.

3:18PM T35.00005 Continuum dislocation dynamics: comparison between models , WOOSONG CHOI, YONG CHEN, STEFANOS PAPANIKOLAOU, JAMES SETHNA, Cornell University — Many continuum theories of dislocation dynamics have been proposed to bridge the gap in between discrete microscopic simulations and macroscale phenomenology. As of yet, however, these theories had limited success in explaining or predicting the physics of microstructure formation and evolution. Recently, we have shown that a simple isotropic continuum model dynamically form walls[1] and exhibit complicated microstructure formation and evolution[2] similar to experiments. Most other continuum theories have not seen such structures emerging, and to what extent this theory explains the physics remains to be answered. We explore several variants of the current theories which have different microscopic physics as to how slip systems, cross-slip, statistically stored dislocations, explicit or effective short range interactions, etc. are treated. Comparisons among simulation results of these models will be presented, and we will discuss the relevant mechanisms and their consequences in the dynamics of microstructures.

[1]S. Limkumnerd and J. P. Sethna, Phys. Rev. Lett. **96**, 095503 (2006)
[2]Y. S. Chen, W. Choi, S. Papanikolaou, and J. P. Sethna, Phys. Rev. Lett. **105**, 105501 (2010)

3:30PM T35.00006 Quantum Monte Carlo calculations of defects in aluminum[1] , RANDOLPH Q. HOOD, Lawrence Livermore National Laboratory, PAUL R.C. KENT, FERNANDO A. REBOREDO, Oak Ridge National Laboratory — We use first-principles fixed-node diffusion quantum Monte Carlo to calculate the energetics of point defects in bulk FCC aluminum demonstrating a very high accuracy when compared to experiment. Aluminum has been well studied experimentally as a "simple" metal prototype for investigating the effects of radiation damage such as void formation and helium embrittlement. Often accuracies at the level of milli-electronvolts are required, which is not achieved even for the simple case of pairs of vacancies in aluminum, using common density functionals. Perhaps surprisingly, even single vacancy energies are not reliable in many simple structural materials. Also presented are results for the bulk properties of aluminum - the equilibrium lattice constant, the cohesive energy, and the bulk modulus. These calculations bring a new level of rigor to the study of defects in metals.

[1]This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences as part of an Energy Frontier Research Center and was performed under the auspices of the U.S. Department of Energy by LLNL under Contract DE-AC52-07NA27344.

3:42PM T35.00007 Molecular dynamics simulation of ablation and spallation in nickel films irradiated by ultra-short laser pulses , BRIAN DEMASKE, VASILY ZHAKHOVSKY, University of South Florida, NAIL INOGAMOV, Landau Institute for Theoretical Physics, CARTER WHITE, Naval Research Laboratory, IVAN OLEYNIK, University of South Florida — Ablation and spallation of micron-sized Ni films irradiated by ultra-short laser pulses were investigated via large-scale molecular dynamics simulations. The interatomic interactions are described by a new embedded atom method potential that was specifically developed to accurately simulate response of Ni to strong compression and tensile waves as well as to high temperatures. It was shown that ablation results from cavitation within strongly stretched molten layer beneath the surface of the Ni film. Owing to a superposition of tensile waves, ablation threshold fluence is an increasing function of film thickness, which asymptotically approaches the experimental value for micron-sized films. Processes of wave-breaking and formation of ultra-short shock waves were also investigated in detail. Fluence threshold for onset of spallation at the rear of the film and spall strength of solid Ni subjected to ultrahigh strain rates were predicted.

3:54PM T35.00008 The thresholds of twinning in *bcc* tantalum[1] , KYLE CASPERSEN, ROBERT RUDD, MIKE SURH, LUIS SANDOVAL, DAVID RICHARDS, Lawrence Livermore National Laboratory — The dominate stress relaxation mechanism for most crystalline materials under most conditions is dislocation motion, or slip. However, materials subjected to extreme conditions (for example, conditions that arise in laser based dynamic compression experiments) can exhibit more complex stress relaxation mechanisms. Specifically, for large stress and large strain rates there is a competition between slip and phase transformations and twinning. The conditions at which phase transformations and twinning become important are not known. Therefore, here we present a molecular dynamics study of thresholds of twinning in *bcc* tantalum under various temperatures, pressures, and strain rates.

[1]Prepared by LLNL under Contract DE-AC52-07NA27344.

4:06PM T35.00009 Development of Phase-Field Crystal model free energy functionals based on molecular dynamics , D.M. NICHOLSON, Oak Ridge National Lab, J.A. DANTZIG, Univ. of Illinois, SARMA GORTI, Oak Ridge Natioanl Lab, BALA RANHAKRISHNAN, Oak Ridge National Lab, D.D. JOHNSON, Ames Lab — The Phase-Field Crystal (PFC) model represents the density as a continuous function, whose spatial distribution evolves in time at diffusional, rather than vibrational time scales. PFC provides a tool to study defect interactions at the atomistic level but over longer time scales than those achievable with MD. We examine the behavior of the PFC model with the goal of relating the PFC parameters to physical parameters for Fe and Mo, derived from molecular dynamics (MD) simulations (using either classical force fields or on density-functioanl-theory-based Hellmann-Feynman forces). MD and PFC results for diffusion rates, energy and volumes of fusion, and melting points as a function ofvacancy concentration are used to validate free energy functionals used in the PFC model. Acknowledgments: This work was supported by the Center for Defect Physics, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Office of Basic Energy Sciences.

4:18PM T35.00010 Terminating Surface Electromigration at the Source[1] , KIRK BEVAN, McGill University / Oak Ridge National Laboratory, WENGUANG ZHU, University of Tennessee / Oak Ridge National Laboratory, HONG GUO, McGill University, ZHENYU ZHANG, Oak Ridge National Laboratory / University of Tennessee / University of Science and Technology of China — Through an extensive search across the periodic table utilizing first-principles density functional theory, we have established a general elemental trend for determining electromigration inhibiting impurities on the technologically important Cu(111) surface – the dominant diffusion pathway in modern nanoelectronics interconnects. Unrecognized thus far, such inhibitors are characterized by energetically favoring (and binding strongly at) the kink sites of step edges. These properties are determined to generally reside in elements that form strong covalent bonds with substrate metal atoms. This finding sheds new light on the possibility of halting surface electromigration via kink blocking impurities.

[1]Funding support from the US Department of Energy and NSERC of Canada is gratefully acknowledged.

4:30PM T35.00011 Coverage Dependent Collective Diffusivity of Dense Pb Wetting Layer on Si(111) , LI HUANG, CAI-ZHUANG WANG, Ames Laboratory, MAOZHI LI, Department of Physics, Renmin University of China, Beijing & Ames Laboratory, KAI-MING HO, Ames Laboratory — The anomalous mass transport in the Pb wetting layer on Si(111) surface observed in recent experiments is studied using dynamical calculations of a generalized Frankel-Kontorova model. Instead of typical random-type diffusion, a novel collective liquid-like motion of the Pb atoms within the dense wetting layers is revealed to give rise to the ultrafast kinetics of the wetting layers even at low temperatures. With this collective spreading mechanism of the dense wetting layer, a simple kinetic Monte-Carlo simulation quantitatively reproduces the experimental observations.

4:42PM T35.00012 Atomic layer deposition of metallic cobalt , JINHEE KWON, the University of Texas at Dallas, MARK SALY, RAVI KANJOLIA, SAFC, YVES CHABAL, the University of Texas at Dallas, THE UNIVERSITY OF TEXAS AT DALLAS COLLABORATION, SAFC COLLABORATION — Metallic cobalt has rich catalytic, electronic and magnetic properties, which makes it critical to have a better control of Co thin film deposition for various applications. This work focuses on the atomic layer deposition (ALD) of cobalt using (tertiarybutylallyl)cobalttricarbonyl (^{t}BuAllyl)Co(CO)$_3$ and dimethylhydrazine (DMHy) on H-terminated Si to uncover the growth mechanisms. The first pulse of (^{t}BuAllyl)Co(CO)$_3$ reacts with surface H–Si bonds completely, forming one monolayer of metallic silicide. In situ infrared absorption spectra show that further deposition of Co is made possible only after linear carbonyl groups which remain after the first (^{t}BuAllyl)Co(CO)$_3$ pulse as the surface ligand are removed by subsequent ALD cycles. Further ALD cycles give rise to metallic Co growth through ligand exchange after a nucleation period of 8–10 cycles. The derived growth rate of cobalt is 0.6 $\pm$ 0.1 Å/cycle. The resultant Co film shows low concentration of carbon and nitrogen impurities in the bulk according to X-ray photoemission spectroscopy.

4:54PM T35.00013 Periodic Stacking Faults in Ag Films Grown on Si(111) Decorated by Atomic Chains , AARON GRAY, University of Illinois Urbana Champaign, MANAMI OGAWA, University of Tokyo, HAWOONG HONG, Argonne National Lab, IWAO MATSUDA, University of Tokyo, TAI CHAING, University of Illinois Urbana Champaign — Thin films grown on a substrate decorated by a periodic array of atomic wires can exhibit unusual properties such as stacking faults and electronic topological phase transitions due to the interfacial modulation. We report a study of Ag films grown on an array of atomic In chains on Si(111). Prior STM studies have suggested an array of stacking faults in the Ag films that allow the film lattice structure to match the interfacial modulations. STM however can only probe the surface. Our work uses x-ray diffraction to elucidate the internal 3-dimensional structure of this system. The measurements are found to be best explained by a model in which the unit cell contains a single stacking fault.

5:06PM T35.00014 Measurement of the Spectral Distribution of Low Energy Electrons emitted as a result of NVV Auger Transitions in Ag (100)[1] , S. KALASKAR, Univ Of Texas at Arlington, S.L. HULBERT, Q. DONG, Brookhaven National Lab, NY, B.R. BARTYNSKI, Rutgers University, NJ, A.H. WEISS, Univ of Texas at Arlington — Auger Photoelectron Coincidence Spectroscopy (APECS) was used to investigate the physics of the Low Energy Tail (LET) of the Auger spectrum of Ag (100) at the National Synchrotron Light Source, Brookhaven National Lab, NY. The incident photon energy was set at 180eV. The APECS spectrum contains the contributions from electrons excited by the NVV Auger transition plus a background due to true coincidences between photoemitted valence band electrons that undergo inelastic scattering and transfer part of their energy with other valence electrons which exit the sample. A series of coincidence measurements were made with the fixed analyzer set at energies 150,160,171.5 and 175eV. These measurements were used to obtain an estimate of the background due to the inelastically scattered valance band electrons. The estimated background was then subtracted from the NVV APECS data to obtain the spectrum of electrons emitted solely as a result of the NVV Auger transitions, which contains implications for quantitative interpretation of the Auger spectrum.

[1]Welch Y1100 NSF DMR 0907679

5:18PM T35.00015 First measurements of the Low Energy Tail (LET) down to 0 eV using Auger Photoelectron Coincidence Spectroscopy (APECS) in Ag (100) and Cu (100)[1] , K. SHASTRY, S. KALASKAR, Univ of Texas at Arlington, S.L. HULBERT, Brookhaven National Labs, B.R. BARTYNSKI, Rutgers university, A.H. WEISS, Univ of Texas at Arlington — We present the Auger Photoelectron Coincidence Spectroscopy (APECS) measurements of Ag (100) and Cu (100) over a full range of emitted energies from 0 eV to 81eV. The measurements were successful in separating the low energy Auger lines from a large background, due to loss processes unrelated to the Auger transition. The measurements reveal a well formed Auger peak at 60 eV for Cu and an Auger peak at 40 eV for Ag accompanied by a low energy tail (LET). The LET extends to 0 eV with a broad maximum at 6eV and 10 eV in the case of Cu and Ag respectively. The integrated intensity of the LET in Cu (100) and Ag (100) were 6 and 2 times larger than that of the Auger peak itself. The origin of this LET is discussed in terms of extrinsic mechanisms in which electrons from the peak lose energy as they propagate to the sample surface, as well as intrinsic mechanisms in which multi-electron Auger processes distribute the energy gained by the filling of the core-hole to multiple valence electrons.

[1]Welch Y1100, NSF DMR 0907679

Wednesday, March 23, 2011 2:30PM - 5:18PM –

Session T36 DMP: Focus Session: Graphene Growth, Characterization, and Devices: Structure, Interfaces and Transfer C142

2:30PM T36.00001 Rotated graphene bilayers : from independent layers to electronic localization , LAURENCE MAGAUD, Institut Neel, CNRS, FRANCE — Graphene outstanding electronic properties rely on its pristine honeycomb lattice. Interaction with the environment - substrate, other C layers- and how it affects graphene properties will form the guiding line of the talk. While some interactions might degrade graphene properties, others can open new and interesting possibilities. We focus first on graphene on SiC. The atomic and electronic structures of the interface and of the first C-layers will be discussed on the basis of ab initio calculations (VASP) and STM experiments. At variance with the Si face, the interaction with the substrate is weak on the C face so that the first C-layer already presents graphene properties. We propose a model for the interface which explains the observed rotational disorder. We then discuss the effect of a rotation between two graphene layers to show how it can lead to an effective decoupling of these layers and a linear graphene like dispersion. To tackle very small rotation angles, we developed a tight binding scheme based on ab initio calculations. Three regimes can be defined as a function of the rotation angle. In the first one (teta$>$15°) the two layers are decoupled and behave like independent graphene layers. In the second one (1$<$teta$<$15°) the Dirac velocity of the bilayer is renormalised with respect to the velocity of a monolayer while in the last one (teta$\sim$1° or smaller) the velocity drops to zero which results in localisation. Theses three regimes will be discussed in the light of analytical developments. Experimental evidence or discrepancies with these three regimes will be given.

3:06PM T36.00002 Atomic Scale Transport in Graphene on Stepped SiC(0001) Surfaces , SHUAIHUA JI, JAMES B. HANNON, RUUD M. TROMP, ARTHUR W. ELLIS, MARK C. REUTER, FRANCES M. ROSS, IBM T. J. Watson Research Center, Yorktown Heights, NY — Thermal decomposition of SiC is a promising route to wafer-scale epitaxial graphene. However, the initial SiC surface contains steps, and graphene formation induces additional steps. Here we consider how these steps affect current transport in graphene. 1-2ML graphene was grown by annealing SiC above 1300°C in disilane. Low energy electron microscopy was used to determine graphene thickness, and transport through 1ML thick regions was measured by scanning tunneling potentiometry. In this technique a bias is applied between two fixed probes while a third, scanning probe measures the local electrochemical potential as well as topography. This allows us to determine the resistivity of the graphene sheet on terraces and across substrate steps. Single steps with 0.5nm height show very weak scattering. However, multiple steps of height 1.0 and 1.5nm scatter strongly, exhibiting a potential drop equivalent to $\sim$80nm and 120nm respectively of terrace graphene. Thus, step bunching is important, and steps separated by less than a few hundred nm can dominate transport through a graphene sheet.

3:18PM T36.00003 Twisting and Interlayer Coupling of Few Layer Graphene[1] , MINGHU PAN, XIAOTING JIA, VINCENT MEUNIER, MILDRED S. DRESSELHAUS, JING KONG — Few layer graphene (FLG) can be synthesized by chemical vapor deposition methods. Considering a graphene bilayer with a small angle rotation between the layers—a stacking defect was observed by high resolution scanning tunneling microscopy. Low-energy Van Hove singularities in twisted graphene layers are identified as two sharp peaks in the density of states by low temperature scanning tunneling spectroscopy. Electronic instabilities at the crossing of the Fermi energy with a Van Hove singularity in the density of states often lead to new phases of matter such as charge/spin density waves. We here observe the coexistence of a charge density wave (CDW) phase and a normal phase on the top graphene layer. By analyzing the Moiré pattern in a normal region, a twisting between the two layers by a relative large angle about 3.9° is identified. This implies that the interlayer coupling for twisted layers is playing a role in the formation of different electronic phases in FLG.

[1]This research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Division of Scientific User Facilities, U.S. Department of Energy.

3:30PM T36.00004 Electronic structure of twisted bilayer graphene with doping and under electric fields , LEDE XIAN, SALVADOR BARRAZA-LOPEZ, MEI-YIN CHOU, Georgia Tech — Rotational stacking faults of graphene layers in epitaxial graphene are believed to electronically decouple adjacent layers, thus single-layer graphene-like behavior can be observed. In addition, the layers close to the SiC substrate are known to be electron doped. Using density functional theory and a pi-electron, highly tuned tight-binding model, we study the modifications of the band structure in rotational stack-faulted bilayer graphene induced by doping and by external electric fields. In particular, the interlayer coupling, the magnitude of the Fermi velocity, and the possible impact on charge transport will be discussed.

3:42PM T36.00005 Imaging the first few layers of Multilayer Epitaxial Graphene grown on SiC $(000\bar{1})$, JEREMY HICKS, M. SPRINKLE, B. ZHANG, Georgia Institute of Technology, A. TEJEDA, A. TALEB-IBRAHIMI, P. LE FÉVRE, F. BERTRAN, Synchrotron SOLEIL, W.A. DE HEER, E.H. CONRAD, Georgia Institute of Technology — Multilayer Epitaxial Graphene (MEG) grown on the C-terminated $(000\bar{1})$ face of SiC has been shown to behave as a series of nearly independent graphene sheets, distinguishing it from few-layer graphite. We present photoemission data from MEG films of 10 Å or less, finding that the first few graphene layers on top of SiC are easily visible and are n-doped in a similar fashion to graphene grown on the Si-terminated face. Combined with the characteristic diversity of rotations in MEG films, we have obtained numerous different combinations of cone doping and rotation angles, allowing us to explore a variety of phenomena associated with the graphene-SiC interface interaction. We find that, unlike similarly-doped graphene grown on the Si-terminated face, there exists no large mismatch between the conduction and valence bands. Other potential effects of the substrate are discussed, as well as efforts in modifying the graphene-SiC interface.

3:54PM T36.00006 ABSTRACT WITHDRAWN –

4:06PM T36.00007 Epitaxial graphene on SiC(0001): More than just honeycombs , L. LI, University of Wisconsin, Milwaukee, WI 53211, Y. QI, R.H. RHIM, G.F. SUN, M. WEINERT — Combing scanning tunneling microscopy using transition-metal (Fe, Cr)-coated W tips and first-principles calculations, we show that the interface of epitaxial graphene/SiC(0001) is a warped graphene layer with periodic inclusions of hexagon-pentagon-heptagon ($H_{5,6,7}$) defects [1]. These defects break the six-fold honeycomb symmetry, thereby inducing a gap and two states below E_F near the Dirac point. Furthermore, we show that the next graphene layer assumes the perfect honeycomb lattice, but its interaction with the warped interfacial layer modifies the linear dispersion about the Dirac point, leading to parabolic dispersion and an apparent gap of $\sim$0.25 eV. These results explain recent angle-resolved photoemission and carbon core-level shift data, and resolve the long-standing issue of the interfacial structure of epitaxial graphene on SiC(0001).

[1] Qi et al., Phys. Rev. Lett. **105**, 085502 (2010).

4:18PM T36.00008 Interfacial Structures of Graphene on 4H- SiC Substrates: SCED-LCAO Molecular Dynamics[1] , MING YU, University of Louisville, SEAN FANCHER, Purdue University, JOSEPH H. BUTERA, C.S. JAYANTHI, S.Y. WU, University of Louisville — The purpose of this work is to obtain a microscopic understanding of the interface between the graphene and Si-terminated as well as C-terminated 4H-SiC substrates by studying several cases of nearly commensurate overplayed structures. Relative energies of these different structures are calculated using the SCED-LCAO method [PRB **74**, 15540; PHYSE **42**,1] to gain insight into the role played by the lattice mismatch in releasing the strain and thus lowering the energy of the system. Further insight into the interfacial properties is obtained by analyzing the local strain in terms local atomic and bonding arrangements [PRB **59**, 7745] which will be correlated to the lattice mismatch. Our results will be compared with current experimental [PRL **100**, 176802; PRB **77**, 155303; J. Phys: Condens Matter **21**, 134016; PRB **78**, 205424; J. Phys: Condens Matter **20**, 323202] and theoretical [PRL **99**, 076802; PRL **99**, 126805; PRB **77**, 235412; PRL **100**, 176802] results.

[1]This work is supported by the Research Corporation (RC19902).

4:30PM T36.00009 Epitaxial graphene on SiC(0001): It takes a Si jump , G.F. SUN, Y. LIU, S.H. RHIM, University of Wisconsin, Milwaukee, WI 53211, J.F. JIA, Q.K. XUE, Tsinghua University, Beijing 100084, P. R. China, M. WEINERT, L. LI, University of Wisconsin, Milwaukee, WI 53211 — Using scanning tunneling microscopy with transition metal (Fe, Cr)-coated W tips and first-principles calculations, we have recently shown that interface of epitaxial graphene/SiC(0001) is a warped graphene layer with periodic inclusions of hexagon-pentagon-heptagon ($H_{5,6,7}$) defects that break the six-fold honeycomb symmetry [1]. Here we show that this unique structure facilitate a novel pathway for the disposal of Si during growth: the diffusion of Si vertically through the warped interfacial layer via a series of configurations that involve the dissociation and formation of C-C and Si-C bonds within the pentagon and heptagon of the $H_{5,6,7}$ complex. The calculated energy barrier for this diffusion path is 4.7 eV. These results and their implications on the self-limiting growth of epitaxial graphene on SiC(0001) will be presented at the meeting.

[1] Qi et al., Phys. Rev. Lett. **105**, 085502 (2010).

4:42PM T36.00010 Inhomogeneous strain fields in epitaxial graphene[1] , DIEDRICH A. SCHMIDT, Ruhr-University Bochum Dept. Physical Chemistry II, TAISUKE OHTA, LAURA B. BIEDERMANN, THOMAS E. BEECHEM, STEPHEN W. HOWELL, GARY L. KELLOGG, Sandia National Laboratories — We report a large, inhomogeneous in-plane compressive strain (up to 0.5%) and its local variation at micrometer length scales in single layer graphene films on silicon carbide (SiC) (0001). The strain, due to the difference in lattice constants and thermal expansion coefficients of graphene and SiC substrate, is probed using Raman scattering and low energy electron diffraction. We show that both the growth mechanism and the relaxation along the mismatched symmetry of the graphene and underlying substrate can affect the exact amount of local strain. The large compressive strain implies that monolayer graphene is tightly grafted to the underlying interface layer and SiC substrate; otherwise it would delaminate to relieve the strain. The magnitudes of the structural strain and its local variation are significant and need to be taken into account for electronics applications of the graphene-SiC(0001) system.

[1]This work was supported by BMBF grants 05KS7PC2 and 05K10PCA, the LDRD program at SNL, and the US DOE Office of Basic Energy Sciences' Division of Materials Science and Engineering (Contract No. DE-AC04-94AL85000).

4:54PM T36.00011 Direct Printing of Graphene onto Plastic Substrates. , DANIEL HINES, Laboratory for Physical Sciences, EVGENIYA LOCK, SCOTT WALTON, MIRA BARAKET, MATTHEW LASKOSKI, SHAWN MULVANEY, PAUL SHEEHAN, WOO LEE, JEREMY ROBINSON, Naval Research Laboratory — Graphene films have been synthesized on metal foils using CVD growth and have the potential to be compatible with roll-to-roll printing. To be usable in electronic devices, these films need to be removed from the metallic substrate. Currently this is accomplished by spin coating a polymer film over the graphene and chemically etching away the metal substrate. We have developed a direct printing method that allows graphene films to be printed off the metal substrate onto a polymer substrate. This printing process does not generate chemical waste, is compatible with roll-to-toll processing and renders the metal foil reusable. Adhesion of the graphene film to the polymer substrate is established by attaching perfluorophenylazides (PFPA) azide linker molecules to a plasma activated polymer surface. The transfer printing was performed by placing the PFPA treated polymer surface in contact with a graphene covered Cu foil and heating under pressure. Graphene films successfully printed onto a polystyrene substrate have been characterized by Raman spectroscopy and electrical measurements revealed the presence of Gr on the polymer surface. Details of the printing process along with characteristics of the graphene film after printing will be presented.

5:06PM T36.00012 Improved methods of transfer of graphene from growth substrate to other surfaces and devices , YUJIE REN, HUIFENG LI, Univ. of Texas at Austin, WEIWEI CAI, Xiamen University, SHANSHAN CHEN, RICHARD PINER, RODNEY RUOFF, Univ. of Texas at Austin — Transfer of graphene films from the growth substrate to other surfaces has turned out to be one of the important challenges to creating graphene based devices. In this talk we will review new techniques which we are developing to meet these challenges. In addition to describing the best technique we have to date, we will show data demonstrating the effectiveness of these techniques. Our analysis includes scanning micro-Raman spectroscopy, electronic measurements with FET devices created with our techniques and other microscopic techniques. FET measurements indicate a strong influence of transfer technique on the doping of the device.

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T37 DMP: Focus Session: Graphene Structure, Dopants, and Defects: Nanoribbons

C146

2:30PM T37.00001 Atomically Precise Bottom-up Fabrication of Graphene Nanoribbons , JINMING CAI, Empa, Swiss Federal Laboratories for Materials Science and Technology — Graphene nanoribbons (GNRs) – narrow stripes of graphene – are predicted to exhibit remarkable properties making them suitable for future electronic applications. Contrary to their two-dimensional (2D) parent material graphene, which exhibits semimetallic behavior, GNRs with widths smaller than 10 nm are predicted to be semiconductors due to quantum confinement and edge effects. Despite significant advances in GNR fabrication using chemical, sonochemical and lithographic methods as well as recent reports on the successful unzipping of carbon nanotubes into GNRs, the production of sub-10 nm GNRs with chemical precision remains a major challenge. In this talk, we will present a simple GNR fabrication method that allows for the production of atomically precise GNRs of different topologies and widths [1]. Our bottom-up approach consists in the surface-assisted coupling of suitably designed molecular precursors into linear polyphenylenes and their subsequent cyclodehydrogenation, and results in GNRs whose topology, width and edge periphery are defined by the precursor monomers. By means of STM and Raman characterization, we demonstrate that this fabrication process allows for the atomically precise fabrication of complex GNR topologies. Furthermore, we have developed a reliable procedure to transfer GNRs fabricated on metal surfaces onto other substrates. It will for example be shown that millimeter sized sheets of crosslinked GNRs can be transferred onto silicon wafers, making them available for further processing, e.g. by lithography, prototype device fabrication and characterization.

Coauthors: Pascal Ruffieux, Rached Jaafar, Marco Bieri, Thomas Braun, and Stephan Blankenburg, Empa, Swiss Federal Laboratories for Materials Science and Technology, 3602 Thun and 8600 Dübendorf, Switzerland; Matthias Muoth, ETH Zurich, Department of Mechanical and Process Engineering, 8092 Zurich, Switzerland; Ari P. Seitsonen, University of Zurich, Physical Chemistry Institute, 8057 Zurich, Switzerland; Moussa Saleh, Max Planck Institute for Polymer Research, 55124 Mainz, Germany; Ivan Shorubalko, Empa, Swiss Federal Laboratories for Materials Science and Technology, 3602 Thun and 8600 Dübendorf, Switzerland; Shuping Pang, Xinliang Feng, and Klaus Müllen, Max Planck Institute for Polymer Research, 55124 Mainz, Germany; and Roman Fasel, Empa, Swiss Federal Laboratories for Materials Science and Technology, 3602 Thun and 8600 Dübendorf, Switzerland and University of Bern, Department of Chemistry and Biochemistry, 3012 Bern, Switzerland.

[1] J. Cai *et.al*, Nature **466,** 470-473 (2010)

3:06PM T37.00002 Templated graphene nanoribbon growth on SiC , MING RUAN, MIKE SPRINKLE, YIKE HU, JOHN HANKINSON, MIGUEL RUBIO-ROY, BAIQIAN ZHANG, RUI DONG, ZELEI GUO, Georgia Institute of Technology, CLAIRE BERGER, Georgia Institute of Technology & CNRS- Institut Néel, WALT DE HEER, Georgia Institute of Technology — We demonstrate a photo-lithography fabrication method of graphene nanoribbon. Epitaxial graphene is grown selectively on SiC (1-10n) facets. For this, SiC is patterned to define 3-dimensional structures. Epitaxial graphene nanoribbons grow preferentially on the exposed sidewalls recrystallized facets that avoids post-processing lithography damage of graphene ribbons. Graphene ribbons narrower than 30nm were produced with this method and all-graphene interconnected structures are fabricated. Metal contacts are evaporated on large graphene areas seamlessly connected to nanoribbons. Transport measurement shows gap opening and high mobility. SiC crystal faceting was also explored. Low index crystal facets where found to be energetically favored.

3:18PM T37.00003 Influence of size effects and substrate morphology on the conductance of epitaxial graphene nanoribbons , SARAH BRYAN, YINXIAO YANG, RAGHU MURALI, Georgia Institute of Technology — To utilize graphene's superior electrical properties and achieve transistor operation comparable to that of silicon, the properties of graphene nanoribbons need to be better understood and optimized. Lithographically patterned nanoribbons suffer from line edge roughness which can result in a detrimental effect on the graphene conductivity. In addition to edge-induced scattering, the morphology of the silicon carbide substrate appears to have a strong effect on the line width scaling behavior. In this talk, we present experimental data that clearly shows the interplay between substrate morphology and line edge roughness in epitaxial graphene nanoribbons. Resistivity is shown to strongly increase as nanoribbon line width is reduced, although the line width at which this behavior sets in varies depending upon the substrate morphology. We also propose a model which can be used to predict the dependence of graphene nanoribbon resistivity on line width.

3:30PM T37.00004 Large-scale production of Graphene Nanoribbons with controlled width: Electrical Properties of Graphene Nanoribbon Films[1] , VIKAS BERRY, NIHAR MOHANTY, ASHVIN NAGARAJA, Kansas State University, DAVID MOORE, University of Kansas — In this talk, we will demonstrate a novel large scale production (10^7 ribbons/ sec) scheme for several microns long, smooth-edged graphene nanoribbons (GNRs) with controlled widths (from 5 – 50 nm). We will then present detailed structural, optical and electrical properties of GNR-films $\sim$ 100 nm thick produced from 5, 15, and 45 nm wide GNRs; including their band-gap evolution and electrical transport mechanism. The high throughput method to synthesize GNR of high-quality will be a quantum leap in the graphene research. The work indents to bridge the gaps in the understanding of monodisperse-GNR film properties.

[1]NSF CMMI 0939523

3:42PM T37.00005 Correlated crystallographic etching of graphene and nanoribbon formation , STEPHEN JOHNSON, D. PATRICK HUNLEY, University of Kentucky, JOSEPH STIEHA, ABHISHEK SUNDARARAJAN, ARUNITA KAR, University of Kentucky, A.T. CHARLIE JOHNSON, University of Pennsylvania , DOUGLAS STRACHAN, University of Kentucky — Catalytic etching is a promising method for constructing crystallographically defined graphene structures such as nanoribbons. Catalytic etching experiments are performed and shown to contain significant correlation yielding crystallographic graphene nanoribbons. This correlation is investigated as a function of etching conditions and compared to simulations with possible sources discussed. Supported in part by NSF Award No. DMR-0805136, the Kentucky NSF EPSCoR program, the University of Kentucky Center for Advanced Materials, and the University of Kentucky Center for Nanoscale Science and Engineering.

3:54PM T37.00006 Aligned, ultra-long graphene nanoribbon network fabrication by nanowire etch masks , JOSHUA WOOD, SEAN SIVAPALAN, VINCENT DORGAN, CATHERINE MURPHY, ERIC POP, JOSEPH LYDING, University of Illinois at Urbana-Champaign — Patterning semi-metallic graphene into quasi one-dimensional structures known as nanoribbons (GNRs) can open a ∼0.5 eV bandgap by quantum confinement [1]. To circumvent GNR lithographic difficulties, Si nanowires (NWs) were used previously as an etch mask for exfoliated graphene [2], but with no scalability or alignment control. Conversely, we transfer ∼1 in^2 graphene sheets off copper to silicon dioxide, giving us a template for array fabrication. We meniscus align both Au NWs (<w>=20 nm, <l>=400 nm) and Ag NWs (<w>=200 nm, <l>=10 μm), respectively, on the graphene surface. By reactive ion etch (RIE), we remove the unmasked graphene, and we etch the NWs. Based on the starting NWs, the resulting GNR arrays have lengths ranging from 200 nm to tens of microns, and widths from 10 nm to 250 nm. We create single GNRs that can span micron-separated contacts and GNR networks, similar to a graphene nanomesh. Using atomic force microscopy and Raman spectroscopy, we determine that we have monolayer GNRs with a high disorder intensity I_D/I_G ∼1, indicating rough edges and graphene grain boundaries, which are deleterious to transport. [1] K.A. Ritter and J.W. Lyding, Nat. Mat. 8, 235 (2009). [2] J. Bai et al., Nano Lett. 9, 2083 (2009).

4:06PM T37.00007 Polymer electrolyte enhanced performance in graphene nanoribbon field-effect transistors[1] , CHENG LING, MING-WEI LIN, YIYANG ZHANG, XUEBIN TAN, MARK MING-CHENG CHENG, ZHIXIAN ZHOU, Wayne State University — Graphene nanoribbon Field-effect transistors were fabricated from unzipped multiwall carbon nanotubes on Si/SiO2 substrate by standard electron beam lithography and metal deposition. A small drop of polymer electrolyte consisting of poly(ethylene oxide) and lithium perchlorate was applied to the graphene nanoribbon devices. Electrical transport properties of the polymer electrolyte covered devices were measured using both the Si-back-gate and polymer-electrolyte-gate configurations. We observed dramatic increase of carrier mobility, significant reduction of the peak-width of the resistance as a function of the back-gate voltage, and the shift of the charge neutrality point toward zero gate-voltage in polymer electrolyte covered graphene nanoribbon devices. These experimental results will be presented and discussed in the context of ionic and dielectric screening of charged impurities on or near the graphene nanoribbons.

[1]ZZ acknowledges the support of the WSU new faculty startup funds.

4:18PM T37.00008 Enhanced Conductance Fluctuation by Quantum Confinement Effect in Graphene Nanoribbons[1] , GUANGYU XU, Dept. Electrical Engineering, UCLA, CARLOS TORRES JR., JIANSHI TANG, UCLA EE, JINGWEI BAI, Dept. Material Science and Engineering, UCLA, EMIL SONG, UCLA EE, YU HUANG, UCLA MSE, XIANGFENG DUAN, Dept. Chemistry and Biochemistry, UCLA, YUEGANG ZHANG, Molecular Foundry, LBNL, WANG KANG, UCLA EE, UCLA EE TEAM, UCLA MSE TEAM, UCLA CHEM TEAM, LBNL TEAM — Conductance fluctuations are usually unavoidable in graphene nanoribbons (GNR) due to the presence of disorder along its edges. By measuring the low-frequency noise in GNR devices, we find that the conductance fluctuations are strongly correlated with the density-of-states of GNR [1]. In single-layer GNR, the gate-dependence of noise shows peaks whose positions quantitatively match the subband positions in the band structures of GNR. This correlation provides a robust mechanism to electrically probe the band structure of GNR, especially when the subband structures are smeared out in conductance measurement.

[1]. G. Xu et al. Nano Lett. 2010, 10, 4590–4594.

[1]This work was in part supported by MARCO Focus Center on Functional Engineered Nano Architectonics and the Office of Basic Energy Sciences, of the U.S. Department of Energy.

4:30PM T37.00009 Doping Level Dependence of Transfer Characteristic of n-type Graphene Nanoribbon Field Effect Transistors , LU WANG, RUI QIN, JING ZHOU, HONG LI, JIAXIN ZHENG, JING LU, State Key Laboratory for Mesoscopic Physics and Department of Physics, Peking University, Beijing 100871, P. R. China, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, Nebraska 68182-0266, SHIGERU NAGASE, Department of Theoretical and Computational Molecular Science, Institute for Molecular Science, Okazaki 444-8585, Japan — By performing first principles calculations and electron transport simulations, we demonstrate that the transfer curves of graphene nanoribbon field effect transistors can be controlled by changing the concentration of potassium atoms and cobaltocene molecules doping, or nanoribbon edge carbon atoms substitution by nitrogen. We reveal that Dirac point shift downward from 0 to -12 V when the impurity concentration increase from 0 to 1.37%, while the transfer curves maintain bipolar characteristics with reasonably high on/off ratios. Moreover, we observed strong charge transfer from the adsorbed atoms and molecules that facilitates n-type characteristics in graphene nanoribbons. Thus, we suggest that an effective way to achieve tunable n-type graphene nanoribbons field effects transistors is to dope them with electron donors.

4:42PM T37.00010 The search for stable sp2 zigzag edge graphene nanoribbon termination , CHENGING CHIA, VINCENT CRESPI, Department of Physics, Penn State University — The zig-zag edge of a graphene ribbon has attracted much attention, since it is predicted to support a spin-polarized edge state. However, it is difficult to produce thermodynamic conditions that favor a pure sp^2 termination of a graphene sheet, since the edge carbons generally prefer to bond to two hydrogen atoms, in sp^3 hybridization, rather than one hydrogen, as sp^2. We examine several candidate alternative termination groups which can modify the thermodynamics of various edge configurations to favor the sp^2 edge termination. Ab-initio calculations demonstrate these alternative terminations can support robust edge states across a broad range of synthetic conditions.

4:54PM T37.00011 High resolution thermal properties study of Joule self-heated graphene nanoribbon[1] , YOUNG-JUN YU, MELINDA Y. HAN, STÉPHANE BERCIAUD, TONY F. HEINZ, LOUIS E. BRUS, Columbia University, KWANG S. KIM, Pohang University of Science and Technology, PHILIP KIM, Columbia University — We present high resolution thermal properties of Joule self-heated graphene nanoribbons (GNRs) by scanning thermal microscope (SThM) which enables local temperature survey within 100 nm spatial resolution. In order to calibrate the SThM probes, we employ the micro-Raman spectroscopy to measure the temperature distribution across a standard graphene device as a function of applied electrical power. This calibrated SThM measurement allows us to scrutinize the temperature distributions in GNRs attributed to Joule heating variation in the channel due to the locally enhanced scattering which forms hot spot formation. We also estimate the junction thermal resistance between GNR and SiO_2 substrate from the temperature distribution of the GNR devices. In addition, we will discuss simultaneous SThM and scanning Kelvin probe microscopy study of high quality exfoliated graphene on hexagonal boron nitride substrate.

[1]This work is supported by Global Research Laboratory and FENA.

5:06PM T37.00012 Thermal transport in graphene nanoribbons: R-Matrix theory approach[1] , K.G.S.H. GUNAWARDANA, Homer L .Dodge Department of Physics and Astronomy, Center for Semiconductor Physics in Nanostructures, The University of Oklahoma, KIERAN MULLEN, Homer L. Dodge Department of Physics and Astronomy, Center for Semiconductor Physics in Nanostructures, The University of Oklahoma — We have developed a new theoretical tool based on R-Matrix theory to calculate phonon scattering on the atomic scale. As device sizes shrink, boundary and interface scattering have become bottlenecks to thermal transport. Therefore, calculating thermal transport considering the atomistic constitution of a device is very important. In this R-Matrix approach, we consider a finite region, which is the main scattering center of the system, connected to semi-infinite leads. We develop interior region solutions (normal modes of the finite system) and lead solutions(periodic waves with dispersion) independently that can be matched at predefined boundaries to extract the transmission probabilities of each phonon modes in the lead. In this work we demonstrate the implementation of the theory for graphene nanoribbons.

[1]This work is supported in part by the US National Science Foundation under Grant MRSEC DMR-0080054.

5:18PM T37.00013 Strong suppression of thermal conductivity in edgedisordered graphene nanoribbons: Order-N methodology and thermoelectric properties , HALDUN SEVINCLI, Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany, WU LI, STEPHAN ROCHE, GIANAURELIO CUNIBERTI, Institute for Materials Science and Max Bergmann Center of Biomaterials, TU-Dresden, 01062 Dresden, Germany — We investigate electron and phonon transport through edge disordered graphene nanoribbons. Electronic transport is calculated using Green's functions[1] while for phonons we develop an efficient linear scaling method [2-3] which is based on the Chebyshev polynomial expansion of the time evolution operator and the Lanczos tridiagonalization scheme. We show that edge disorder dramatically reduces phonon thermal transport in both armchair and zigzag ribbons, while in zigzag graphene nanoribbons edge disorder is only weakly detrimental to electronic conduction. The behavior of the electronic and phononic elastic mean free paths points to the possibility of realizing an electron-crystal coexisting with a phonon-glass. The calculated thermoelectric figure of merit (ZT) values qualify zigzag graphene nanoribbons as a promising material for thermoelectric applications.

[1] H. Sevinçli and G. Cuniberti Phys. Rev. B 81, 113401 (2010). [2] W. Li, H. Sevinçli, G. Cuniberti and S. Roche, Phys. Rev. B 82, 041410 (2010). [3] W. Li, H. Sevinçli, S. Roche and G. Cuniberti, arXiv:1011.1116

Wednesday, March 23, 2011 2:30PM - 4:06PM –

Session T38 DCP DBP: Focus Session: Quantum Coherence in Biology IV A130/131

2:30PM T38.00001 Biophysics of Magnetic Orientation: Radical Pairs, Biogenic Magnetite, or both? , JOE KIRSCHVINK, California Institute of Technology — Two major biophysical mechanisms for magnetoreception in terrestrial animals, one based on biogenic magnetite and another on radical-pair biochemical reactions, have been the subject of experiment and debate for the past 30 years. The magnetite hypothesis has stood the test of time: biogenic magnetite is synthesized biochemically in Bacteria, Protists, and numerous Animal phyla, as well as in some plants. Chains of single-domain crystals have been detected by clean-lab based SQUID magnetometry in animal tissues in all major phyla, followed by high-resolution TEM in selected model organisms, as well as by electrophysiological studies demonstrating the role of the ophthalmic branch of the trigeminal nerve in the magnetoreceptive process. Pulse-remagnetization - configured to uniquely flip the polarity of single-domain ferromagnets - has dramatic effects on the behavior of many birds, honeybees, mole rats, turtles, and bats, to cite a growing list. Magnetite-containing cells in the vicinity of these neurons in fish are now the subject of intense study by our consortium. The existence of a specialized class of magnetite-containing magnetoreceptor cells in animal tissues is no longer controversial. In contrast, less success has been achieved in gaining experimental support across a range of taxa for the radical-pair hypothesis. Although this mechanism was proposed to explain an early observation that birds would not respond to complete inversion of the magnetic vector, many organisms (even some birds) do indeed respond to the field polarity. We also note that few, if any, of these critical experiments have been done using fully double-blind methods. This is joint work with: M. M. Walker (University of Auckland, New Zealand) and M. Winklhofer (LMU Munich, Germany).

3:06PM T38.00002 Magnetic compasses in biological systems: Does quantum physics play a role? , THORSTEN RITZ, Dept of Physics and Astronomy, University of California, Irvine — One hypothesis of the process underlying the magnetic compass of animals surmises that the magnetic field is perceived by its effect on the coherent spin evolution within a non-equilibrium photochemical radical pair reaction. If this hypothesis were proven, it would be a dramatic demonstration of a quantum process with clear biological significance. We will review the physics of the radical pair mechanism and the current state of evidence supporting it. Experimentally, we will focus on the use radio-frequency magnetic fields to affect a radical-pair based mechanism in birds and discuss the approach and its limitations. Theoretically, we will focus on the question of how one should design a radical pair to be optimally sensitive to the direction of a weak magnetic field. Regardless of whether or not a radical pair mechanism is indeed used by birds or other animals, optimal design features could be used to manufacture biologically inspired, but man-made magnetic compass systems.

3:42PM T38.00003 Quantum Control and Entanglement in a Chemical Compass , GIAN GIACOMO GUERRESCHI, JIANMING CAI, HANS J. BRIEGEL, University of Innsbruck, Institute for Quantum Optics and Quantum Information (IQOQI) of the Austrian Academy of Science — The radical-pair mechanism is one of the two main hypotheses to explain the navigability of animals in weak magnetic fields, enabling, e.g., birds to see Earth's magnetic field. It also plays an essential role in spin chemistry. Here, we show how quantum control can be used to either enhance or reduce the performance of such a chemical compass, providing a new route to further study the radical-pair mechanism and its applications. We study the role of radical-pair entanglement in this mechanism, and demonstrate its intriguing connections with the magnetic-field sensitivity of the compass. Beyond their immediate application to the radical-pair mechanism, these results also demonstrate how state-of-the-art quantum technologies could potentially be used to probe and control biological functions.

3:54PM T38.00004 A Biochemical Double Slit , IANNIS KOMINIS, University of Crete - Physics Department — Radical-ion-pair reactions, fundamental in photosynthesis and at the basis of the avian magnetic compass mechanism, have been recently shown to offer a rich playground for applying methods and concepts from quantum measurement/quantum information science. We will demonstrate that radical-ion-pair reactions are almost the exact analog of the optical double slit experiment, i.e. Nature has already engineered biochemical reactions performing the act of quantum interference. We will further elaborate on the non-trivial quantum effects pertaining in these reactions and the recent debate on their fundamental theoretical description that these effects have sparked.

Wednesday, March 23, 2011 2:30PM - 5:18PM –

Session T39 DBP: Computational Molecular Biophysics A124/127

2:30PM T39.00001 Simulation of pH-dependent Behavior of Liposome , REJWAN ALI, Fordham University & Queensborough Community College of CUNY — Optimized liposome for biomedical delivery applications has been a field of vigorous research for past few decades. While experimental techniques of fluorescence spectroscopy, differential scanning calorimetry and dynamic light scattering report physical suitabilities in several applications of liposomes, molecular dynamics simulation can provide more detailed feature at atomistic level for such biophysical systems. In recent times, experimental results of liposome's physical properties in different pH environment have widely been reported. The system draws interest for potential applications in several biomedical areas. We will present our molecular simulation results for such system highlighting the effect of pH on hydrogen bonding as well as correlation of dynamics to observed phase behavior.

2:42PM T39.00002 *In silico* investigation of molecular effects caused by missense mutations in creatine transporter protein[1] , ZHE ZHANG, Clemson University, CHARLES SCHWATZ, Greenwood Genetic Center, EMIL ALEXOV, Clemson University — Creatine transporter (CT) protein, which is encoded by SLC6A8 gene, is essential for taking up the creatine in the cell, which in turn plays a key role in the spatial and temporal maintenance of energy in skeletal and cardiac muscle cells. It was shown that some missense mutations in CT cause mental retardation, while others are harmless non-synonymous single nucleoside polymorphism (nsSNP). Currently fifteen missense mutations in CT are known, among which twelve are disease-causing. Sequence analysis reveals that there is no clear trend distinguishing disease-causing from harmless missense mutations. Because of that, we built 3D model of the CT using highly homologous template and use the model to investigate the effects of mutations of CT stability and hydrogen bond network. It is demonstrated that disease-causing mutations affect the folding free energy and ionization states of titratable group in much greater extend as compared with harmless mutations.

[1]Supported by grants from NLM, NIH, grant numbers 1R03LM009748 and 1R03LM009748-S1.

2:54PM T39.00003 Investigating the mechanism of DNA bulk hybridization with Forward Flux Sampling , DANIEL HINCKLEY, Department of Chemical and Biological Engineering, University of Wisconsin-Madison — DNA has become increasingly common as a building block for constructing nanomaterials. However, the mechanism by which DNA hybridization occurs is largely unknown, even in the bulk. Previous work using Transition Path Sampling and a coarse grain DNA model has shown that DNA bulk hybridization occurs via a "slithering" mechanism for repetitive sequences and a distinct nucleation event for random sequences. This mechanistic description remains somewhat incomplete as only configurations within the general vicinity of the transition state ensemble have been examined. In this work, we use Forward Flux Sampling and Langevin Dynamics to examine configurations along the entire transition pathway. We find that, for random sequences, barriers to hybridization arise at certain points in the hybridization pathway requiring reorientation of the two strands. Such barriers are not as pronounced for repetitive sequences where rearrangement occurs without the large scale disruption of hydrogen bonding. The formalism which we use has allowed us to calculate reaction constants for hybridization that are consistent with experiments. It has also allowed us to explain the precipitous decay of reaction rates that is observed when molecular weight is increased.

3:06PM T39.00004 A backbone based protein model with explicit solvent , SUMIT SHARMA, Princeton University, SERGEY BULDYREV, Yeshiva University, PETER J. ROSSKY, University of Texas Austin, H. EUGENE STANLEY, Boston University, PABLO G. DEBENEDETTI, Princeton University, C. AUSTEN ANGELL, Arizona State University, SANAT K. KUMAR, Columbia University — The computational expense of folding atomistically detailed protein models is prohibitive. Hence minimalist models of proteins are a popular choice. The minimalist models developed so far have excluded water, and treated the hydrophobic effect as an effective attraction between hydrophobic monomers. This simplified treatment does not capture the temperature-dependent variations in entropy and enthalpy of water molecules. Proteins have a predominantly water-screened hydrophobic core and water-exposed polar groups. This structural feature should alter the dynamics of proteins and surrounding water from that of a hydrophobic homopolymer in water. To include these features in a minimalist model, we designed heteropolymers of polar and hydrophobic monomers in explicit water-like medium. The polar monomers and water molecules were modeled with the Jagla potential, which has been shown to reproduce many water-like thermodynamic properties, and the hydrophobic monomers as hard spheres. We discuss a methodology for optimizing the sequence of these heteropolymers and how the hydrophobic collapse of these heteropolymers differs from that of a random heteropolymer.

3:18PM T39.00005 Connecting ion channel simulations to experiment , PETER HUGO NELSON, Benedictine University — A simple theoretical framework is used to connect MD simulation with ion channel permeation experiments. MD simulations of potassium channels typically exhibit at least two stable selectivity filter states, one with double occupancy and another with triple occupancy. In the association/dissociation (A/D) model, transitions between these two states occur via concerted motion of all three ions in a shunt-on shunt-off mechanism that is consistent with a large group of published MD simulations. This is the simplest model that explains the universal saturating behavior observed experimentally for many ion channels. Published permeation experiments through the MaxiK channel over a wide range of concentrations and positive voltages are shown to be remarkably consistent with the predictions of this model. Published MD simulations of the Kv1.2 potassium channel exhibit an extended shunt-on shunt-off mechanism at one end of the selectivity filter and a pop-off pop-on mechanism at the other end. This two-step mechanism is incorporated into an asymmetric variant of the A/D model that successfully explains published permeation data through the Shaker potassium channel at physiological concentrations, and successfully predicts qualitative changes in the negative current-voltage data (including a transition to super-Ohmic behavior) based solely on a fit to positive voltage data (that appear linear). Support from NSF 0836833 is gratefully acknowledged.

3:30PM T39.00006 On the Minimum Energy Path to Membrane Pore Formation , CHRISTINA TING, ZHEN-GANG WANG, California Institute of Technology — Several experimental methods have been developed to study the mechanical response of vesicles under an applied tension. Of particular note are the micropipette aspiration techniques and the use of a viscous solution to extend the lifetime of pores. MD simulations have also been used to study the energetic and structural properties of these transient pores on a molecular level. However, they often require extremely high tensions beyond the regime where pore formation is a thermally-activated event. We approach the nucleation problem by combining the string method with dynamic self-consistent field (DSCF) theory to obtain the full minimum energy path (MEP) to pore formation for a range of surface tensions γ. We compare our results with classical nucleation theory (CNT). Near the coexistence ($\gamma \to 0$) the rim of the pore is well-defined and the line tension is well approximated by the macroscopic definition given by CNT. However, when the free energy barrier is within $\sim 10\ \mathrm{kT}$, the transition state is somewhere between a stalk-like structure and a thinned membrane leading to a hole that is partially exposed to solvents. These molecular rearrangements involved in the formation of a pore are not captured by CNT.

3:42PM T39.00007 Capturing electrostatic interactions explicitly with the 3SPN model for DNA , GORDON S. FREEMAN, DANIEL M. HINCKLEY, JUAN J. DE PABLO, Department of Chemical and Biological Engineering, University of Wisconsin-Madison — The "Three Sites Per Nucleotide" (3SPN) model for nucleic acid simulation provides a powerful tool for computational studies of biological phenomena. Previously, this model has relied on an implicit representation of the surrounding ionic environment at the level of Debye-Hückel theory. In this work, we eliminate this limitation and implement an explicit representation of ions, both monovalent and divalent. The coarse-grain ion-ion and ion-phosphate$_{DNA}$ potential is adapted after the model of Lenart *et al.* and parameterized to reproduce the key features in the local structure and organization of ions in the bulk and in the presence of DNA. The parameters of the previous generation of 3SPN (3SPN.1) have been modified to reproduce melting temperatures observed experimentally employing a biased parallel tempering scheme. The resulting model is capable of reproducing the local structure observed in fully detailed atomistic simulations as well as the melting temperature of DNA reported experimentally for a range of DNA oligonucleotide lengths, CG-content, Na^+ concentration and Mg^{2+} concentration. The usefulness of the model is demonstrated in the context of confinement of dsDNA within a viral capsid and the exploration of pathways between dehybridized and hybridized DNA.

3:54PM T39.00008 Intrinsic noise in stochastic models of gene expression with molecular memory and bursting , TAO JIA, RAHUL V. KULKARNI, Department of Physics, Virginia Polytechnic Institute and State University — Regulation of intrinsic noise in gene expression is essential for many cellular functions. Correspondingly, there is considerable interest in understanding how different molecular mechanisms of gene expression impact variations in protein levels across a population of cells. In this work, we analyze a stochastic model of bursty gene expression which considers general waiting-time distributions governing arrival and decay of proteins. By mapping the system to models analyzed in queueing theory, we derive analytical expressions for the noise in steady-state protein distributions. The derived results extend previous work by including the effects of arbitrary probability distributions representing the effects of molecular memory and bursting. The analytical expressions obtained provide insight into the role of transcriptional, post-transcriptional and post-translational mechanisms in controlling the noise in gene expression.

4:06PM T39.00009 First-Principles Study of Muon Trapping in Singlet and Triplet States of Oxyhemoglobin , S.R. BADU, Department of Physics and Astronomy, University of Utah, ACHANA DUBEY, Department of Physics, UCF, LEE CHOW, Physics Department, UCF, R.H. PINK, Physics Department, SUNY Albany, R.H. SCHEICHER, Department of Physics and Astronomy, Uppsala University, K. NAGAMINE, Physics Department, UCR, N. SAHOO, UTMD Anderson, T.P. DAS[1], Department of Physics, SUNY Albany — Observation of muon spin-lattice relaxation effects in Oxyhemoglobin by the muon-spin rotation (μSR) technique [1] has sparked current interest in the possibility of magnetic character in Oxyhemoglobin (OxyHb). First-Principles variational Hartree-Fock Many Body Perturbation Theory (VHFMBPT) technique investigations on the singlet and triplet states of pure (OxyHb) have shown [2] that the triplet state is considerably higher than the singlet state ruling out magnetic character. However the charge distribution obtained by the VHFMBPT procedure in both states show a number of sites that have negative charges where the trapping of muon is being investigated to examine if the energy gap in the ordering of singlet and triplet states can be reduced or reversed leading to magnetic effects. Other possible sources of magnetism in Oxyhemoglobin will also be discussed. [1] K. Nagamine et al. Proc. Japan. Acad. B-Physics 83, 120 (2007); [2] S.R. Badu et al. Reported at Third Joint HFI-NQI International Conference, CERN, Geneva, September 2010.

[1]Also Department of Physics, University of Central Florida

4:18PM T39.00010 Binding-rebinding dynamics of proteins interacting non-specifically with a long DNA molecule , AZITA PARSAEIAN, Department of Materials Science and Engineering, Northwestern University, JOHN F. MARKO, D, MONICA OLVERA DE LA CRUZ, Department of Materials Science and Engineering, Northwestern University — Protein interactions with DNA chains and/or fibers regulate a large number of cell functions, and are also important in the understanding of experiments that reveal biochemical and physical cell processes. In order to determine the time range and length range of interactions between proteins and DNA, we analyze the adsorption and de-sorption of units (proteins) that bind reversibly to linear chains (DNA fibers) via non specific interactions through Monte Carlo simulations. We assume the particles are random walkers and that bind reversibly to stretched DNA fiber. In particular we determine the number of re-bindings events. We find that the number of protein re-bindings have a logarithmic dependence on DNA fiber length.

4:30PM T39.00011 Regulation of gene expression by small RNAs via coupled stoichiometric degradation: a variational approach , THIERRY PLATINI, Virginia Bioinformatics Institute, TAO JIA, RAHUL V. KULKARNI, Department of Physics, Virginia Tech — Regulatory genes called small RNAs (sRNAs) are known to play critical roles in cellular responses to changing environments. For several bacterial sRNAs, regulation is effected by coupled stoichiometric degradation with messenger RNAs (mRNAs). The nonlinearity inherent in this regulatory scheme implies that exact analytical solutions for the corresponding stochastic models are intractable. Based on the mapping of the master equation to a quantum evolution equation, we use the variational method (introduced by Eyink) to analyze a well-studied stochastic model for regulation by sRNAs. Results from the variational ansatz are in excellent agreement with stochastic simulations for a wide range of parameters, including regions of parameter space where mean-field approaches break down. The results derived provide new insights into sRNA-based regulation and will serve as useful inputs for future studies focusing on the interplay of stochastic gene expression and regulation by sRNAs.

4:42PM T39.00012 Spatial gradients of Ran-GTP-importin-β complex around chromosomes in a cell of spheroidal shape[1] , GUILLERMO RAMIREZ-SANTIAGO, GERARDO SOSA, Instituto de Fisica, UNAM, Mexico — The concept of signaling gradients of a diffusible and slowly degraded chemical plays an important role in the description of cell signal transduction. It has been suggested that the generation of spatial gradients around chromosomes of the complex, Ran-GTP-importin-β, promotes microtubule nucleation and growth of the mitotic-spindle in Xenopus egg extracts. Here we solved the appropriate reaction-diffusion equation in spheroidal coordinates, and use measured values of the diffusion coefficients and activities to find out how the magnitude of the gradients depend upon the shape and geometry of the chromatin and cytoplasm. We found that the greater the eccentricity the smaller the magnitude of the stationary gradient. When the chromatin becomes spherical the magnitude of the gradient of the complex appears to be optimized.

[1]Work supported by DGAPA-UNAM contract IN118410.

4:54PM T39.00013 Kinetic simulations of tension-induced DNA strand-unpeeling transition , YUANYUAN QU, Department of Physics, National University of Singapore, HONGXIA FU, Mechanobiology Institute, Singapre, National University of Singapore, JIE YAN, Mechanobiology Institute, Singapore, Department of Physcis, National University of Singapore — Sequence- and salt- dependent kinetic simulation assuming strand-unpeeling from B-DNA using the Gellispie's stochastic kinetics simulation algorism was performed for DNA fragments of a few hundred base pairs. Similar to DNA unzipping experiments, sequence-dependent energy barriers resulted stepwise extension changes were observed during the transition. The simulations were compared with recent single-molecule studies of overstretching transition of the same DNAs occurring at around 65 pN. The results quantitatively reproduced the dynamics of overstretching transition of the same DNAs under conditions when overstretching led to strand separation, and were distinct from that when the transition led to a double-stranded overstretched DNA called "S-DNA" through the B-S transition pathway. We conclude that the strand separation transition pathway was a strand-unpeeling transition from the two free ends of DNA. Further, our results suggest that the B-S transition pathway does not involve base-pair separation.

5:06PM T39.00014 Determination of NMR chemical shifts for cholesterol crystals from first-principles , EMINE KUCUKBENLI, STEFANO DE GIRONCOLI, International School for Advanced Studies (SISSA) and CNR-IOM DEMOCRITOS Simulation Center, via Bonomea 265, 34136 Trieste, Italy — Solid State Nuclear Magnetic Resonance (NMR) is a powerful tool in crystallography when combined with theoretical predictions. So far, empirical calculations of spectra have been employed for an unambiguous identification. However, many complex systems are outside the scope of these methods. Our implementation of ultrasoft and projector augmented wave pseudopotentials within *ab initio* gauge including projector augmented plane wave (GIPAW) method in Quantum Espresso simulation package allows affordable calculations of NMR spectra for systems of thousands of electrons. We report here the first *ab initio* determination of NMR spectra for several crystal structures of cholesterol. Cholesterol crystals, the main component of human gallstones, are of interest to medical research as their structural properties can shed light on the pathologies of gallbladder. With our application we show that *ab initio* calculations can be employed to aid NMR crystallography.

Wednesday, March 23, 2011 2:30PM - 5:06PM –

Session T40 DBP: Physics of Proteins V: Protein-Protein Interaction, and Protein Aggregation

A122/123

2:30PM T40.00001 Early aggregation studies of diabetic amyloid in solution , SADANAND SINGH, JUAN DE PABLO, University of Wisconsin-Madison — Islet amyloid polypeptide (IAPP, also known as amylin) is responsible for pancreatic amyloid deposits in type II diabetes. The deposits, as well as intermediates in their assembly, are cytotoxic to pancreatic β-cells and contribute to the loss of β-cell mass associated with type II diabetes. To better understand the mechanism and cause of such aggregation, molecular simulations with explicit solvent models were used to compare monomer structure and early aggregation mechanism. Using free-energy maps generated through a variety of novel, enhanced sampling free-energy calculation techniques, we have found that, in water, the peptide adopts three major structures. One has a small α-helix at the N-terminus and a small β-hairpin at the other end. The second and the most stable one, is a complete β-hairpin, and the third is a random coil structure. Transition Path Sampling simulations along with reaction coordinate analysis reveal that the peptide follows a "zipping mechanism" in folding from α-helical to β-hairpin state. From studies of the dimerization of monomers in water, we have found that the early aggregation proceeds by conversion of all α-helical configurations to β-hairpins, and by two β-hairpins coming together to form a parallel β-sheet. Several aspects of the proposed mechanism have been verified by concerted 2D IR experimental measurements, thereby adding credence to the validity of our predictions.

2:42PM T40.00002 Applied Electric Fields and the Aggregation of Highly Charged Proteins , LOUIS NEMZER, BRET FLANDERS, CHRISTOPHER SORENSEN, Kansas State University — The abnormal aggregation of misfolded proteins is associated with the onset of Alzheimer's disease, along with other neurodegenerative disorders, and there is increasing evidence that prefibrillar clusters, rather than fully-formed amyloid plaques, are primarily responsible. Therefore, weakly invasive methods, such as dynamic light scattering, which can probe the size distribution and structure factor of early nuclei and proto-aggregate clusters, can serve an important role in understanding this process, and may lead to insights regarding future therapeutic interventions. Here we study a highly charged model protein, lysozyme, under the influence of applied AC and DC fields in an effort to evaluate general models of protein aggregation, including the coarse-grained "patchy protein" method of visualizing charge heterogeneity. This anisotropy in the interprotein interaction can lead to frustrated crystalline order, resulting in low density phases. Dynamic measurements of the size distribution and structure factor can reveal local ordering, hierarchical clustering, and fractal properties of the aggregates. Early results show that applied fields affect early cluster growth by modulating local protein and counterion concentrations, in addition to their influence on protein alignment.

2:54PM T40.00003 Ion Specificity in Protein Aggregation Predicted from Diffusivity Measurements in Stable Protein Solutions , JONATHAN RUBIN, ADRIANA SAN MIGUEL, ANDREAS BOMMARIUS, SVEN BEHRENS, Georgia Tech — The aggregation of therapeutic proteins in solution represents a major challenge in pharmaceutical development, as the mid- and long-term stability of these proteins is crucial for their efficacy and for compliance with FDA requirements. Monitoring slow aggregation experimentally is notoriously time-consuming, yet often unavoidable, since no theory with predictive power is currently available. In the present work, diffusion and aggregation kinetics of the globular model proteins lysozyme and BSA were studied in sodium-salt solutions of different composition and ionic strength using dynamic light scattering. We find a strong correlation between the concentration dependent protein diffusivity in stable solutions and the kinetics of protein aggregation in unstable solutions of similar composition but higher salt content. Our findings suggest a fast and convenient new way to assess a protein's specific tendency to aggregate in different types of electrolytes and buffer solutions.

3:06PM T40.00004 ABSTRACT WITHDRAWN –

3:18PM T40.00005 Controlling Protein Oligomerization with Surface Curvature on the Nanoscale , MARTY KURYLOWICZ, JOHN DUTCHER, University of Guelph — We investigate the effect of surface curvature on the conformation of beta-lactoglobulin (βLG) using Single Molecule Force Spectroscopy. βLG is a model interfacial protein which stabilizes oil droplets in milk and is known to undergo structural rearrangement when adsorbed onto a surface. We reliably control nanoscale surface curvature by creating close-packed monolayers of monodisperse polystyrene (PS) nanoparticles with diameters of 20, 40, 60, 80 and 140 nm, which are stable in aqueous buffer. By adsorbing βLG onto these hydrophobic surfaces and collecting force-extension curves in the fluid phase we can compare the conformation of βLG on 5 different surface curvatures with that on a flat PS film. We demonstrate a transition from oligomeric to monomeric βLG as the surface curvature is increased. Histograms of contour length from fits to peaks in the force-extension curves show a single maximum near 30 nm for βLG adsorbed onto nanoparticles with diameters less than 80 nm. For the larger nanoparticles, the histogram approaches that observed for βLG adsorbed onto a flat PS film, with maxima indicative of βLG dimers and trimers.

3:30PM T40.00006 Computational Analysis of β-Peptide Self-Assembly[1] , MICHAEL MCGOVERN, University of Wisconsin-Madison — $\beta-$peptides are a class of synthetic oligomers that are capable of folding in precise patterns. The wide variety of side chains that are available for insertion into β-peptide sequences along with the stability of these folded secondary structures allow precise control over the nanoscale presentation of various chemical functional groups in three dimensional space. Some β-peptides have been shown to spontaneously fold into complex supramolecular structures, and others have been shown to be effective antimicrobial agents that are believed to act by aggregating in certain types of cell membranes. However, more work is needed to understand what drives this assembly in order to design β-peptides that assemble in particular ways. Using molecular simulations, the process of β-peptide aggregation is examined in a variety of environments that allow for direct comparison to experiment. Using new simulation techniques, the structure of the aggregates formed by several β-peptides are predicted in both bulk solutions, and at interfaces. Free energy surfaces are generated using multiple geometric parameters to directly compare the favorability of different modes of aggregation. By analyzing these results, we gain an understanding of the factors that drive self-assembly and aggregation.

[1]Nanoscale Science and Engineering Center on Templated Synthesis and Assembly at the Nanoscale. We gratefully acknowledge funding from the National Science Foundation, DMR-0832760

3:42PM T40.00007 Electrospun Synthetic Polypeptide Nanofibrous Biomaterials , DHAN KHADKA, DONALD HAYNIE, University of South Florida — Water-insoluble nanofiber mats of synthetic polypeptides of defined composition have been prepared from fibers electrospun from aqueous solution in the absence of organic co-solvents. 20-50 kDa poly(L-glutamate, L-tyrosine) 4:1 (PLGY) but not 15-50 kDa or 50-100 kDa poly(L-glutamate) was spinnable at 20-55% (w/v) polymer in water. Applied voltage and needle-collector distance were crucial for spinnability. Attractive fibers were obtained at 50% polymer. Fiber diameter and mat morphology have been characterized by electron microscopy. Exposure of spun fiber mats to 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide hydrochloride (EDC), which reacts with carboxylate, decreased fiber solubility. Fluorescein-conjugated poly(L-lysine) (FITC-PLL) but not the fluorophore alone was able bind PLGY fiber mats electrostatically, judging by fluorescence microscopy. Key advances of this work are the avoidance of an animal source of peptides and of an inorganic co-solvent to achieve polypeptide spinnability. Polypeptide fiber mats are a promising type of nano-structured biomaterial for applications in biomedicine and biotechnology.

3:54PM T40.00008 Exploring the dewetting transition in the hydrophobic collapse of melittin , PATRICK VARILLY, University of California, Berkeley, AMISH J. PATEL, Rensselaer Polytechnic Institute, DAVID CHANDLER, University of California, Berkeley — We present our recent results on understanding the hydrophobic collapse of melittin dimers. Melittin dimers have large, complementary hydrophobic patches, and the dimer collapse mechanism involves a dewetting transition [Liu, Huang, Zhou and Berne, *Nature* **437**, 159–162 (2005)]. As a result, melittin has become a model system for studying dewetting transitions in proteins. We apply our recently- developed tools for probing density fluctuations in water [Patel, Varilly and Chandler, *JPCB* **114**, 1632–1637 (2010)] to understand this dewetting transition in terms of free energy surfaces, their bistability and their barrier heights. We show how the hydrophobic character of melittin's tetramerization surface results in an enhanced probability of density depletion next to that surface. When two dimers come together, the density depletion is further enhanced, so that even at large separations, there is a metastable dry phase in the region between the dimers. As the dimers come together, the dry phase is stabilized and eventually the wet phase is destabilized, leading to the collapse of the dimers. We explore how mutations that have been observed to suppress the dewetting transition affect the corresponding free energy surfaces and discuss our ongoing efforts to fully map out the reaction coordinate of melittin collapse.

4:06PM T40.00009 Effect of the ordered interfacial water layer in protein complex formation: a non-local electrostatic approach , ALEXANDER RUBINSTEIN, RENAT SABIRIANOV, University of Nembraska at Omaha — Using a non-local electrostatic approach that incorporates the short-range structure of the contacting media, we evaluated the electrostatic contribution to the energy of the complex formation of two model proteins. In this study, we have demonstrated that the existence of an low-dielectric interfacial water layer at the protein-solvent interface [1] reduces the charging energy of the proteins in the aqueous solvent, and consequently increases the electrostatic contribution to the protein binding (change in free energy upon the complex formation of two proteins). This is in contrast with the finding of the continuum electrostatic model, which suggests that electrostatic interactions are not strong enough to compensate for the unfavorable desolvation effects [2].

[1] Rubinstein and Sherman, Biophys. J. 87, 1544, 2004
[2] Rubinstein et al., Phys. Rev. E 82, 021915, 2010).

4:18PM T40.00010 Modeling virus capsids and their protein binding – the search for weak regions within the HIV capsid , OTTO F. SANKEY, DARYN E. BENSON, C. MICHAEL GILBERT, Arizona State University — Viruses remain a threat to the health of humans worldwide with 33 million infected with HIV. Viruses are ubiquitous, infecting animals, plants, and bacteria. Each virus infects in its own unique manner making the problem seem intractable. However, some general physical steps apply to many viruses and the application of basic physical modeling can potentially have great impact. The aim of this theoretical study is to investigate the stability of the HIV viral capsid (protein shell). The structural shell can be compromised by physical probes such as pulsed laser light [1,2]. But, what are the weakest regions of the capsid so that we can begin to understand vulnerabilities of these deadly materials? The atomic structure of HIV capsids is not precisely known and we begin by describing our work to model the capsid structure. We have constructed three representative viral capsids of different CA protein number – HIV-900, HIV-1260 and HIV-1740. The complexity of the assembly requires a course grained model to investigate protein interactions within the capsid which we will describe.
[1] K-T. Tsen, WS.-D. Tsen, O.F. Sankey, J.G. Kiang, Journal of Physics – Condensed Matter, 19 472201 (2007).
[2] E.C. Dykeman, D.Benson, K.-T. Tsen, and O.F. Sankey, Physical Review E 80, 041909 (2009).

4:30PM T40.00011 Low-Frequency Raman Spectroscopy of Trialanine.[1] , RACHEL M. STEPHENSON, ANGELA R. HIGHT WALKER, NIST — The effect of sample conditions on the structural conformation of trialanine has been investigated with visible Raman spectroscopy. Trialanine is used here as a simple protein-mimetic system in order to more easily isolate the backbone amide vibrational modes, low-frequency tortional modes and modes from hydrogen bonding. Crystalline trialanine is known to exist with both parallel (p-Ala$_3$) and antiparallel (ap-Ala$_3$) β-sheet crystal structures, depending on the solvent composition during crystallization. The *ap*-sheet form of trialanine co-crystallizes with water, which is easily removed under vacuum, offering a further opportunity to examine the effect of solvation on the vibrational spectra, especially when also compared with trialanine in solution. By collecting Raman spectra in different sample phases, and at different concentrations, pH and temperatures, the vibrational modes most sensitive to the secondary structure can be identified. The collected data will be compared to the literature, including other vibrational spectroscopic data and high-level simulations.

[1]This work was supported in part by the National Research Council Postdoctoral Research Associateship.

4:42PM T40.00012 Fast X-ray Photon Correlation Spectroscopy measurements from the diffusion of concentrated Alpha Crystallin suspensions[1] , VIDANAGE NUWAN KARUNARATNE, JANAE DEBARTOLO, JUSTIN BERRY, LAURENCE LURIO, Northern Illinois University, GEORGE THURSTON, Rochester Institute of Technology, SURESH NARAYANAN, ALEC SANDY, JOHN WEIZEORICK, Advanced Photon Source — Alpha Crystallin constitute up to half of the total protein found in the mammalian eye lens. It has chaperone like behavior and may play a key role in maintaining lens transparency by preventing condensation of other lens proteins. We report here Fast X-ray Photon Correlation Spectroscopy (XPCS) measurements of protein diffusion within concentrated suspensions of Alpha Crystallin. Bovine calf eye lens cortices were homogenized, centrifuged and ultra-filtered to obtain concentrated Alpha Crystallin suspensions. Diffusion of proteins within these suspensions was measured as a function of temperature. The overall observed diffusion rates imply that the proteins exist in a glassy or gel phase, even at concentrations where equivalent hard sphere system would still be liquid. We interpret these results within the context of strongly interacting proteins, with protein-protein interactions possibly mediated by subunit exchange among Alpha Crystallin oligormers.

[1]NSF Grant DMR-0706369, ANL/NIU Joint Fellowship

4:54PM T40.00013 Ultrasound and Hypersound Speeds in Lysozyme Solutions , ALFONS SCHULTE, Department of Physics and College of Optics, University of Central Florida, Orlando, CHRISTIAN PRUNER, EMMERICH WILHELM, AUGUSTINUS ASENBAUM, Department of Materials Science and Physics, University of Salzburg, A-5020 Salzburg — Ultrasound velocimetry and Brillouin spectroscopy provide information on the compressibility of proteins and the surrounding hydration layer. Employing both techniques we investigate the sound speeds at GHz (hypersound) and MHz (ultrasound) frequencies in lysozyme solutions (250 mg / ml, pH 7) and pure water over the temperature range from 275 K to 335 K. Compared to water the Brillouin peaks in the lysozyme solutions are shifted by about 400 MHz towards higher frequencies. This shift reflects the change in sound speed and is attributed to the influence of the compressibility of the protein and bound water in the hydration shell. In addition, we measure a dispersion of the sound velocity in the lysozyme solution. The higher sound speed at GHz frequencies, as measured by Brillouin scattering, may indicate additional relaxation processes as compared to pure bulk water, where no sound dispersion between ultrasound speed and hypersound speed is observed.

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T41 DCP: Focus Session: The Role of Water in Energy Production and Utilization I

2:30PM T41.00001 Deciphering the morphology of ice films on metal surfaces[1] , KONRAD THÜRMER, Sandia National Laboratories, CA — Although extensive research has been aimed at the structure of ice films [1], questions regarding basic processes that govern film evolution remain. Recently we discovered how ice films as many as 30 molecular layers thick can be imaged with STM [2]. The observed morphology yields new insights about water-solid interactions and how they affect the structure of ice films. This talk gives an overview of this progress for crystalline ice films on Pt(111) [2-5]. STM reveals a first molecular water layer very different from bulk ice: besides the usual hexagons it also contains pentagons and heptagons [3]. Slightly thicker films ($\sim$1nm, at T>120K) are comprised of $\sim$3nm-high crystallites, surrounded by the one-molecule-thick wetting layer. These crystals dewet by nucleating layers on their top facets [4]. Measurements of the nucleation rate as a function of crystal height provide estimates of the energy of the ice-Pt interface. For T>115K surface diffusion is fast enough that surface smoothing and 2D-island ripening is observable [5]. By quantifying the T-dependent ripening of island arrays we determined the activation energy for surface self-diffusion. The shape of these 2D islands varies strongly with film thickness. We attribute this to a transition from polarized ice at the substrate towards proton disorder at larger film thicknesses. Despite fast surface diffusion ice multilayers are often far from equilibrium. For example, ice grows between $\sim$120 and $\sim$160 K in its cubic variant rather than in its equilibrium hexagonal form. We found this to be a consequence of the mismatch in the atomic Pt-step height and the ice-bilayer separation and propose a mechanism of cubic-ice formation via growth spirals around screw dislocations [2].

[1] A. Hodgson and S. Haq, Surf. Sci. Rep. 64, 381 (2009).
[2] K. Thürmer and N. C. Bartelt, Phys. Rev. B 77, 195425 (2008).
[3] S. Nie, P. J. Feibelman, N. C. Bartelt and K. Thürmer, Phys. Rev. Lett. 105, 026102 (2010).
[4] K. Thürmer and N. C. Bartelt, Phys. Rev. Lett. 100, 186101 (2008).
[5] S. Nie, N. C. Bartelt, and K. Thürmer, Phys. Rev. Lett. 102, 136101 (2009).

[1]Joint work with N.C. Bartelt and S. Nie, Sandia Natl. Labs, CA. This work was supported by the Office of Basic Energy Sciences, Division of Materials Sciences, U.S. DOE under Contracts No. DEAC04-94AL85000.

3:06PM T41.00002 *A Priori* Method for First Principles Study of Aqueous Electrochemistry: Application to Biofuels and Catalysis , KENDRA LETCHWORTH WEAVER, RAVISHANKAR SUNDARARAMAN, TOMAS ARIAS, Cornell University — We present a novel description of water which will allow the first *a priori* studies of catalysis of biofuels in aqueous electrochemical environments. Our method offers a computationally efficient alternative to the thermal sampling required by molecular dynamics yet provides a more realistic description of bulk water than including explicit frozen water or traditional continuum solvation models. Into Joint Density Functional Theory (JDFT), which joins an electron density-functional for the solute with classical density-functional theories for liquid water[1] into a single variational principle for the free energy of the combined system, we introduce the innovation of an *a priori* form of the coupling functional between the quantum-mechanical system and liquid water based on a local density approximation to the Hohenberg-Kohn density-only functional. Without any fits to solvation data whatsoever, this new method predicts solvation energies of small organic molecules well compared to state-of-the art empirical quantum-chemical cavity approaches. The site interaction potentials produced closely resemble the widely used TIP3P site potentials for water without requiring any empirical parameters.

[1]R. Sundararaman et al, unpublished, to be presented at the APS March Meeting (2011)

3:18PM T41.00003 *A priori* classical density functionals of water: toward first principles exploration of aqueous based energy systems , RAVISHANKAR SUNDARARAMAN, KENDRA LETCHWORTH WEAVER, TOMAS ARIAS, Cornell University — The microscopic structure of inhomogeneous water plays a critical role in the properties of a wide variety of important energy systems including fuel cells and photoelectrochemical cells. Joint density functional theory has proven to be an efficient tool for the quantum-mechanical modeling of systems such as Pt electrodes in the presence of water, but requires theories for water which go beyond semi-empirical continuum solvation models, and accurate models for the coupling between water and electronic systems [1]. Toward this end, we present a new density-functional description of liquid water capable of predicting interatomic correlation functions, the linear and nonlinear dielectric response, and solvation energies without empirical fit parameters. The functional itself is built upon the site-potential representation of the ideal gas, a hard sphere reference fluid for the repulsive correlations, and an equation of state that reproduces the bulk properties of water over the entire extent of its liquid phase. Hydrogen bonding, the local tetrahedral structure and orientational correlations are captured *a priori* by a density-functional reformulation of the Kirkwood model for the dielectric constant.

[1]K. L. Weaver et al, to be presented at APS March Meeting 2011

3:30PM T41.00004 Quasicrystal and ice phases tiled with pentagons in confined water , VALERIA MOLINERO, Department of Chemistry, University of Utah — Bulk water is known to form a wealth of ice polymorphs and two distinct amorphous phases. Less is known of the structures that confined and interfacial water can adopt, and whether there is a correspondence between the structures and phase diagrams of water in bulk and in confinement. In this talk I will present a molecular simulations study of the phase behavior of a water bilayer confined between two non-hydrogen bonding walls and demonstrate that a water bilayer also presents rich polymorphism, including an ice crystal fully tiled by pentagons and a quasicrystal, the first ever reported for water. The water quasicrystal and the ice polymorph tiled with pentagons are not templated by the confining surfaces. This indicates that these novel phases are intrinsically favored in bilayer water and suggests that they may be formed, without confinement, on surfaces.

[1] J.C. Johnston, N. Kastelowitz and V. Molinero, "Liquid to quasicrystal transition in bilayer water," J. Chem. Phys. 133, 154516 (2010)
[2] N. Kastelowitz, J. C. Johnston and V. Molinero, "The anomalously high melting temperature of bilayer ice," J. Chem. Phys. 132, 124511 (2010).

4:06PM T41.00005 The role of interfacial water in "nano" , ALENKA LUZAR, Virginia Commonwealth University, JIHANG WANG, CHRIS DAUB, DUSAN BRATKO, CHEMISTY DEPARTMENT, VCU TEAM — To understand the role of interfacial water on nanostructred surfaces is important for materials science and biology. The talk will describe some of our recent progress in predicting and understanding the effects of nanopatterning on topologically or chemically heterogeneous surfaces on wetting via *in silico* experiments.

4:18PM T41.00006 Ordering of confined water between metallic surfaces[1] , ADRIEN POISSIER, MARIA V. FERNANDEZ-SERRA, Stony Brook University — It has been pointed out (PCCP 2010, Poissier et al.) that the hydrogen bonding type interaction occuring at water/metal interface makes the two type of interfacial water orderings (hydrophobic or hydrophilic overlayers) very close in energy. The most stable, hydrophobic, overlayer has very small net dipole moment perpendicular to the surface, while the least stable (in vacuum) hydrophilic interface has a large ($\approx 1.8D$) net dipole moment. First principles molecular dynamics simulations of liquid water confined between two Pd surfaces have been performed and structural and electronic water properties have been studied in detail. We show that water confinement in this situation results in a spontaneous symmetry breaking of the system, inducing an electric field across the liquid water slab. We discuss the origin of this spontaneous polarization and show its dependence with the confinement distance along the direction perpendicular to the planes of the surfaces.

[1]This work is supported by DOE award number DE-SC0003871

4:30PM T41.00007 Exploring hydration at the nanoscale[1] , PETER ROSSKY, University of Texas at Austin — It is widely appreciated that water molecules contribute a critical element to the forces governing chemical processes in an aqueous environment, and the purported differences in water structure induced by the presence of confining surfaces are correspondingly likely to play a role in interfacial chemistry. The development of a detailed understanding of the organization of fluid water at the interface with real materials is therefore of great interest. In this presentation, results obtained from fully atomistic computer simulations of water in the presence of confining interfaces will be discussed, with the goal of elucidating the molecular level influence of surface character on water structure and energetics. Further, we emphasize the extension of studies to temperatures and pressures well outside the conventional realm of the ambient solvent thermodynamic state. The interface examples to be considered in this presentation emphasize systematic studies designed to elucidate guiding principles. These include extended and nanoscale hydrophobic and hydrophilic crystalline surfaces and interfaces with systematically patterned hydrophobicity.

[1]This work is the result of support for Collaborative Research by the US National Science Foundation.

5:06PM T41.00008 ABSTRACT WITHDRAWN –

5:18PM T41.00009 Energy transport during sessile-water-droplet evaporation[1] , HADI GHASEMI, Unversity of Toronto, CHARLES WARD, University of Toronto — Energy transport mechanisms for a steadily evaporating water droplet maintained on Cu or Au(111) surfaces are compared. In the absence of buoyancy-driven convection, thermal conduction and thermocapillary convection are the active modes of energy transport. The dominant mode varies along the liquid-vapor interface. Although thermal conduction is the dominant mode in regions far from the contact line, thermocapillary convection is by far the larger mode of energy transport near the three-phase contact line. The latter region is where most of the droplet evaporation occurs. Evaporation experiments on both Cu and Au(111) suggest that the thermocapillary convection provides more than 92% of the total energy required for the evaporation.

[1]We gratefully acknowledge the support Natural Sciences and Engineering Council of Canada and the Canadian Space Agency

Wednesday, March 23, 2011 2:30PM - 4:18PM –

Session T42 DCP DBP: Focus Session: The Physics of Evolution I A302/303

2:30PM T42.00001 Insights into protein evolution landscapes from folding models , EUGENE KOONIN, National Center for Biotechnology Information, National Library of Medicine, National Institutes of Health — Off-lattice models of protein folding were employed to investigate the origins of the evolutionary rate distributions and fitness landscapes. For each robust folder, the network of sequences that share its native structure is identified. The fitness of a sequence is a simple function of the number of misfolded molecules produced to reach a characteristic protein abundance. Fixation probabilities of mutants are computed under a simple population dynamics model, and the fold-averaged evolution rate is computed a using a Markov chain on the fold network. The distribution of the logarithm of the evolution rates exhibits a peak with a long tail on the low rate side and resembles the universal empirical distribution of the evolutionary rates more closely than either distribution resembles the log-normal distribution. We next addressed the question of the extent of determinism in protein evolution. Limited empirical studies suggest that the fitness landscapes of protein evolution are significantly smoother, or more additive, than random landscapes. However, widespread sign epistasis seems to restrict evolution to a small fraction of available trajectories, thus making the evolutionary process substantially deterministic. Access to complete fitness landscapes within the model framework enables exhaustive analysis of evolutionary trajectories. The model landscapes were compared to a continuum of artificial landscapes of varying smoothness. In maximally smooth, fully additive landscapes, evolution cannot be predicted because all paths are accessible. However, a small amount of noise can make most paths inaccessible while preserving the overall structure of the landscape. Although the model landscapes are almost additive, most paths are non-monotonic with respect to fitness, so evolutionary trajectories can be approximately predicted. Thus, protein folding physics seems to dictate the universal distribution of the evolutionary rates of protein-coding genes and the quasi-deterministic character of evolution.

3:06PM T42.00002 A mechanism for the evolution of allosteric control in proteins , KIMBERLY REYNOLDS, RAMA RANGANATHAN, Green Center for Systems Biology, and Department of Pharmacology, University of Texas Southwestern Medical Center — Co-evolution analysis indicates a general architecture for natural proteins in which sparse networks of physically contiguous amino acids underlie basic aspects of structure and function. These networks, termed sectors, are spatially organized such that active sites are linked to many surface sites distributed throughout the protein structure. Here, we propose that sectors represent an evolutionarily conserved "wiring" mechanism that effectively functionalizes a large but non-random fraction of the protein surface - that is, perturbation at sector-connected surface positions should preferentially yield coupling to the active site. To test this premise, we conducted a comprehensive "domain insertion scan," and show that sector-connected surface sites are statistically significant locations for the emergence of allosteric control in vivo. This finding suggests practical guidelines for the engineering of new allosteric systems, and permits description of a plausible model for the evolution of intermolecular communication and regulation.

3:18PM T42.00003 Biophysical Aspects of Spindle Evolution , REZA FARHADIFAR, Harvard University, CHARLIE BAER, University of Florida, DANIEL NEEDLEMAN, Harvard University — The continual propagation of genetic material from one generation to the next is one of the most basic characteristics of all organisms. In eukaryotes, DNA is segregated into the two daughter cells by a highly dynamic, self-organizing structure called the mitotic spindle. Mitotic spindles can show remarkable variability between tissues and organisms, but there is currently little understanding of the biophysical and evolutionary basis of this diversity. We are studying how spontaneous mutations modify cell division during nematode development. By comparing the mutational variation - the raw material of evolution - with the variation present in nature, we are investigating how the mitotic spindle is shaped over the course of evolution. This combination of quantitative genetics and cellular biophysics gives insight into how the structure and dynamics of the spindle is formed through selection, drift, and biophysical constraints.

3:30PM T42.00004 The relationship between relative solvent accessibility and evolutionary rate in protein evolution , CLAUS WILKE, The University of Texas at Austin — Recent work with the yeast Saccharomyces cerevisiae shows a linear relationship between the evolutionary rate of sites and the relative solvent accessibility (RSA) of the corresponding residues in the folded protein. Here, we aim to develop a mathematical model that can reproduce this linear relationship. We first demonstrate that two models that both seem reasonable choices (a simple model in which selection strength correlates with RSA and a more complex model based on RSA-dependent amino-acid distributions) fail to reproduce the observed relationship. We then develop a model based on observed site-specific amino-acid distributions and show that this model behaves appropriately. We conclude that evolutionary rates are directly linked to the distribution of amino acids at individual sites. Because of this link, any future insight into the biophysical mechanisms that determine amino-acid distributions will improve our understanding of evolutionary rates.

4:06PM T42.00005 Quantum Darwinian Evolution Implies Tumor Origination , W. GRANT COOPER, International Physics — Quantum uncertainty limits operating on metastable amino DNA protons drive the arrangement, keto-amino ? enol-imine, which contributes to time-dependent stochastic mutations. Product enol-imine protons participate in coupled quantum oscillations at frequencies of about 1013 s-1 until "measured by" an evolutionarily selected quantum reader, the transcriptase. This introduces entanglement states between coherent protons and transcriptase components, which ultimately yield an ensemble of decohered, non-reequilibrated enol and imine isomers that participate in "molecular clock" base substitutions at G'-C' and *G-*C sites. This introduces a quantum Darwinian evolution model which (a) simulates incidence of cancer data and (b) implies insight into quantum origins of evolutionary extinction. Data identify an inherited "genetic space," s, which is initially mutation-free and satisfies the inequality, 1 = s = 0.97. When accumulated stochastic mutations cause s-values to approach their evolutionarily allowed threshold limit, s 0.97 + e, age-related degenerative disease is manifested. This implies a gain in evolutionary advantage which protects the gene pool against acquiring unsafe levels of mutation. Data requiring coherent states imply that classical duplex DNA contains an embedded microphysical subset of electron lone-pairs and hydrogen bonded protons that govern time-dependent genetic specificity in terms of quantum probability laws.

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T43 DBP: Physics of Bacteria A306/307

2:30PM T43.00001 Guided Motion of Individual and Collective Swimmers in Funnel Arrays , CYNTHIA OLSON REICHHARDT, Los Alamos National Laboratory, THUC MAI, Syracuse University, CHARLES REICHHARDT, Los Alamos National Laboratory — We generalize a model of swimming bacteria in asymmetric arrays of obstacles [1] to include different rules of motion, including various rules for collective behvaiors. For individual noninteracting swimmers, we observe guided motion and rectification by the asymmetric barriers when the particles align with the walls they contact, but we find no rectification if the particles are reflected by the walls or bounce off the walls. For collectively interacting swimmers, it is possible for the particles to form large swimming clumps that can move against the normal rectification direction of the asymmetric barrier array. In general, the rectification by the barriers is lost when the length scale of the swarms of collectively moving particles is significantly larger than the length scale of the funnel shaped barriers. A particle swarm can become trapped inside a funnel; however, individual strings of particles that follow each other can escape from the trap and move against the funnel direction.

[1] M.B. Wan, C.J. Olson Reichhardt, Z. Nussinov, and C. Reichhardt, Phys. Rev. Lett. 101, 018102 (2008).

2:42PM T43.00002 Surface motility of Myxococcus Xanthus , MAXSIM GIBIANSKY, University of California, Los Angeles, Bioengineering Department, WILLIAM HU, University of California, Los Angeles, School of Dentistry, FAN JIN, University of California, Los Angeles, Bioengineering Department, KUN ZHAO, WENYUAN SHI, University of California, Los Angeles, School of Dentistry, GERARD WONG, University of California, Los Angeles, Bioengineering Department — We examine the surface motility of Myxococcus Xanthus, a bacterium species found in soil that exhibits a broad range of self-organizing behavior, including predatory "swarms" and survival-enhancing "fruiting bodies." To quantify the effects of exopolysaccharides (EPS) on surface adhesion and motility, we use modified versions of particle tracking algorithms from colloid physics to analyze bacterial trajectories, and compare the wild type (WT) strain to EPS knockout and EPS overproducer strains. We find that EPS deficiency leads to an increase in the number of "standing" bacteria oriented normal to the surface, attached by one end with minimal motility. EPS overproduction, by contrast, suppresses this phenotype. A detailed investigation of the influence of EPS on Myxococcus social motility will be presented.

2:54PM T43.00003 Dynamics of microorganisms with autochemotactic interactions , JOHANNES TAKTIKOS, Technical University Berlin, Germany, VASILY ZABURDAEV, Harvard University, HOLGER STARK, Technical University Berlin, Germany — Our work aims at the description of the early stage of bacterial biofilm formation. In light of this, we model bacteria as self-propelled particles that move on a surface with constant speed and whose directions of motion diffuse on the unit circle. Individual cells communicate by autochemotaxis, so they follow the gradient of a chemical which is produced by the microorganisms themselves. We investigate how the autochemotactic coupling influences the mean squared displacement of a single particle and show that the long-time dynamics is diffusive. We present theoretical predictions for the diffusion coefficient and compare them to numerical results. To incorporate the size of bacteria, we model them as disks that experience a harmonic repulsion force when they start to overlap. Our repulsion mechanism for particles in contact assumes a linear relationship between force and velocity. For such a soft model microorganism, we present numerical results on two-particle collisions and study the cluster formation in a multi-particle system.

3:06PM T43.00004 Shear flow influences the twitching motility of *Pseudomonas Aeruginosa*[1] , YI SHEN, Princeton University, SIGOLENE LECUYER, Harvard University, ALBERT SIRYAPORN, ZEMER GITAI, HOWARD STONE, Princeton University — Twitching motility is one of the mechanisms by which bacteria can spread on surfaces and is important in the process of biofilm formation. Flow is often involved in biofilm formation, for instance when bacteria contaminate medical devices or water systems. We have studied the twitching mobility of *Pseudomonas aeruginosa* in straight microfluidic channels under laminar shear flow at low Reynolds number. We tracked all the bacteria adhering and moving on the immersed glass surface. We observed that upon applying a flow, a significant fraction of bacteria started to twitch, and that many twitched upstream, opposite to the flow direction. By measuring the displacement and residence time of the bacteria staying on the surface, we found that the flow not only tuned the direction of twitching by orienting bacteria, but also that the shear rate significantly influenced the fraction of bacteria moving upstream, with an optimal shear rate about $500s^{-1}$.

[1]Princeton University MAE Complex fluids group

3:18PM T43.00005 Biofilm growth: a lattice Monte Carlo model , YUGUO TAO, GARY SLATER, University of Ottawa — Biofilms are complex colonies of bacteria that grow in contact with a wall, often in the presence of a flow. In the current work, biofilm growth is investigated using a new two-dimensional lattice Monte Carlo algorithm based on the Bond-Fluctuation Algorithm (BFA). One of the distinguishing characteristics of biofilms, the synthesis and physical properties of the extracellular polymeric substance (EPS) in which the cells are embedded, is explicitly taken into account. Cells are modelled as autonomous closed loops with well-defined mechanical and thermodynamic properties, while the EPS is modelled as flexible polymeric chains. This BFA model allows us to add biologically relevant features such as: the uptake of nutrients; cell growth, division and death; the production of EPS; cell maintenance and hibernation; the generation of waste and the impact of toxic molecules; cell mutation and evolution; cell motility. By tuning the structural, interactional and morphologic parameters of the model, the cell shapes as well as the growth and maturation of various types of biofilm colonies can be controlled.

3:30PM T43.00006 Transitions in biofilm formation , VERNITA GORDON, TRAVIS THATCHER, BENJAMIN COOLEY, Center for Nonlinear Dynamics and Department of Physics, University of Texas at Austin — Biofilms are multicellular, dynamic communities formed by interacting unicellular organisms bound to a surface. Forming a biofilm is a developmental process, characterized by sequential changes in gene expression and behavior as bacteria and yeast progress from discrete, free-swimming cells though stages that arrive at a mature biofilm. We are developing automated metrics to identify key transitions in early biofilm formation as cells attach to a surface, populate that surface, and adhere to each other to form early microcolonies. Our metrics use high-throughput tracking and analysis of microscopy movies to localize these transitions in space and time. Each of these transitions is associated with a loss of entropy in the bacterial system and, therefore, with biological activity that drives this loss of entropy. Better understanding of these transitions will allow automated determination of the strength and turn-on of attractive cell-surface and cell-cell interactions as biofilm development progresses.

3:42PM T43.00007 Changes in the Mechanical Properties of Pseudomonas aeruginosa Bacterial Cells Induced by Antimicrobial Peptides , SHUN LU, JOHN DUTCHER, University of Guelph — In our research group, we have developed an atomic force microscopy nano-creep technique [1] to study the mechanical properties of individual Pseudomonas aeruginosa bacterial cells in a liquid environment. In the present study, we have used this technique to measure changes to the mechanical properties of the cells produced by exposing the cells to well-studied antimicrobial peptides: polymyxin B (PMB) and its derivative polymyxin B nonapeptide (PMBN). We find that the creep response of cells under a fixed applied load is very different after exposure of the cells to PMB and PMBN, which is possibly due to the disruption of its outer membrane. To describe the viscoelastic properties of the cells exposed to PMB and PMBN, we found that it was necessary to use a four element spring and dashpot model, instead of the three element standard linear solid model that describes the viscoelastic properties of cells in Millipore water [1]. We also found that PMB and PMBN have qualitatively different effects on the stiffness of the cell membrane. These measurements provide a first step towards understanding the different mechanisms of action of PMB and PMBN on bacterial cells.

[1] V. Vadillo-Rodriguez, T. J. Beveridge, and J. R. Dutcher, J. Bacteriol., 190, 4225-4232, 2008.

3:54PM T43.00008 Nanofabrication and Detection of Molecular Shuttles powered by Kinesin Motor Proteins , DANIEL OLIVEIRA, WPI - Advanced Institute for Materials Research, Tohoku University, Sendai, Japan, KIM DOMYOUNG, Dept. of Biomolecular Engineering, Tohoku University, Sendai, Japan, MITSUO UMETSU, WPI - Advanced Institute for Materials Research and Dept. of Biomolecular Engineering, Tohoku University, Sendai, Japan, TADAFUMI ADSCHIRI, WPI - Advanced Institute for Materials Research, Tohoku University, Sendai, Japan, WINFRIED TEIZER, WPI - Advanced Institute for Materials Research, Tohoku University, Sendai, Japan and Dept of Physics, Texas A&M University, College Station, TX, USA — The intracellular cargo delivery performed by kinesin motor proteins can be biomimetically employed to engineer tailor-made artificial nanotransport systems. Kinesin (expressed on an *Escherichia coli* system) and microtubules (obtained from the polymerization of tubulin proteins) were prepared and characterized. We report recent results and explore the aim of the construction of Nanoelectromechanical Systems and their potential applications, e.g. as drug delivery systems. This work was supported by the WPI Program.

4:06PM T43.00009 Electrodynamics of Nanosystems , SAMINA MASOOD, Univ. of Houston Clear Lake — We use Electrodynamics to study the nanosystems. Quantum nature of electrodynamics has been used to describe the physics of nanosystems including carbon nanotubes as well as the cellular growth. We use bacterial cell as an example and test a part of our theory on the bacterial growth experimentally. Preliminary results of these experiments are also mentioned here.

4:18PM T43.00010 Long range electronic transport in microbial nanowires bridging an electrode and scanned probe[1] , JOSHUA VEAZEY, SANELA LAMPA-PASTIRK, KATHY WALSH, JIEBING SUN, PENGPENG ZHANG, GEMMA REGUERA, STUART TESSMER, Michigan State University — The filament-like appendages known as pili, expressed by the bacterium *Geobacter sulfurreducens*, are believed to act as electrically conductive nanowires [1]. Previously, we used scanning tunneling microscopy to study the local density of states at different positions along the wire. However, the long range electron transfer believed to occur in this protein has not been directly observed. Here we discuss a system for verifying long range transport using a scanning probe technique. Transport at distances of more than a few nanometers would require a novel biological electron transfer process.

[1] G. Reguera, K.D. McCarthy, T. Mehta, J.S. Nicoll, M.T. Tuominen, and D.R. Lovley, Nature 435, 1098 (2005)

[1]The authors gratefully acknowledge support from the National Science Foundation (MCB-1021948) and the Michigan State University Foundation (Strategic Partnership Grant)

4:30PM T43.00011 Heterogeneous diversity of spacers within CRISPR , MICHAEL DEEM, JIANKUI HE, Rice University — Clustered regularly interspaced short palindromic repeats (CRISPR) in bacterial and archaeal DNA have recently been shown to be a new type of anti-viral immune system in these organisms. We here study the diversity of spacers in CRISPR under selective pressure. We propose a population dynamics model that explains the biological observation that the leader-proximal end of CRISPR is more diversified and the leader-distal end of CRISPR is more conserved. This result is shown to be in agreement with recent experiments. Our results show that the CRISPR spacer structure is influenced by and provides a record of the viral challenges that bacteria face. 1) J. He and M. W. Deem, Phys. Rev. Lett. 105 (2010) 128102

4:42PM T43.00012 Filament depolymerization can pull a chromosome during bacterial mitosis , EDWARD BANIGAN, University of Pennsylvania, MICHAEL GELBART, Harvard University, ZEMER GITAI, Princeton University, ANDREA LIU, NED WINGREEN, Princeton University — Chromosome segregation is fundamental to all cells, but the force-generating mechanisms underlying chromosome translocation in bacteria remain mysterious. *Caulobacter crescentus* utilizes a depolymerization-driven process in which a ParA protein structure elongates from the new cell pole and binds to a ParB-decorated chromosome, and then retracts via disassembly, thus pulling the chromosome across the cell. This poses the question of how a depolymerizing structure can robustly pull the chromosome that is disassembling it. We perform Brownian dynamics simulations with a simple and physically consistent model of the ParABS system. The simulations suggest that the mechanism of translocation is "self-diffusiophoretic": by disassembling ParA, ParB generates a ParA concentration gradient so that the concentration of ParA is higher in front of the chromosome than behind it. Since the chromosome is attracted to ParA via ParB, it moves up the ParA gradient and across the cell. We find that translocation is controlled by the product of an effective relaxation time for the chromosome and the rate of ParA disassembly. Our results provide a physical explanation of the mechanism of depolymerization-driven translocation and suggest physical explanations for recent experimental observations.

4:54PM T43.00013 Polymerization and oscillation stuttering in a filamentous model of the subcellular Min oscillation , ANDREW RUTENBERG, Dalhousie University, SUPRATIM SENGUPTA, Jawaharlal Nehru University, ANIRBAN SAIN, Indian Institute of Technology - Bombay, JULIEN DERR, Harvard University — We present a computational model of the *E. coli* Min oscillation that involves polymerization of MinD filaments followed by depolymerization stimulated by filament-end zones of MinE. Our stochastic model is fully three-dimensional, and tracks the diffusion and interactions of every MinD and MinE molecule. We recover self-organized Min oscillations. We investigate the experimental phenomenon of oscillation stuttering, which we relate to the disruption of MinE tip-binding at the filament scale.

5:06PM T43.00014 Effect of Antimicrobial Agents on MinD Protein Oscillations in E. coli Bacterial Cells , COREY KELLY, MEGAN MURPHY, MAXIMILIANO GIULIANI, JOHN DUTCHER, University of Guelph — The pole-to-pole oscillation of the MinD proteins in E. coli determines the location of the division septum, and is integral to healthy cell division. It has been shown previously that the MinD oscillation period is approximately 40 s for healthy cells [1] but is strongly dependant on environmental factors such as temperature, which may place stress on the cell [2,3]. We use a strain of E. coli in which the MinD proteins are tagged with green fluorescent protein (GFP), allowing fluorescence visualization of the MinD oscillation. We use high resolution total internal reflection fluorescence (TIRF) microscopy to observe the effect of exposure to antimicrobial agents on the MinD oscillation period and, more generally, to analyze the time variation of the spatial distribution of the MinD proteins within the cells. These measurements provide insight into the mechanism of antimicrobial action.

[1] Raskin, D.M.; de Boer, P. (1999) Proc Natl. Acad. Sci. 96: 4971-4976.
[2] Colville, K.; Tompkins, N.; Rutenberg, A. D.; Jericho, M. H. (2010) Langmuir 2010:26.
[3] Downing, B.; Rutenberg, A.; Touhami, A.; Jericho, M. (2009) PLoS ONE 4: e7285.

5:18PM T43.00015 Pattern Transitions in Bacterial Oscillating System under Nanofluidic Confinement[1] , JIE-PAN SHEN, CHIA-FU CHOU, Academia Sinica — Successful binary fission in E. coli relies on remarkable oscillatory behavior of the MinCDE protein system to determine the exact division site. The most favorable models to explain this fascinating spatiotemporal regulation on dynamic MinDE pattern formation in cells are based on reaction-diffusion scenario. Although not fully understood, geometric factors caused by bacterial morphology play a crucial role in MinDE dynamics. In the present study, bacteria were cultured, confined and reshaped in various micro/nanofluidic devices, to mimic either curvature changes of cell peripherals. Fluorescence imaging was utilized to detail the mode transitions in multiple MinDE patterns. The understanding of the physics in multiple pattern formations is further complemented via in silico modeling. The study synergizes the join merits of in vivo, in vitro and in silico approaches, to grasp the insight of stochastic dynamics inherited from the noisy mesoscopic biophysics.

[1]We acknowledge support from the Foresight Project, Academia Sinica.

Wednesday, March 23, 2011 2:30PM - 5:42PM –
Session T44 DBP: Evolutionary and Ecological Systems A309

2:30PM T44.00001 Spatial Disorder in Cyclic Three-Species Predator-Prey Models[1] , QIAN HE, Department of Physics, Virginia Tech, MAURO MOBILIA, Department of Applied Mathematics, University of Leeds, U.K., UWE C. TÄUBER, Department of Physics, Virginia Tech — By numerically studying the oscillatory dynamics of several variants of cyclic three-species predator-prey models with conserved total particle density, we investigate the effects of spatial variability of the reaction rates and site occupancy restrictions on the system's co-evolutionary dynamics. It is shown that both quenched disorder in the reaction rates and lattice site occupancy restrictions have only minor effects on the dynamics of cyclic competing systems. This result is starkly different from the finding in two-species predator-prey model where spatial disorder can greatly enhance species fitness. We also numerically compute the dependence of the mean extinction time, for small systems, on system size.
Reference: Phys. Rev. E **82**, 051909 (2010).

[1]Research in part supported through Virginia Tech's Institute for Critical Technology and Applied Science (ICTAS).

2:42PM T44.00002 A Two-Species Social Dominance Model , SWAPNIL JAWKAR, Department of Physics, Virginia Tech, GEOFFREY ADAMS, Department of Neurobiology, Duke University, UWE C. TÄUBER, Department of Physics, Virginia Tech — We study the general properties of a stochastic two-species social-domination model defined on a d-dimensional lattice. The introduction of spatial degrees of freedom and allowance of stochastic fluctuations surprisingly does not invalidate the deterministic mean-field picture. In the active state, where the dominant and submissive species coexist, no patch formation is observed, with correlation lengths restricted to a few lattice sites. Oscillations seen in the submissive population density are strongly damped and restricted to a small section of the parameter space. Observations are explained to be a result of the two-particle reactions being restricted to the same social group.

2:54PM T44.00003 Cooperation and cheating in microbes , JEFF GORE, Massachusetts Institute of Technology — Understanding the cooperative and competitive dynamics within and between species is a central challenge in evolutionary biology. Microbial model systems represent a unique opportunity to experimentally test fundamental theories regarding the evolution of cooperative behaviors. In this talk I will describe our experiments probing cooperation in microbes. In particular, I will compare the cooperative growth of yeast in sucrose and the cooperative inactivation of antibiotics by bacteria. In both cases we find that cheater strains—which don't contribute to the public welfare—are able to take advantage of the cooperator strains. However, this ability of cheaters to out-compete cooperators occurs only when cheaters are present at low frequency, thus leading to steady-state coexistence. These microbial experiments provide fresh insight into the evolutionary origin of cooperation.

3:06PM T44.00004 Cooperative Bacterial Growth Dynamics Predict the Evolution of Antibiotic Resistance , TATIANA ARTEMOVA, YLAINE GERARDIN, SOPHIA HSIN-JUNG LI, JEFF GORE — Since the discovery of penicillin, antibiotics have been our primary weapon against bacterial infections. Unfortunately, bacteria can gain resistance to penicillin by acquiring the gene that encodes beta-lactamase, which inactivates the antibiotic. However, mutations in this gene are necessary to degrade the modern antibiotic cefotaxime. Understanding the conditions that favor the spread of these mutations is a challenge. Here we show that bacterial growth in beta-lactam antibiotics is cooperative and that the nature of this growth determines the conditions in which resistance evolves. Quantitative analysis of the growth dynamics predicts a peak in selection at very low antibiotic concentrations; competition between strains confirms this prediction. We also find significant selection at higher antibiotic concentrations, close to the minimum inhibitory concentrations of the strains. Our results argue that an understanding of the evolutionary forces that lead to antibiotic resistance requires a quantitative understanding of the evolution of cooperation in bacteria.

3:18PM T44.00005 Slowly switching between environments facilitates reverse evolution in small populations , LONGZHI TAN, JEFF GORE, Department of Physics, Massachusetts Institute of Technology — The rate at which a physical process occurs usually changes the behavior of a system. In thermodynamics, the reversibility of a process generally increases when it occurs at an infinitely slow rate. In biological evolution, adaptations to a new environment may be reversed by evolution in the ancestral environment. Such fluctuating environments are ubiquitous in nature, although how the rate of switching affects reverse evolution is unknown. Here we use a computational approach to quantify evolutionary reversibility as a function of the rate of switching between two environments. For small population sizes, which travel on landscapes as random walkers, we find that both genotypic and phenotypic reverse evolution increase at slow switching rates. However, slow switching of environments decreases evolutionary reversibility for a greedy walker, corresponding to large populations (extensive clonal interference). We conclude that the impact of the switching rate for biological evolution is more complicated than other common physical processes, and that a quantitative approach may yield significant insight into reverse evolution.

3:30PM T44.00006 Bacterial cheating limits the evolution of antibiotic resistance , HUI XIAO CHAO, MANOSHI DATTA, EUGENE YURTSEV, JEFF GORE, Department of Physics, Massachusetts Institute of Technology — The widespread use of antibiotics has led to the evolution of resistance in bacteria. Bacteria can gain resistance to the antibiotic ampicillin by acquiring a plasmid carrying the gene beta-lactamase, which inactivates the antibiotic. This inactivation may represent a cooperative behavior, as the entire bacterial population benefits from removing the antibiotic. The cooperative nature of this growth suggests that a cheater strain–which does not contribute to breaking down the antibiotic–may be able to take advantage of cells cooperatively inactivating the antibiotic. Here we experimentally find that a "sensitive" bacterial strain lacking the plasmid conferring resistance can invade a population of resistant bacteria, even in antibiotic concentrations that should kill the sensitive strain. We observe stable coexistence between the two strains and find that a simple model successfully explains the behavior as a function of antibiotic concentration and cell density. We anticipate that our results will provide insight into the evolutionary origin of phenotypic diversity and cooperative behaviors found in nature.

3:42PM T44.00007 A slowly evolving host moves first in symbiotic interactions , JAMES DAMORE, JEFF GORE, MIT — Symbiotic relationships, both parasitic and mutualistic, are ubiquitous in nature. Understanding how these symbioses evolve, from bacteria and their phages to humans and our gut microflora, is crucial in understanding how life operates. Often, symbioses consist of a slowly evolving host species with each host only interacting with its own sub-population of symbionts. The Red Queen hypothesis describes coevolutionary relationships as constant arms races with each species rushing to evolve an advantage over the other, suggesting that faster evolution is favored. Here, we use a simple game theoretic model of host- symbiont coevolution that includes population structure to show that if the symbionts evolve much faster than the host, the equilibrium distribution is the same as it would be if it were a sequential game where the host moves first against its symbionts. For the slowly evolving host, this will prove to be advantageous in mutualisms and a handicap in antagonisms. The model allows for symbiont adaptation to its host, a result that is robust to changes in the parameters and generalizes to continuous and multiplayer games. Our findings provide insight into a wide range of symbiotic phenomena and help to unify the field of coevolutionary theory.

3:54PM T44.00008 How do the effects of mutations add up? , ANDREA VELENICH, MIT, MINGJIE DAI, Harvard University, JEFF GORE, MIT — Genetic mutations affect the fitness of any organism and provide the variability necessary for natural selection to occur. Given the fitness of a wild type organism and the fitness of mutants A and B which differ from the wild type by a single mutation, predicting the fitness of the double mutant AB is a fundamental problem with broad implications in many fields, from evolutionary theory to medicine. Analysis of millions of double gene knockouts in yeast reveals that, on average, the fitness of AB is the product of the fitness of A and the fitness of B. However, most pairs of mutations deviate from this mean behavior in a way that challenges existing theoretical models. We propose a natural generalization of the geometric Fisher's model which accommodates the experimentally observed features and allows us to characterize the fitness landscape of yeast.

4:06PM T44.00009 Theory of cooperation in a micro-organismal snow-drift game[1] , ZHENYU WANG, NIGEL GOLDENFELD, Department of Physics, Center for the Physics of Living Cells and Institute for Genomic Biology, University of Illinois at Urbana-Champaign — We present a mean field model for the phase diagram of a community of micro-organisms, interacting through their metabolism so that they are, in effect, engaging in a cooperative social game. We show that as a function of the concentration of the nutrients glucose and histidine, the community undergoes a phase transition separating a state in which one strain is dominant to a state which is characterized by coexisting populations. Our results are in good agreement with recent experimental results, correctly predicting quantitative trends and the phase diagram.

[1]We thank Jeff Gore for sharing with us his experimental data. This work was supported in part by the National Science Foundation through grant number NSF-EF-0526747.

4:18PM T44.00010 Spatial population genetics in a petri dish , KIRILL KOROLEV, MIT, JOAO XAVIER, MELANIE MULLER, NILAY KARAHAN, OSKAR HALLATSCHEK, KEVIN FOSTER, ANDREW MURRAY, DAVID NELSON — The evolution of natural populations involves more than mutations followed by natural selection: Stochasticity and spatial migrations are also important. The effects of fluctuations and spatial structure become especially pronounced when organisms expand to new territories. The fluctuations are enhanced because the number of organisms at the front of the expansion is typically small, and the spatial structure is more pronounced due to dimensional reduction from two to one spatial dimension (because colonization occurs along the quasi-one-dimensional periphery of the population). The interplay of fluctuations and space leads to spatial segregation of different genotypes, which significantly alters the evolutionary dynamics of the population. We investigate this process by combining theory, simulations, and experiments on microbial expansions on the surface of a Petri dish. In particular, I will discuss how one can use simple microbiology experiments to measure important parameters of microbial populations such as the strength of fluctuations, migration rate, and relative fitness.

4:30PM T44.00011 The Goldilocks Principle and Rapid Evolution of Antibiotic Resistance in Bacteria[1] , QIUCEN ZHANG, ROBERT AUSTIN, Department of Physics, Princeton University — Goldilocks sampled the three bear's wares for the "just right" combination of taste, fit and comfort. Like Goldilocks's need for the just right parameters, evolution proceeds most rapidly when there is the just right combination of a large number of mutants and rapid fixation of the mutants. We show here using a two-dimensional micro-ecology that it is possible to fix resistance to the powerful antibiotic ciprofloxacin (Cipro) in wild-type E. coli in 10 hours through a combination of extremely high population gradients, which generate rapid fixation, convolved with the just right level of antibiotic which generates a large number of mutants and the motility of the organism. Although evolution occurs in well-stirred chemostats without such Goldilocks conditions, natural environments are rarely well stirred in nature.For complex environments such as the Galapagos Islands, spatial population gradients and movement of mutants along these population gradients can be as important as genomic heterogeneity in setting the speed of evolution. The design of our micro-ecology is unique in that it provides two overlapping gradients, one an emergent and self generated bacterial population gradient due to food restriction and the other a mutagenic antibiotic gradient. Further, it exploits the motility of the bacteria moving across these gradients to drive the rate of resistance to Cipro to extraordinarily high rates.

[1]The research described was supported by Award Number U54CA143803 from the National Cancer Institute.

4:42PM T44.00012 Evolution on a Lattice under Strong Mutation[1] , JAKUB OTWINOWSKI, STEFAN BOETTCHER, Emory University — The most common approach to study biological evolution in a population considers mutations to arise one at a time, and spread to the whole population. However, recent experimental work has shown that under conditions of strong mutation and strong selection, multiple mutations may arise simultaneously. Such overlapping mutations compete with each other and make the results difficult to analyse. Theorists are working on understanding the relationships between different parameters such as population size, mutation rate, and selection coefficients, in the way they affect observables such as the speed of evolution, and the probability of fixation. We have shown with simulations that under additional spatial constraints the dynamics are very different compared to well-mixed populations. A surface in fitness space evolves, akin to surface growth phenomena, with non-trivial power-law exponents. The result is that the speed of evolution is restricted and the probability of fixation is reduced.

[1]With support from the NSF through grant DMR-0812204

4:54PM T44.00013 Modeling Political Populations with Bacteria , CHRIS CLEVELAND, Princeton University, DAVID LIAO, U. California San Francisco — Results from lattice-based simulations of micro-environments with heterogeneous nutrient resources reveal that competition between wild-type and GASP rpoS819 strains of E. Coli offers mutual benefit, particularly in nutrient deprived regions. Our computational model spatially maps bacteria populations and energy sources onto a set of 3D lattices that collectively resemble the topology of North America. By implementing Wright-Fishcer re- production into a probabilistic leap-frog scheme, we observe populations of wild-type and GASP rpoS819 cells compete for resources and, yet, aid each other's long term survival. The connection to how spatial political ideologies map in a similar way is discussed.

5:06PM T44.00014 Mutualistic Interactions and Community Structure in Biological Metacommunities[1] , PER ARNE RIKVOLD, Florida State Univ., ELISE FILOTAS, Univ. du Quebec a Montreal, MARTIN GRANT, McGill Univ., LAEL PARROTT, Univ. de Montreal — The role of space in determining species coexistence and community structure is well established. However, previous studies mainly focus on simple competition and predation systems, and the role of mutualistic interspecies interactions is not well understood. Here we use a spatially explicit metacommunity model, in which new species enter by a mutation process, to study the effect of fitness-dependent dispersal on the structure of communities with interactions comprising mutualism, competition, and exploitation [1]. We find that the diversity and interaction network undergo a nonequilibrium phase transition with increasing dispersal rate. Low dispersion rate favors spontaneous emergence of many dissimilar, strongly mutualistic and species-poor local communities. Due to the local dissimilarities, the *global* diversity is high. High dispersion rate promotes local biodiversity and supports similar, species-rich local communities with a wide range of interactions. The strong similarity between neighboring local communities leads to reduced global diversity.

[1]. E. Filotas, M. Grant, L. Parrott, P.A. Rikvold, J. Theor. Biol. **266**, 419 (2010); Ecol. Modell. **221**, 885 (2010).

[1]Supported by NSERC (Canada), FQRNT (Québec), NSF (U.S.A.)

5:18PM T44.00015 Universal Description of Interactive Growth[1] , CARLOS CONDAT, LUCAS BARBERIS, FaMAF - Universidad Nacional de Cordoba and IFEG - CONICET — Although the existence of organism-organism interactions during ontogenesis is well documented, ontogenetic growth models usually focus exclusively on the organism-environment interaction. We develop a new formalism to describe the interactive growth of two or more organisms in a given environment. Using a vector formulation of the Phenomenological Universalities concept, we are able to characterize the joint growth of two or more interacting organisms and assess the direct mutual influences between them, as well as the indirect influences that operate through environment modifications. The resulting equations describe synergetic, antagonistic, and cooperative growth, and can be applied to biological and ecological problems. As an example, we examine the growth dynamics in a mixed-species plantation.

[1]This work was supported by ANPCyT and CONICET (Argentina)

5:30PM T44.00016 Large fluctuations and fixation in evolutionary games , MICHAEL ASSAF, MAURO MOBILIA — One of the most striking effects of fluctuations in evolutionary game theory is the possibility for mutants to fixate (take over) an entire population. In this work we use a semi-classical theory to study fixation in evolutionary games under non-vanishing selection, and investigate the relation between selection intensity and demographic (random) fluctuations. This approach allows the accurate treatment of rare large fluctuations and yields the probability and mean time of fixation beyond the weak-selection limit, often considered in previous works. The power of the theory is demonstrated on prototypical models of cooperation dilemmas with multiple absorbing states, and we find excellent agreement between the theoretical predictions and numerical simulations. Furthermore, we show that our treatment is superior to the Fokker-Planck approximation for finite selection intensity. M. Assaf and M. Mobilia, J. Stat. Mech. P09009 (2010). M. Mobilia and M. Assaf, Euro. Phys. Lett. 91, 10002 (2010).

Wednesday, March 23, 2011 2:30PM - 5:30PM –

Session T45 GMAG DAMOP: Focus Session: Magnetic and Spin Ordering in Atomic and Optical Systems A310

2:30PM T45.00001 Macroscopic quantum phenomenon in a spin-orbit coupled Bose-Einstein condensate , SHIZHONG ZHANG, TIN-LUN HO, Department of Physics, the Ohio-State University — It is well-known in electron physics in semiconductors that the spin-orbit coupling gives rise to many exciting new physics, for example, the topological insulator that is now being actively studied. With the advent of artificial gauge field that can be generated using Raman lasers for neutral bosonic atoms, we can now study the corresponding effects in the boson system. In this talk, I shall discuss the structure of the spinor condensate with spin-orbit coupling. In particular, we show that the system develops stripe structure in each spin component, as a result of the fact that the ground state consists of two dressed states carrying different momentum. We also work out the phase diagram of the system, which compares well with the recent experiment.

2:42PM T45.00002 Spin-orbit coupled spinor Bose-Einstein condensate , HUI ZHAI, CHUNJI WANG, CHAO GAO, CHAO-MING JIAN, Institute for Advanced Study, Tsinghua University — An effective spin-orbit coupling can be generated in cold atom system by engineering atom-light interactions. We study spin-1/2 and spin-1 Bose-Einstein condensates with Rashba spin-orbit coupling, and find that the condensate wave function will develop non-trivial structures. From numerical simulation we have identified two different phases. In one phase the ground state is a single plane wave, and often we find the system splits into domains and an array of vortices plays the role as domain wall. In this phase, time-reversal symmetry is broken. In the other phase the condensate wave function is a standing wave and it forms spin stripe. The transition between them is driven by interactions between bosons. We also provide an analytical understanding of these results and determines the transition point between the two phases.

2:54PM T45.00003 Phase transitions of spin-orbit coupled Bose-Einstein Condensate in an external trap potential , XIANGFA ZHOU, The Department of Physics, University of Science and Technology of China, IAN MONDRAGON-SHEM, The Department of Physics, Cornell University, CONGJUN WU, The Department of Physics, Univeristy of California, San Diego — Recently, the experimental realization of artificial magnetic fields using laser beams in a Rb87 Bose-Einstein condensate provides a valuable opportunity to investigate the rich physics of atomic gases in the presence of external Abelian and Non-Abelian gauge fields. We investigate the ground state properties of two-component BECs with Rashba spin-orbit coupling in the presence of external trapping potential. In the presence of density-density interaction between particles, the competitions among interaction, spin-orbit coupling and trap potential results in phase transitions of the ground states from a spiral spin-density wave state to a skyrmion type spin texture with rotational symmetry. We numerically solve the Gross-Pitaevskii equation and plot the phase diagram. The corresponding physics with asymmetrical Rashba coupling is also discussed.

3:06PM T45.00004 Artificial Staggered Magnetic Field for Ultracold Atoms in Optical Lattices[1] , CRISTIANE MORAIS SMITH, ITP, Utrecht University — Uniform magnetic fields are ubiquitous in nature, but this is not the case for staggered magnetic fields. In this talk, I will discuss an experimental set-up for cold atoms recently proposed by us [1], which allows for the realization of a "staggered gauge field" in a 2D square optical lattice. If the lattice is loaded with bosons, it may be described by an effective Bose-Hubbard Hamiltonian, with complex and anisotropic hopping coefficients. A very rich phase diagram emerges: besides the usual Mott-insulator and zero-momentum condensate, a new phase with a finite momentum condensate becomes the ground-state at strong gauge fields [2]. By using the technique of Feshbach resonance, the dynamics of a coherent superposition of a vortex-carrying atomic condensate and a conventional zero-momentum molecular condensate can also be studied within the same scheme [3]. On the other hand, if the lattice is loaded with fermions, a highly tunable, graphene-like band structure can be realized, without requiring the honeycomb lattice symmetry [2]. When the system is loaded with a mixture of bosons and two-species fermions, several features of the high-Tc phase diagram can be reproduced. A dome-shaped unconventional superconducting region arises, surrounded by a non-Fermi liquid and a Fermi liquid at low and high doping, respectively [4].

[1] A. Hemmerich and C. Morais Smith, Phys. Rev. Lett. 99, 113002 (2007).
[2] Lih-King Lim, A. Hemmerich, and C. Morais Smith, Phys. Rev. Lett. 100, 130402 (2008), Phys. Rev. A 81, 023404 (2010).
[3] Lih-King Lim, T. Troppenz, and C. Morais Smith, arXiv:1009.1471.
[4] Lih-King Lim, A. Lazarides, A. Hemmerich, and C. Morais Smith, EPL 88, 36001 (2009) and Phys. Rev. A 82, 013616 (2010)

[1]We acknowledge financial support from the Netherlands Organization for Scientific Research (NWO).

3:42PM T45.00005 Itinerant ferromagnetism in a Fermi gas with contact interaction: Magnetic properties in a dilute Hubbard model[1] , CHIA-CHEN CHANG, SHIWEI ZHANG, Department of Physics, College of William and Mary, DAVID M. CEPERLEY, Department of Physics, University of Illinois Urbana-Champaign — Motivated by recent experiments addressing the issue of itinerant ferromagnetism in a dilute ultra-cold Fermi gas with contact interaction, we examine ground state properties of the repulsive Hubbard model on a cubic lattice [1] by means of a very accurate auxiliary-field quantum Monte Carlo method [2]. We focus on low-density systems with varying on-site interaction U/t, in the range relevant to the experiments. Twist-averaged boundary conditions are used to eliminate open-shell effects and large lattice sizes are studied to reduce finite-size effects. The sign problem is controlled by a generalized constrained path approximation [2]. We find no ferromagnetic phase transition in this model. The ground-state correlations are consistent with those of a paramagnetic Fermi liquid.

[1] Chia-Chen Chang, Shiwei Zhang, and David M. Ceperley, arXiv:1009.1409
[2] Chia-Chen Chang and Shiwei Zhang, Phys. Rev. B 78, 165101 (2008).

[1]C.C. and S.Z. are supported by ARO, D.M.C. is supported by OLE program.

3:54PM T45.00006 Magnetic instabilities in spin imbalanced ultracold Fermi gases[1] , INTI SODEMANN VILLADIEGO, DMYTRO PESIN, ALLAN MACDONALD, University of Texas at Austin — We study the possibility of preparing magnetic states of spin imbalanced ultracold Fermi gases near a broad Feshbach resonance by analyzing the unstable collective magnetization modes developed when the system is placed on the BEC side. Within the approximation of momentum independent interatomic scattering, transverse magnetization instabilities appear at lower critical interaction strengths than those corresponding to the longitudinal instabilities, suggesting that the former ones are primarily responsible for driving the system into a textured state with inhomogeneous magnetization direction. The critical interaction for the onset of transverse instabilities increases with polarization. However the system already has ferromagnetic character below these interaction strengths because of a change in sign of the spin stiffness which occurs close to the Stoner transition of the corresponding unpolarized gas. We also discuss the behavior expected beyond the momentum independent scattering approximation across the resonance for, both, the superfluid and ferromagnetic instabilities present in the system and the implication of these results for experiments.

[1]Work supported by Welch Foundation grant F1473

4:06PM T45.00007 Energy decay constant in sodium spinor condensates , JIE JIANG, YINGMEI LIU, Department of Physics, Oklahoma State University, Stillwater, OK 74078, EDUARDO GOMEZ, D.A. QUINONES , Instituto de Fisica, Universidad Autonoma de San Luis Potosi, San Luis Potosi 78290, P.D. LETT, Joint Quantum Institute, University of Maryland and National Institute of Standards and Technology, Gaithersburg, MD 20899 — Spinor condensates of F=1 sodium atoms display rich spin dynamics due to the antiferromagnetic nature of the interactions in this system. Damped spin oscillations are observed in sodium spinor condensates, which eventually lead to the mean-field ground state. In recent experiments we have been able to track and observe the time evolution of atom number fluctuations, which enables the first quantitative measure of energy dissipation in the spinor condensate. We also develop a method to extract the energy in spinor dynamics from experimental data, and characterize the energy dissipation with a decay constant. This decay constant appears to follow a power-law dependence with the energy of spinor condensates. This power-law dependence has been experimentally checked for a wide range of the spinor energy, by varying the applied magnetic field strength, the magnetization and the density of the spinor condensate.

4:18PM T45.00008 Tunneling properties of collective spin wave excitations in the supercurrent state of a spin-1 spinor BEC , SHOHEI WATABE, Keio University, and CREST(JST), YUSUKE KATO, The University of Tokyo, YOJI OHASHI, Keio University, and CREST(JST) — We theoretically investigate tunneling properties of spin wave excitations through a barrier in the supercurrent state of a spin-1 BEC. In the ferromagnetic phase, we show that the transverse spin wave always exhibits perfect transmission, when the spin- wave momentum p coincides with the momentum of supercurrent q. This is quite different from the case of the Bogoliubov mode, where the so-called anomalous tunneling phenomenon always occurs when $p = 0$, unless the system is in the critical current state ($q = q_c$). In the polar phase, spin wave modes always exhibit perfect transmission when $p = 0$, as in the case of the Bogoliubov mode. However, this anomalous tunneling behaviors of spin wave modes are shown to still hold even in the critical current state, in contrast to the breakdown of the perfect transmission of the Bogoliubov mode at q_c. Only when the Gross-Pitaevskii equation for the spin-1 BEC is integrable, perfect transmission of the spin wave is absent at q_c. Using a simple $delta$-functional barrier, we also discuss similarity between the condensate wave function in the supercurrent state and the wave functions of spin wave excitations when perfect transmission occurs.

4:30PM T45.00009 Quantum rotor theory of spinor condensates in tight traps , RYAN BARNETT, HOI-YIN HUI, CHIEN-HUNG LIN, JAY D. SAU, S. DAS SARMA, Joint Quantum Institute and Condensed Matter Theory Center — In this talk, we theoretically construct exact mappings of many-particle bosonic systems onto quantum rotor models. In particular, we analyze the rotor representation of spinor Bose-Einstein condensates. There is an exact mapping of a spin-one condensate of fixed particle number with quadratic Zeeman interaction onto a quantum rotor model. We use the rotor mapping to describe the different dynamical regimes recently observed in ^{23}Na condensates. We also suggest a way to experimentally observe quantum mechanical effects (collapse and revival) in spinor condensates. We classify three distinct physical limits of the rotor model: the Rabi, Josephson, and Fock regimes. The last regime corresponds to a fragmented condensate and is thus not captured by the Bogoliubov theory. The semiclassical limit of the rotor problem is discussed and connections with the quantum wave functions are made through use of the Husimi distribution function. Finally, we describe how to extend the analysis to higher-spin systems and derive a rotor model for the spin-two condensate. This work was supported by the NSF JQI Physics Frontier Center.

4:42PM T45.00010 Spin susceptibility of spin-1/2 fermions with dipole interactions[1] , BENJAMIN M. FREGOSO, University of Chicago, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign — The general form of the spin susceptibility is found for spin- 1/2 fermions with dipole interactions. In the paramagnetic phase and partially magnetized phase (ferro-nematic) the spin susceptibility is explicitly computed in the Random Phase Approximation. Important modifications to the static susceptibility are discussed which are relevant for future experiments. Unconventional collective modes in the paramagnetic and ferro-nematic phases are also discussed.

[1]NSF DMR 0758462

4:54PM T45.00011 Quasi-two-dimensional fermionic dipolar gases in the Hartree-Fock approximation: band renormalization, inter-subband excitons and the liquid-solid phase diagram , MEHRTASH BABADI, EUGENE DEMLER, Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA — We study quasi-two-dimensional systems of fermionic dipolar gases in the Hartree-Fock approximation for various trap frequencies and dipolar interactions at finite temperatures and evaluate the energy dispersions of the renormalized subbands. We also study the inter-subband excitation spectrum of the system in the Time-Dependent Hartree-Fock approximation and predict the energy absorption rates in lattice modulation spectroscopy experiments. It is shown that the spectrum consists of inter-subband particle-hole excitation continuums as well as excitonic modes, and that their observation is highly likely in current experiments. Finally, we calculate the liquid-solid phase diagram of the system and find novel features such as multiple crystalline orders and re-entrant crystallization.

5:06PM T45.00012 Probing non-Abelian statistics of Majorana fermions in ultracold atomic superfluid , SHI-LIANG ZHU, School of Physics, South China Normal University, L.B. SHAO, Z.D. WANG, Department of Physics, The University of Hong Kong, LU-MING DUAN, Department of Physics, Michigan University — We propose an experiment to directly probe the non-Abelian statistics of Majorana fermions by braiding them in an s-wave superfluid of ultracold atoms. We show different orders of braiding operations give orthogonal output states that can be distinguished through Raman spectroscopy. Realization of Majorana bound states in an s-wave superfluid requires strong spin-orbital coupling and a controllable Zeeman field in the perpendicular direction. We present a simple laser configuration to generate the artificial spin-orbital coupling and the required Zeeman field in the dark state subspace.

5:18PM T45.00013 Magnetism and Cooper pairing in one-dimensional large spin fermions with repulsive interactions , HSIANG-HSUAN HUNG, The department of Physics, Univeristy of California, San Diego, YUPENG WANG, Institute of Physics, Chinese Academy of Sciences, Beijing, China, CONGJUN WU, The department of Physics, Univeristy of California, San Diego — The recent experimental realization of ultracold large-spin fermionic systems provides a new opportunity to investigate exotic magnetism and Cooper pairing physics. By means of exact diagonalizaton and the density matrix renormalization group, we systematically study the magnetic properties of the Mott-insulating state of the simplest large-spin systems with hyperfine spin $F = 3/2$ in one-dimension and at quarter filling. Such a system is characterized by an exact $SO(5)$ symmetry. The ground state shows various profiles at various $\theta = \tan^{-1} J_0/J_2$, where J_0/J_2 is the ratio of exchange strengths of the singlet ($S_T = 0$) and quintet ($S_T = 2$) channels. As $\theta > 45^\circ$ the ground state is a gapped state with dimerization patterns whereas as $\theta \leq 45^\circ$ it is a gapless Luttinger liquid state. Furthermore, we found that in the Luttinger liquid phase the static correlation functions show power-law decays with a four-site periodicity, which is similar to an SU(4) chain. We also study the spin-$3/2$ model with doping. In the regime of $\theta > 45^\circ$ and at moderate doping, the singlet pairing correlations indicate power-law decays whereas the quintet pairing correlations have exponential decays. On the other hand, in the regime of $\theta \leq 45^\circ$ the quintet pairing correlations are more robust than the singlet pairing correlations.

Wednesday, March 23, 2011 5:45PM - 6:45PM –

Session U1 APS: Nobel Prize Session: Graphene: Materials in the Flatland Ballroom C1

5:45PM U1.00001 Graphene: Materials in the Flatland , KONSTANTIN NOVOSELOV, University of Manchester, Manchester —

6:15PM U1.00002 Discussion –

Wednesday, March 23, 2011 7:30PM - 9:00PM –

Session U55 APS: "Trends" in the APS Publication Physics Hyatt Regency Dallas Reunion A-D

7:30PM U55.00001 Topological order, topological insulators, and the search for the Majorana fermion , JOEL E. MOORE, University of California — In condensed matter physics complex order often emerges from simple interactions. Recent experiments show that topological order, previously seen only in 2D electron systems in high magnetic field, can exist in zero field and even in bulk 3D materials called topological insulators, in which spin-orbit coupling induces the topological order. Topologically ordered phases can support new kinds of emergent particles, such as the Majorana fermion. Current experiments in condensed matter, in both fractional quantum Hall systems and strong spin-orbit materials, are probing the physics of Majorana fermions, which may eventually enable a topological approach to quantum computing.

8:00PM U55.00002 Quantum information in solid-state systems , DANIEL LOSS, University of Basel — I review the theoretical concepts for spin qubits and scalable quantum computers in nanostructures and highlight the experimental progress in this fast moving field [1]. I describe the standard model of quantum computing and the basic criteria for its potential realization in solid state systems such as GaAs heterostructures, carbon nanotubes, InAs or SiGe nanowires, etc. Other alternative formulations such as measurement-based and adiabatic quantum computing are mentioned briefly. I then focus on qubits formed by individual electron spins in single and double GaAs quantum dots. Introducing the problem of decoherence arising from spin orbit and hyperfine interactions I discuss ways to overcome it, such as state narrowing and nuclear magnetism induced by strong correlations [2].

[1] R. Zak, B. Röhlisberger, S. Chesi, and D. Loss, Rivista del Nuovo Cimento 033, 345 (2010).
[2] B. Braunecker, P. Simon, and D. Loss, Phys. Rev. B 80, 165119 (2009).

8:30PM U55.00003 Graphene: Deep physics from the all-surface material , MICHAEL S. FUHRER, University of Maryland, College Park — The 2010 Nobel Prize in Physics was awarded to Andre Geim and Kostya Novoselov for their experiments on graphene, a single-atom plane of graphite. I will discuss why graphene has generated such excitement in condensed matter physics. Graphene is different: graphene's electrons mimic massless Dirac Fermions. But graphene is also amazingly tunable: Bandgaps can be generated by nanostructuring. Interactions can be tuned by the surrounding dielectric. Strain generates effective "pseudomagnetic" fields up to 300 Tesla. The work function can be tuned over a large range. Such tunability promises that graphene will remain interesting as a laboratory for condensed matter physics.

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V1 DCMP: Iron Pnictides versus Iron Chalcogenides: Magnetism and Pairing Fluctuation Ballroom A1

8:00AM V1.00001 Symmetry and structure of the pairing gap in Fe-based superconductors[1] , ANDREY CHUBUKOV, University of Wisconsin — I review recent works on the symmetry and structure of superconducting gap in Fe-pnictides and related compounds. I show that the gap very likely has s-wave symmetry, and is either nodal or has nodes along the two electron Fermi surfaces, depending on the parameters. I argue that the nodal gap is most likely outcome in systems with less pronounced tendency towards antiferromagnetism. I compare 4-and 5-pocket models for Fe-pnictides and argue that the parameter range where the gap is nodal is much wider in 4-pocket models. I review recent experiments aimed to understand whether the gap has nodes, e.g., experiments on the variation in the field-induced component of the specific heat C(H) with the direction of the applied field in $FeSe_{0.4}Te_{0.6}$. I show that, for extended s-wave gap, C(H) has $\cos 4\phi$ component, where ϕ is the angle between H and the direction between hole and electron Fermi surfaces, but only if the gap has no nodes. When the gap has accidental nodes, the $\cos 4\phi$ variation does not hold. I also plan to discuss the interplay between direct Coulomb interaction at large momentum transfer and spin-fluctuation contribution to the pairing, and the interplay between antiferromagnetism and superconductivity. In particular, I show that in 4-pocket (but not in 5-pocket) model superconductivity becomes the leading instability in some range of parameters even at perfect nesting, i.e, antiferromagnetism is not a pre-condition for superconductivity. This agrees with functional RG studies.

[1]In collaboration with Ilya Eremin and Saurabh Maiti

8:36AM V1.00002 Anisotropic Superconducting Gap Revealed by Angle Resolved Specific Heat, Point Contact Tunneling and Scanning Tunneling Microscope in Iron Pnictide Superconductors[1] , HAI-HU WEN, Institute of Physics, CAS — Angle resolved specific heat was measured in $FeSe_{0.55}Te_{0.45}$ single crystals. A four-fold oscillation of C/T, with the minimum locating at the Fe-Fe bond direction, was observed when the sample was rotated at 9 T, which can be understood as due to the gap modulation on the electron pocket within the scheme of S$\pm$ pairing. Accordingly, by measuring the point contact Andreev reflection spectrum on the $BaFe_{2-x}Ni_xAs_2$ single crystals in wide doping regimes, we found a crossover from nodeless to nodal feature of the superconducting gap. In K-doped $BaFe_2As_2$ single crystals, we performed the low temperature STM measurements and observed a well ordered vortex lattice in local region. In addition, the statistics on over 3000 dI/dV spectra illustrate clear evidence of two gaps with magnitude of 7.6 meV and 3.3 meV, respectively. Detailed fitting to the tunneling spectrum shows an isotropic superconducting gap. Work collaborated with B. Zeng, C. Ren, L. Shan, Y. L. Wang, B. Shen, G. Mu, H. Q. Luo, T. Xiang, H. Yang, I. I. Mazin and P. C. Dai. References:

[1] B. Zeng, et al., arXiv:1007.3597, Nature Communications, 2010, in press.
[2] C. Ren, et al., to be published.
[3] L. Shan, et al., arXiv:1005.4038.

[1]This work was supported by the Natural Science Foundation of China, the Ministry of Science and Technology of China (2011CB605900, No. 2006CB921802), and Chinese Academy of Sciences. IIM was supported by the Office of the Naval Research.

9:12AM V1.00003 From magnetism to superconductivity in $FeTe_{1-x}Se_x$[1] , DIMITRI ARGYRIOU[2], European Spallation Source ESS AB P.O Box 117, SE-221 00 Lund, Sweden — The iron chalcogenide $FeTe_{1-x}Se_x$ is structurally the simplest of the Fe-based superconductors and exhibits a Fermi surface similar to iron pnictides. Despite this similarity, the parent compound $Fe_{1+y}Te$ orders antiferromagnetically with an in-plane magnetic wave vector (π,0) with an ordered moment of $\sim 2\mu_B$/Fe, suggestive of a localized rather than itinerant character of the magnetic order. This contrasts the pnictide parent compounds where the magnetic order has an in-plane magnetic wave vector (π,π) that likely arises from Fermi Surface nesting. Regardless both the pnictide and chalcogenide Fe superconductors exhibit a superconducting spin resonance around (π,π) as probed by neutron scattering. A central question in this burgeoning field is therefore how (π,π) superconductivity emerges from a (π,0) magnetic instability ? Using neutron scattering we show that incommensurate magnetic excitations around (π,π) are found even in the undoped parent compound $Fe_{1+y}Te$. With increasing x, the (π,0)-type magnetic long-range order becomes unstable and correlates with a weak charge carrier localization, while the mode at (π,π) becomes dominant for x>0.29. Our results suggest a common magnetic origin for superconductivity in iron chalcogenide and pnictide superconductors. This work was carried out in close collaboration with the groups of W.Bao (Renmin), Arno Hies (ILL), Zhiqiang Mao (Tulane), C. Brohom (John Hopkins) and I. Eremin (MPI-Dresden/Bochum).

[1]Authors thanks Helmholtz Zentrum Berlin and the DFG (under SPP 1458) for support.
[2]On leave from the Helmholtz-Zentrum Berlin.

9:48AM V1.00004 The nature of electronic nematic states in iron-pnictides , JIANGPING HU, Purdue University — We show that the electronic nematic states in iron-pnictides is driven by frustrated spin fluctuations. A three dimensional effective spin model is constructed to explain the nematicity. This model explains the relation between the structural and magnetic transitions, and the spin excitations measured in recent neutron scattering experiments. Moreover, the model naturally predicts the separation between the two transitions are controlled by the c-axis magnetic exchange coupling , and the existence of an non-collinear magnetic state before spin-glass state upon replacing irons by nonmagnetic impurities. The experimental evidence supporting the predictions and the relation to orbital ordering and superconductivity will also be addressed.

10:24AM V1.00005 Differences in the degree of correlations between Pnictides and Chalcogenides: LaFeAsO vs. FeSe[1] , MARKUS AICHORN, TU Graz, Institute of theoretical and computational physics — The discovery of high-temperature superconductivity in iron-based compounds triggered an enormous amount of research in condensed matter physics. A very intriguing property of these new compounds is the rather high flexibility concerning elemental substitutions, leading to several families of superconductors, termed "1111," "122," "11," and so on, depending on their chemical composition. In this talk we will analyse the single-particle properties of prominent iron-based superconductors using a combination of density-functional theory with the Dynamical Mean-Field Theory, where also the interaction parameters are calculated ab-initio. This approach enables us to understand also these more complex materials at a first-principle level. We will show that there are significant differences in the electronic properties, when going from more weakly correlated members as LaFeAsO, to more correlated ones like FeSe. For reasonable Coulomb parameters, the properties range from Fermi-liquid like to incoherent bad-metal like.

[1]Supported by the Austrian Science Fund, project J2760.

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V2 DCMP: Fermi Surface Reconstruction and Competing Orders in High Tc Cuprates

Ballroom A2

8:00AM V2.00001 Broken rotational and translational symmetries in the pseudogap phase of cuprates[1] , LOUIS TAILLEFER, University of Sherbrooke and Canadian Institute for Advanced Research — A large in-plane anisotropy of the Nernst coefficient in YBCO is found to set in precisely at the pseudogap temperature $T^\star$ throughout the doping phase diagram [1]. This implies that the pseudogap phase is an electronic state that breaks the four-fold rotational symmetry of the copper-oxide planes. At a somewhat lower temperature, of order $T^\star/2$, the positive Hall and Seebeck coefficients of YBCO start dropping, and they reach large negative values at $T = 0$, in the normal state accessed by applying high magnetic fields [2,3]. We interpret this in terms of an electron pocket forming in the Fermi surface of YBCO as a result of a Fermi-surface reconstruction caused by some order which breaks the translational symmetry of the lattice. Because very similar transport anomalies are observed in Eu-LSCO [4], where they coincide with the onset of stripe order, we infer that some form of stripe order is also at play in YBCO, and argue that the pseudogap phase is a precursor region of stripe (or spin-density-wave) fluctuations [5].

[1] R. Daou *et al.*, Nature **463**, 519 (2010).
[2] J. Chang *et al.*, Physical Review Letters **104**, 057005 (2010).
[3] D. LeBoeuf, arXiv:1009.2078.
[4] O. Cyr-Choinière *et al.*, Nature **458**, 743 (2009).
[5] L. Taillefer, Annual Review of Condensed Matter Physics **1**, 51 (2010); arXiv:1003.2972.

[1]In collaboration with F. Laliberte, N. Doiron-Leyraud, J. Chang, R. Daou, O. Cyr-Choiniere, D. LeBoeuf, B. Vignolle, C. Proust, I. Sheikin, L. Malone, K. Behnia, B. J. Ramshaw, R. Liang, D. A. Bonn, W. N. Hardy, S. Pyon, T. Takayama, Y. Tanaka, H. Takagi.

8:36AM V2.00002 Quantum oscillation measurements and their reconciliation with ARPES results in underdoped cuprates[1] , SUCHITRA SEBASTIAN, University of Cambridge — A current conundrum relating to the normal state electronic structure of the underdoped cuprates is the apparent dichotomy between photoemission and quantum oscillations measurements. New quantum oscillation measurements performed over an extended regime on underdoped YBCO are presented that bring results of these two techniques into closer agreement. Further, from the latest quantum oscillation results, we are able to distinguish between various scenarios involving single or multiple carrier types – we show that the experimental findings are only consistent with one of these possibilities. *Work performed in collaboration with N. Harrison, M. Altarawneh, P. A. Goddard, R. Liang, W. N. Hardy, D. A. Bonn, and G. G. Lonzarich

[1]Funding from The Royal Society, DOE BES '100T', and NSF is acknowledged

9:12AM V2.00003 Magnetic phase diagram and magnetic dynamics of $YBa_2Cu_3O_{6+x}$: Implications for the mechanism of high-T_c superconductivity , BERNHARD KEIMER, Max Planck Institute for Solid State Research, Stuttgart, Germany — We will present a comprehensive study of the magnetic phase diagram of the high-temperature superconductor $YBa_2Cu_3O_{6+x}$. Using elastic neutron scattering, we show that the phase diagram includes incommensurate spin density wave and electronic liquid-crystal states, in addition to the well-known antiferromagnetic, d-wave superconducting, and paramagnetic phases [1]. Using a combination of inelastic neutron scattering and resonant inelastic x-ray scattering, we have also arrived at a comprehensive picture of the magnetic excitation spectrum in all of these phases [2]. The dispersion relations and spectral weights of all compounds, including the slightly overdoped superconductor $YBa_2Cu_3O_7$, are closely similar to those of magnons in undoped, antiferromagnetically ordered $YBa_2Cu_3O_6$. The results are in excellent agreement with the spin excitations obtained by exact diagonalization of the t-J Hamiltonian on finite-sized clusters. A numerical solution of the Eliashberg equations based on the experimental spin excitation spectrum of $YBa_2Cu_3O_7$ reproduces its superconducting transition temperature T_c within a factor of two, strongly supporting magnetic Cooper pairing models for the cuprates. Neutron scattering data of the buckling phonon in $YBa_2Cu_3O_7$ suggest that coupling to this phonon does not substantially enhance d-wave pairing [3].

[1] D. Haug, V. Hinkov, Y. Sidis, P. Bourges, N. B. Christensen, A. Ivanov, T. Keller, C. T. Lin, B. Keimer, New J. Phys. **12**, 105006 (2010).
[2] M. Le Tacon, G. Ghiringhelli, J. Chaloupka, M. Moretti Sala, V. Hinkov, M. W. Haverkort, M. Minola, M. Bakr, K. J. Zhou, S. Blanco-Canosa, C. Monney, Y. T. Song, G. L. Sun, C. T. Lin, G. M. De Luca, M. Salluzzo, G. Khaliullin, T. Schmitt, L. Braicovich, B. Keimer, to be published.
[3] M. Raichle *et al.*, to be published.

9:48AM V2.00004 The spin density wave quantum phase transition in two dimensional metals , SUBIR SACHDEV, Harvard University — The mean-field theory for the onset of spin density wave order in a metal describes a quantum phase transition which reconstructs the "large" Fermi surface to small Fermi pockets. Fluctuations near this transition are described by a quantum field theory of fermions near the reconstruction points, and the bosonic order parameter. This field theory is shown to be strongly-coupled in two spatial dimensions. We find an instability near the quantum critical point to d-wave pairing: this is a "log-squared" instability, stronger than the familiar logarithmic BCS instability. A similar instability is also found towards a modulated bond order. We also discuss an alternative route for the onset of spin density wave order, via intermediate non-Fermi liquid phases which have small Fermi pockets but without long-range spin density wave order.

M. A. Metlitski and S. Sachdev, Physical Review B **82**, 075128 (2010)
S. Sachdev, M. A. Metlitski, Y. Qi, and C. Xu, Physical Review B **80**, 155129 (2009)

10:24AM V2.00005 Quantum Oscillations and High Magnetic Field Heat Capacity in Underdoped YBCO , GREGORY BOEBINGER, National High Magnetic Field Laboratory — This abstract not available.

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V3 DCMP: Controlling Quantum Interactions of Single Spins and Photons in Diamond

Ballroom A3

8:00AM V3.00001 Spin quantum measurements on diamond defects , JOERG WRACHTRUP, University of Stuttgart — Diamond defects allow for precise measurement of single electron and nuclear spin quantum states. The excellent controllability of these spins as well as efficient decoupling from environment make them an ideal playground for engineering complex quantum states and development of elaborate control schemes. The talk will describe how nuclear spin states can be efficiently read-out and used as Qbits in spin clusters. Routs towards the controlled engineering of extended spin arrays as well as coupling to control structures will be discussed.

8:36AM V3.00002 Observation of spin-light coherence for single spin measurement and control in diamond[1] , BOB BUCKLEY[2], Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — The long spin coherence and optical addressability of nitrogen-vacancy (NV) centers in diamond makes them excellent candidates for studies of quantum information science with potential technological applications. We demonstrate the coherent coupling of light to the electronic spin of a single NV center for both non-destructive, single-spin readout via the Faraday effect and unitary, single-spin control via the optical Stark effect[3]. By monitoring the Faraday effect of laser light focused on a single NV center and detuned from optical resonances, we are able to read out an NV center's spin state without destroying it, in contrast to traditional spin readout techniques which polarize the spin during measurement. In a complimentary way, the spin coherently rotates in response to the light through the optical Stark effect, which we demonstrate as a method of all-optical spin control. These measurements have important consequences for future single-spin quantum non-demolition measurements and spin-photon entanglement schemes in diamond that may be exploited for the development of quantum repeater technologies and photonic coupling of spins over large distances.

[1]Work supported by AFOSR, DARPA, and ARO.

[2]In collaboration with G. D. Fuchs, L. C. Bassett, and D. D. Awschalom

[3]B. B. Buckley, G. D. Fuchs, L. C. Bassett, D. D. Awschalom, *Science Express* (DOI: 10.1126/science.1196436)

9:12AM V3.00003 Quantum entanglement between an optical photon and a solid-state spin qubit , EMRE TOGAN, Harvard University — Quantum entanglement is among the most fascinating aspects of quantum theory. In this work quantum entanglement between the polarization of a single optical photon and a solid-state spin qubit is realized. The experimental entanglement verification demonstrates that a high degree of control over interactions between a solid-state qubit associated with the single electronic spin of a nitrogen vacancy centre in diamond and the quantum light field can be achieved. The reported entanglement source can be used in studies of fundamental quantum phenomena and provides a key building block for the solid-state realization of quantum optical networks.[1]

[1]Quantum entanglement between an optical photon and a solid-state spin qubit, Nature 466, 730-734, (2010)

9:48AM V3.00004 Coupling single electron spins in diamond to integrated optical structures , RAY BEAUSOLEIL, HP Laboratories — Diamond is an attractive material for some electronic and photonic applications because of its excellent chemical stability and high thermal conductivity and carrier mobility. Diamond appears to be an excellent material for quantum information processing and magnetic sensing applications as well, with many optically active paramagnetic centers. Of these, the most carefully studied to date has been the nitrogen-vacancy (NV) color center, since it is optically addressable and can exhibit electron spin coherence lifetimes exceeding 1 ms at room temperature. This long-lived coherence is usually attributed to the nuclear spin-zero environment of the diamond lattice, which can be further improved with isotopic purification. These capabilities have recently allowed for some remarkable demonstrations in this system such as controlled coupling between single electronic and nuclear spins. For quantum information technologies, NV centers that are mutually optically coupled could enable long-distance quantum communication through repeaters. However, given the low branching ratio of natural emission from NV centers in bulk diamond into the zero phonon line, coupling these centers to cavities with at least moderately large Purcell factors is a critically important step. In this talk I will describe our recent progress in realizing microcavities with low loss and small mode volume in two hybrid systems: silica microdisks coupled to diamond nanoparticles, and gallium phosphide microdisks coupled to single-crystal diamond. In both cases, we have demonstrated coupling between NV centers and whispering-gallery-type cavity modes. Finally, I will present our most recent progress toward fabricating waveguides and microcavities directly in diamond.

10:24AM V3.00005 Quantum control and decoherence of a single spin in diamond[1] , VIATCHESLAV DOBROVITSKI, Ames Laboratory US DOE and Iowa State University — Nitrogen-vacancy (NV) impurity centers in diamond have recently emerged as a unique platform for investigating quantum dynamics and quantum control of single spins in solid-state environments. NV centers demonstrate an unusual combination of spin-dependent optical properties, individual addressability, and long spin coherence times. The NV spin state can be manipulated both optically and magnetically, and very fast quantum control operations can be performed with high fidelity [1,2]. Due to these uniquely favorable properties, quantum dynamics of a single NV spin can be investigated in great detail. I will present the results of our work on decoherence of NV spins by spin baths of atomic nitrogen impurities (P1 centers) and the spins of ^{13}C nuclei, and discuss different regimes of the decoherence dynamics. We will consider modern dynamical decoupling techniques which aim at preserving coherence of quantum spins, and the experimental implementation of the decoupling protocols, as well as more advanced quantum control of NV spins. Using a variety of analytical and numerical tools, we can characterize and optimize the factors which limit our control over these quantum spin systems [2]. We will also examine how the quantum control approaches can be used to elucidate the quantum dynamics of NV centers and the properties of the spin bath [3].

[1] G. D. Fuchs, V. V. Dobrovitski, D. M. Toyli, F. J. Heremans, and D. D. Awschalom, Science 326, 1520 (2009).
[2] V. V. Dobrovitski, G. de Lange, D. Riste, and R. Hanson, Phys. Rev. Lett. 105, 077601 (2010).
[3] G. de Lange, Z. H. Wang, D. Riste, V. V. Dobrovitski, and R. Hanson, Science 330, 60 (2010).

[1]Work at Ames Laboratory was supported by the Department of Energy-Basic Energy Sciences under Contract No. DE-AC02-07CH11358

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V4 DPOLY: Dynamics of Polymers: Phenomena Due to Confinement Ballroom A4

8:00AM V4.00001 Direct measurement of molecular motion in freestanding polystyrene thin films , MARK EDIGER, University of Wisconsin-Madison — An optical photobleaching technique has been used to measure the reorientation of dilute probes in freestanding polystyrene films as thin as 14 nm. Temperature-ramping and isothermal anisotropy measurements reveal the existence of two subsets of probe molecules with differing dynamics. While the slow subset shows bulk-like dynamics, the more mobile subset reorients within a few hundred seconds even at Tg-25 K (Tg is the glass transition temperature of bulk polystyrene). At Tg -5 K, the mobility of these two subsets differs by 4 orders of magnitude. These data are consistent with the presence of a high mobility layer at the film surface whose thickness is independent of polymer molecular weight and total film thickness. The thickness of the mobile surface layer increases with temperature and equals 7 nm at Tg.

8:36AM V4.00002 Molecular dynamics at nanometric length-scales , FRIEDRICH KREMER, Universität Leipzig — Broadband Dielectric Spectroscopy, Spectroscopic vis-Ellipsometry, X-Ray Reflectometry, Alternating and Differential Scanning Calorimetry are combined to study glassy dynamics and the glass transition in nanometric thin ($\geq$5 nm) layers of polystyrene (PS) having widely varying molecular weights and Polymethylmethacrylate (PMMA) deposited on different substrates. For the dielectric measurements two sample geometries are employed, the common technique using evaporated electrodes and a recently developed approach taking advantage of nanostructures as spacers. *All* applied methods deliver the concurring result that deviations from glassy dynamics and from the glass transition of the bulk never exceed margins of $\pm$3 K *independent* of the layer thickness, the molecular weight of the polymer under study and the underlying substrate. Our findings are discussed in the context of the highly controversial literature and prove that an appropriate sample preparation is of paramount importance in order to avoid artefacts.

[1] Erber et al., *Macromolecules* **43**, 7729 (2010).
[2] Mapesa et al., *Europ. Phys. J. - Special Topics* **189**, 173-180 (2010).
[3] Treß et al., *Macromolecules* (2010). DOI:10.1021/ma 102031k.

9:12AM V4.00003 Gas Permeation in Thin Glassy Polymer Films , DONALD PAUL, University of Texas at Austin — The development of asymmetric and composite membranes with very thin dense "skins" needed to achieve high gas fluxes enabled the commercial use of membranes for molecular level separations. It has been generally assumed that these thin skins, with thicknesses of the order of 100 nm, have the same permeation characteristics as films with thicknesses of 25 microns or more. Thick films are easily made in the laboratory and have been used extensively for measuring permeation characteristics to evaluate the potential of new polymers for membrane applications. There is now evidence that this assumption can be in very significant error, and use of thick film data to select membrane materials or predict performance should be done with caution. This presentation will summarize our work on preparing films of glassy polymers as thin as 20 nm and characterizing their behavior by gas permeation, ellipsometry and positron annihilation lifetime spectroscopy. Some of the most important polymers used commercially as gas separation membranes, i.e., Matrimid® polyimide, polysulfone (PSF) and poly(2,6-dimethyl-1,4-phenylene oxide) (PPO), have been made into well-defined thin films in our laboratories by spin casting techniques and their properties studied using the techniques we have developed. These thin films densify (or physically age) much faster than thicker films, and, as result, the permeability decreases, sometimes by several-fold over weeks or months for thin films. This means that the properties of these thin films can be very different from bulk films. The techniques, interpretations and implications of these observations will be discussed. In a broader sense, gas permeation measurements can be a powerful way of developing a better understanding of the effects of polymer chain confinement and/or surface mobility on the behavior of thin films.

9:48AM V4.00004 Surface Dynamics in Glass forming Materials[1] , JAMES FORREST, University of Waterloo — There is mounting evidence that the surface of glassy polymers exhibits enhanced dynamics compared to the bulk material at the same temperature. Using nanoparticle embedding and relaxation of nanodeformations on the surface, we have developed a detailed characterization of the dynamics of glassy polymers (polystyrene (PS), isotactic-poly(methyl methacrylate)). This includes the effects of temperature, molecular weight and film thickness on the surface dynamics. We have extended the studies to the molecular glass former TNB, which display striking similarities to PS. The results of these studies allow us to begin to develop an understanding of the surface properties of glassy material, and how these properties may lead to observed changes in thin film polymer properties.

Work done in collaboration with Chad Daley and Dongping Qi, University of Waterloo; Zahra Fakhraaim, University of Pennsylvania; and Mark Ilton, University of Waterloo.

[1]Funded by NSERC (Canada)

10:24AM V4.00005 Confinement effects on polymer structure and glassy dynamics[1] , ALEXEY LYULIN, Eindhoven University of Technology — We have performed molecular-dynamics simulations to explore the influence of confinement on the glass-transition temperature T_g for supported atactic-polystyrene thin films of different thickness (1 nm $\div$ 10 nm) and different strengths of attraction to the substrate (0.1 kcal/mol $\div$ 3.0 kcal/mol). The films have been equilibrated in a melt at 540 K and further cooled down with a constant cooling velocity of 0.01 K/ps below T_g to room temperature, 300 K. Based on the density measurements we have defined three different (substrate, middle and surface) layers for each film. We found that the monomers close to the surface and in the substrate layer are partially oriented, which leads to more effective monomer packing. For the whole film the average T_g value remains almost constant for films down to 2 nm thickness, where middle layer vanishes. For the middle layer itself T_g does not depend on the total film thickness, while an increase up to 70 K is measured for the substrate layer depending on the strength of attraction to the actual substrate. The surface layer remains liquid-like in the whole temperature range (300 K $\div$ 540 K). We claim that the redistribution of mass in the three film layers may explain the change with film thickness of the average T_g, if the latter is determined from linear fits of the average glass and melt densities. First results on the shear cycling and the rejuvenation phenomena will be discussed as well.

[1]This study is a part of the research program of the Dutch Polymer Institute. This work was also sponsored by the Stichting Nationale Computerfaciliteiten (National Computing Facilities Foundation, NCF) for the use of supercomputer facilities.

Thursday, March 24, 2011 8:00AM - 11:00AM –
Session V5 DMP DCMP: Physics for Everyone Ballroom C1

8:00AM V5.00001 Biomagnetism and Magnetotaxis in Bacteria: What Bacteria Know About Magnetic Materials and Permanent Magnet Design , RICHARD FRANKEL, California Polytechnic State University, San Luis Obispo, CA — Magnetotactic bacteria (mtb) migrate along geomagnetic field lines, i.e., they behave like self-propelled magnetic compass needles. Mtb make single-magnetic-domain crystals of magnetite (Fe_3O_4) and greigite (Fe_3S_4) in intracellular structures called magnetosomes. The magnetosomes are arranged in linear chains that comprise permanent magnetic dipoles with remanent moments approaching the saturation moment, causing the mtb to be oriented in the geomagnetic field as they swim. This allows them to keep their heading and efficiently migrate to, and remain in, a preferred, microaerobic, aquatic habitat. The mtb have solved the difficult problem of designing a permanent magnet that is sufficiently robust to cause the cell to be oriented in the geomagnetic field at ambient temperature, yet fit inside a micron-sized object, and be assembled *in situ* from potentially toxic materials scavenged from the environment. I will describe some recent advances in mtb genetics that illuminate the process by which they make and arrange their magnetosomes.

8:36AM V5.00002 Voodoo Science , ROBERT PARK, American Physical Society — A remarkable scientific result that appears to violate natural law may portend a revolutionary advance in human knowledge. It is, however, more likely an experimental screw up. Error is normal; it can be reduced by repeating measurements and better design of controls, but the success and credibility of science is anchored in a culture of openness. Ideas and observations are freely exposed to independent testing and evaluation by others. What emerges is the book of nature. On its pages we find, if not a simple world, at least an orderly world, in which everything from the birth of stars to falling in love is governed by the same natural laws. These laws cannot be circumvented by any amount of piety or cleverness, they can be understood - with the possible exception of String Theory. For those who elect to work outside the scientific community, errors may go unrecognized. We will examine examples of this, including claims of perpetual motion and cancer caused by cell-phone radiation.

9:12AM V5.00003 MMs Packing and Research with Undergrads , PAUL CHAIKIN, New York University — This abstract not available.

9:48AM V5.00004 Science and Cooking: Motivating the Study of Freshman Physics[1] , DAVID WEITZ, Harvard University — This talk will describe a course offered to Harvard undergraduates as a general education science course, meant to intrduce freshman-level science for non-science majors. The course was a collaboration between world-class chefs and science professors. The chefs introduced concepts of cooking and the professors used these to motivate scientific concepts. The lectures were designed to provide a coherent introduction to freshman physics, primarily through soft matter science. The lectures were supplemented by a lab experiments, designed by a team of very talented graduate students and post docs, that supplemented the science taught in lecture. The course was very successful in motivating non-science students to learn, and even enjoy, basic science concepts.

[1]This course depended on contributions from Michael Brenner, Otger Campas, Amy Rowat and a team of talented graduate student teaching fellows.

10:24AM V5.00005 Making a frothy shampoo or beer[1] , DOUGLAS DURIAN, University of Pennsylvania, Department of Physics and Astronomy — The terms "foam" and "froth" refer to a dispersion of gas bubbles in a liquid. Why do certain liquids show a tendency to foam while others do not? For example, bubbles can be produced in pure water by vigorous agitation, but then they rapidly coalesce and disappear. While foams cannot be produced with pure water, foams associated with beer or shampoo can persist for several minutes or even hours. What ingredient(s) in shampoo and beer make their foams stable, and what physical concepts control their stability? In this talk I'll review three basic mechanisms underlying foam stability, and I'll make connection with current research on coarsening by the diffusion of gas from smaller to larger bubbles.

[1]With thanks to Srinivasa Raghavan, Adam Roth, and NASA Microgravity Fluid Physics Grant NNX07AP20G.

Thursday, March 24, 2011 8:00AM - 11:00AM –
Session V6 DCOMP: Hybrid Functionals Applied to Solids Ballroom C2

8:00AM V6.00001 The shortcomings and advantages of hybrid functionals in the description of solids[1] , GEORG KRESSE, University of Vienna — For extended systems, density functional theory currently possesses the optimal balance between computational efficiency and accuracy. Hence its wide spread acceptance and application in quantum chemistry, materials science and computational catalysis is in no way astonishing. However, it is also well known that standard density functionals underestimate the band gap in particular for small gap systems, and resultantly structural properties related to the band gap are difficult to predict. In quantum chemistry this has long be realized, and hybrid functionals mixing Hartree-Fock and local density functionals are generally preferred over purely local functionals. Such functionals usually predict a much larger band gap than purely local density functionals. With the exception of the Crystal code, hybrid functionals were not available in popular periodic codes, and only recently successful implementations and applications using plane wave based codes, such as VASP, were reported. In this talk, I will survey the expertise we have acquired for hybrid functionals for extended systems. For simple prototypical materials, such as metals, semiconductors, and insulators many ground state properties are indeed found to be in much better agreement with experiment than using purely local functionals. This concerns lattice constants and bulk moduli, but phonon dispersion relations are also often significantly improved, in particular, for those semiconductors where DFT predicts no band gap. Some specific applications will be discussed in detail. This includes the description of (small) polarons in semiconductors, the properties of ferroelectric materials (specifically $BaTiO_3$ and $SrTiO_3$), phonon dispersion relations in the group IV elements, and magnetic impurities in semiconductors.

[1]Support by the Austrian FWF is acknowledged

8:36AM V6.00002 The effects of long-range exact exchange in hybrid-functional methods , THOMAS HENDERSON, Departments of Chemistry and of Physics and Astronomy, Rice University — Over the past several years, hybrid density functional theory, which mixes a fraction of exact exchange into conventional semilocal exchange-correlation functionals, has become the dominant method used in molecular electronic structure calculations. While hybrid functionals are responsible for many successes of modern Kohn-Sham theory, they suffer from several drawbacks as well. The rapid decay of semilocal exchange causes errors in describing many phenomena, including charge transfer and Rydberg excitations, polarizabilities of long chains, and several others. Further, different properties seem to require different amounts of exact exchange; calculations near equilibrium, for example, appear to require less exact exchange than do calculations far from equilibrium. Including long-range exact exchange in finite systems improves accuracy in quantities sensitive to the long-range potential and makes it possible to treat systems both near and away from equilibrium on a fairly even footing. This talk discusses the motivations for including long-range exact exchange, as well as some remarkable successes and notable failures caused by doing so. Alternatives which attempt to retain most of the successes while eliminating most of the failures are also discussed.

9:12AM V6.00003 Structure of oxygen vacancies and electron localization on $CeO_2(111)$[1] , MARIA VERONICA GANDUGLIA-PIROVANO, Humboldt-Universität zu Berlin, Berlin, Germany and Institute of Catalysis and Petrochemistry-CSIC, Madrid, Spain — In the many applications of ceria-based materials in heterogeneous catalysis, the reducibility of ceria is essential to the catalytic function. Thus, having a theoretical approach that is able to describe the changes in the oxidation state of the multivalent cerium atoms appears desirable. The use of density functional theory with hybrid functionals is shown to be adequate [1]. It has been generally accepted that the electrons left behind upon oxygen removal from CeO_2 surfaces, driving the $Ce^{4+} \rightarrow Ce^{3+}$ reduction, localize on cationic sites in next-neighbor distance to the defect. We apply density-functional theory (DFT) with the HSE06 hybrid functional as well as the DFT+U approach and predict that vacancies on $CeO_2(111)$ are likely to be bound to Ce^{4+} ions rather than to Ce^{3+} as priorly suggested. This prediction has been recently confirmed by means of STM imaging and spectroscopy [3]. We further find that subsurface vacancies are energetically preferred when compared to surface vacancies by up to 0.5 eV, and thus provide support for the most recent experimental result [4]. Defect-induced lattice relaxations are crucial to the electron localization on more distant cation sites to the defect and to the subsurface preference.

[1] J. L. F. Da Silva, M. V. Ganduglia-Pirovano, J. Sauer, V. Bayer, G. Kresse, Phys. Rev. B 75, 045121 (2007)
[2] M. V. Ganduglia-Pirovano, J. L. F. Da Silva, J. Sauer, Phys. Rev. Lett. 102, 026101 (2009).
[3] J. F. Jerratsch, X. Shao, N. Nilius, H-J Freund, C. Popa, M. V. Ganduglia-Pirovano, J. Sauer, unpublished.
[4] S. Torbrügge et al., Phys. Rev. Lett. 99, 056101 (2007).

[1]This work has been performed in collaboration with J. L. F. Da Silva, C. Popa and J. Sauer.

9:48AM V6.00004 Orbital-dependent functionals in FLAPW: hybrid functionals and optimized effective potentials[1] , STEFAN BLÜGEL, Institut fuer Festkoerperforschung and Institute for Advanced Simulation, Forschungszentrum Juelich and JARA, 52425 Juelich, Germany — Orbital-dependent functionals are a new class of exchange-correlation (xc) functionals for density-functional theory. Hybrid functionals combine a local or semi-local xc functional with a nonlocal orbital-dependent exchange functional and improve the band gaps of semiconductors and insulators as well as the description of localized states. As an alternative to nonlocal hybrid potentials, one can also construct local optimized effective potentials (OEP) from the exact exchange (EXX) functional. So far, most implementations for periodic systems use a pseudopotential plane-wave approach. We present an efficient all-electron, full-potential implementation of the PBE0 [1] and HSE [2] hybrid functionals as well as the OEP-EXX functional [3] within the FLAPW method (`Fleur` code: www.flapw.de). Results for prototype semiconductors and insulators are in very good agreement with other implementations. We will demonstrate the improvement over conventional local or semilocal functionals for oxide materials and focus in particular on systems where standard functionals yield qualitatively wrong results. In particular, we will discuss the geometric and magnetic structures of EuO and GdN. Additionally, we will address the possibility of using the hybrid-functional ground state as starting point for a GW quasiparticle correction [4] and show results for complex perovskite systems.

[1] M. Betzinger, C. Friedrich, and S. Blügel, Phys. Rev. B 81, 195117 (2010).
[2] M. Schlipf, M. Betzinger, C. Friedrich, M. Lezaic, and S. Blügel, inpreparation.
[3] M. Betzinger, C. Friedrich, S. Blügel, and A. Görling, to be published in Phys. Rev. B.
[4] C. Friedrich, S. Blügel, and A. Schindlmayr, Phys. Rev. B 81, 125102 (2010).

[1]Financial support from the DFG through the Priority Program 1145 and the Helmholtz association through the Young Investigators Group Program, contract VH-NG-409, is gratefully acknowledged.

10:24AM V6.00005 Hybrid functional studies of InGaN alloys and oxides for photochemical watersplitting[1] , POUL GEORG MOSES, Stanford University — Photochemical watersplitting can potentially be a future sustainable energy source, converting sunlight and water into hydrogen. However, in order to have highly efficient devices materials are needed that absorb a large proportion of the solar spectrum while at the same time having valence and conduction bands that straddle the hydrogen and oxygen evolution redox potentials. It is well known that DFT consistently underestimates the band gap (the so-called "band-gap problem"). As a consequence, the positions of the valence and conduction bands (and hence the band offsets) also suffer from uncertainties. To address these deficiencies of the local density approximation (LDA) and generalized gradient approximation (GGA) we use the HSE exchange correlation functional in order to accurately calculate the electronic band structure [1]. We will discuss bowing effects in InGaN alloys based on accurate calculation of band gaps of InGaN alloys and on an analysis of experimental results using our calculated deformation potentials to disentangle the effect of strain and alloying on the band gap. We will also discuss calculations of the absolute position of the valence band maximum and the conduction band minimum. Including a discussion and comparison with generalized gradient and local density approximations results. Finally we show that HSE may be used to understand the nature of surface defects.

[1] J. Heyd, G. E. Scuseria, and M. Ernzerhof, J. Chem. Phys. 118, 8207 (2003)

[1]Acknowledgment is made to the Donors of the American Chemical Society Petroleum Research Fund for support of this research and CNSI Computing Facility, the Teragrid TACC and NCSA supercomputer facilities.

Thursday, March 24, 2011 8:00AM - 11:00AM –
Session V7 GIMS: High Resolution Tunneling Spectroscopy of Dirac Fermions Ballroom C3

8:00AM V7.00001 Strain-Induced Pseudo–Magnetic Fields in Graphene: MegaGauss in Nanobubbles , NIV LEVY[1], Department of Physics, University of California & Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA. — Recent theoretical proposals suggest that strain can be used to modify graphene electronic states through the creation of a pseudo–magnetic field. This effect is unique to graphene because of its massless Dirac fermion-like band structure and particular lattice symmetry (C3v). Scanning tunneling microscopy shows that graphene grown on a platinum (111) surface forms nanobubbles, which are highly strained due to thermal expansion mismatch between the film and the substrate. We find that scanning tunneling spectroscopy measurements of these nanobubbles exhibit Landau levels that form in the presence of strain-induced pseudo–magnetic fields greater than 300 Tesla. This demonstration of enormous pseudo–magnetic fields opens the door to both the study of charge carriers in previously inaccessible high magnetic field regimes and deliberate mechanical control over electronic structure in graphene or so-called "strain engineering".

In collaboration with S. A. Burke[§,2], K. L. Meaker[2], M. Panlasigui[2], A. Zettl[2,3], F. Guinea[4], A. H. Castro Neto[5] and M. F. Crommie[2,3]. §. Present address: Department of Physics and Astronomy and Department of Chemistry, University of British Columbia, Vancouver, BC V6T 121, Canada. 2. Department of Physics, University of California, Berkeley, CA 94720, USA. 3. Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA. 4. Instituto de Ciencia de Materiales de Madrid (CSIC), Madrid 28049, Spain. 5. Department of Physics, Boston University, Boston, MA 02215, USA.

[1]Present address: Center for Nanoscale Science and Technology, NIST, Gaithersburg, MD 20899, USA

8:36AM V7.00002 Scanning tunneling microscopy studies of topological insulators grown by molecular beam epitaxy , XI CHEN, Tsinghua University — I will summarize our recent activities of using scanning tunneling microscope (STM) to study topological insulators grown by molecular beam epitaxy (MBE). The Landau quantization in three-dimensional topological insulators was directly observed in the tunneling spectra. In particular, we discovered the zeroth Landau level, which is predicted to give rise to the half-quantized Hall effect for the topological surface states. The existence of the discrete Landau levels and the suppression of Landau levels by surface impurities strongly support the 2D nature of the topological states. In addition, we studied the quantum interference pattern formed by the topological surface states near the step edges and magnetic impurities in Bi_2Se_3 and Bi_2Te_3. The decay behavior of the standing waves is in good agreement with the Dirac cone structure of the topological surface states. We show that the combination of MBE and high energy resolution scanning tunneling spectroscopy provides a powerful way to probing the novel physics in the topological insulators.

9:12AM V7.00003 Spatially Resolved Spectroscopy of Magnetic States in Epitaxial Graphene , DAVID MILLER, Georgia Institute of Technology — Graphene grown epitaxially on silicon carbide provides a potential avenue toward industrial-scale graphene electronics. A predominant aspect of the multilayer graphene produced on the carbon-terminated $(000\bar{1})$ face of SiC is the rotational stacking faults between graphene layers and their associated moire-pattern superlattice. We use scanning tunneling microscopy (STM) and spectroscopy (STS) in high magnetic fields to obtain detailed information about the massless Dirac fermions that carry charge in graphene. In agreement with prior investigations, we find that for small magnetic fields, the rotational stacking effectively decouples the electronic properties of the top graphene layer from those below. However, in maps of the wavefunction density at magnetic fields above 5 Tesla, we discover atomic-scale features that were not previously known or predicted. A phenomenological theory shows that this high-field symmetry-breaking is a consequence of small cyclotron-orbit wavefunctions, which are sensitive to the local layer stacking internal to the moire superlattice cell.

9:48AM V7.00004 Landau-level spectroscopies of a topological insulator , TETSUO HANAGURI, RIKEN — Topological insulators such as Bi_2Se_3 are characterized by massless Dirac surface state which would give rise to unique quantum phenomena in a magnetic field. Although it was experimentally verified by many ARPES experiments that the surface electrons are indeed massless, there has been a lack of studies exploring their quantum properties due to the inevitable contribution from the bulk electrons in a real material. Using surface-sensitive STM/STS technique, we selectively probed the surface massless electrons in Bi_2Se_3. Under magnetic field perpendicular to the cleaved surface, a series of Landau levels (LLs) has been observed in the tunneling spectra. Remarkably, there is a field-independent LL at the Dirac point, which is a hallmark of Dirac fermions. We developed a scaling analysis scheme of LLs based on the Bohr-Sommerfeld quantization condition which allowed us to determine the energy-momentum dispersion of the surface state [1]. Width of the LL peaks in the spectra becomes smaller near the Fermi energy, which may suggest that electron-electron correlation plays a role. In addition to the narrowing of LLs, the spectra near the Fermi energy exhibit complicated fine structures, which may be responsible for the anomalous magneto-fingerprint effect [2]. This work has been done in collaboration with K. Igarashi, M. Kawamura, H. Takagi and T. Sasagawa.

[1] T. Hanaguri *et al.*, Phys. Rev. B **82**, 081305(R) (2010).
[2] J. G. Checkelsky *et al.*, Phys. Rev. Lett. **103**, 246601 (2009).

10:24AM V7.00005 Scanning Tunneling Spectroscopy of a Gated Single- and Bilayer Graphene Devices in the Quantum Hall Regime , SUYONG JUNG, CNST, NIST — We have performed scanning tunneling spectroscopy (STS) measurements on a gated single- and bilayer graphene devices. The combination of STM/STS capability and an electrostatic back gate enables us to investigate the interactions of Dirac particles with local impurities at the atomic scale in zero magnetic field and in the quantum Hall regime while varying the Fermi-energy with respect to a Dirac (charge neutrality) point. In an applied magnetic field, well-resolved Landau levels (LLs) following the Dirac particle scaling are observed in both single- and bilayer graphene. Additionally, in single layer graphene, spatial dispersion of LLs caused by disorder potential lead to formation of graphene quantum dots (QDs). The tunneling spectra measured as a function of gate and sample biases are governed by Coulomb blockade physics. In contrast, no QDs are seen in bilayer devices. Instead, the main feature of the spectra is an energy gap formed around the charge neutrality point. The possible origin of energy gap will be discussed in a context of broken layer symmetry caused by gate electric field and disorder potential variation. Other noticeable features in the tunneling spectra of single- and bilayer graphene such as the formation of electron- and hole-puddles and the Fermi-level pinning effect will be discussed.

Thursday, March 24, 2011 8:00AM - 11:00AM –
Session V8 FEd FGSA: Enhancing Graduate Education in Physics: Focus on Skills Ballroom C4

8:00AM V8.00001 Teaching graduate students The Art of Being a Scientist[1] , ROEL SNIEDER — Graduate education in the classroom traditionally focuses on disciplinary topics, with non-disciplinary skills only marginally discussed, if at all, between graduate student and adviser. Given the wide range of advisers with different types and quality of communication skill (or lack thereof), the professional coaching delivered to students often is restricted to just the technical aspects of research. Yet graduate students have a great need to receive professional training aimed at, among other things, helping their graduate career be more efficient, less frustrating and less needlessly time-consuming. We have addressed this gap in graduate education by developing the one-credit course "The Art of Being a Scientist." This course covers a diverse range of topics of importance to being an effective and creative researcher. Topics covered include the following: What is science? Choosing a research topic, department, and adviser. The adviser and thesis committee. Making a work plan. Setting goals. Ethics of research. Using the scientific literature. Perfecting oral and written communication. Publishing papers and writing proposals. Managing time effectively. Planning a scientific career. Applying for jobs in academia or industry. In evaluations of the course, students invariably comment that they could have avoided significant problems in their graduate study and saved valuable time if they would have taken the course earlier on. This is an indication that the course not only useful for students, but also that it is best taken early in a their graduate career. The material covered in the course is captured in the book "The Art of Being a Scientist: A Guide for Graduate Students and Their Mentors," published by Cambridge University Press; more information can be found at: `www.mines.edu/~rsnieder/Art_of_Science.html` From this website one can download a description of the curriculum used in the class, including homework exercises. Currently we are expanding of professional education by offering more lectures and workshops in order to better prepare graduate students for a career in science.

[1]Roel Snieder, Tom Boyd, and Ken Larner, Center for Wave Phenomena and Office of the Graduate School, Colorado School of Mines

8:36AM V8.00002 Got Skills? On-the-Job Activities of Physicists , RACHEL IVIE, American Institute of Physics — It goes almost without saying that physics doctorates do a lot more than just physics research or teaching at their jobs. But what exactly do they do? First, I will share basic data showing where physics doctorates are employed. Then I will present data from two of AIP's surveys about the employment of physicists. The first set of data comes from our survey of physics PhDs one year after doctorate. We will consider how often physics doctorates do a variety of activities on the job, including management, technical writing, teamwork, design and development, programming, and advanced mathematics. The second set of data comes from AIP's new survey of PhDs in physics 10 to 13 years after graduation. Data for many of the same activities will be shown for physics doctorates who have been in the workplace about a decade. Depending on the type of job, most industrially employed physics doctorates do some type of physics at work, but they are also very likely to report managing projects, writing for technical audiences, working on a team, and collaborating with non-physicists, among many other activities. This examination of the types of activities physics doctorates perform in the workplace will provide insight on the non-scientific training that would benefit graduate students the most.

9:12AM V8.00003 Communication and Critical Thinking Skills , ELIZABETH H. SIMMONS, Michigan State University — This talk will discuss how faculty can help graduate students (and even postdocs) improve non-technical professional skills required for success in scientific careers. Examples to be covered will include a) planning and delivering high-quality presentations b) listening critically to others' presentations c) writing grant proposals, cover letters, and CV's d) reviewing manuscripts and responding to referee reports. The faculty member(s) involved must be prepared to project a welcoming attitude, to convey the importance of these skills, and to make a consistent investment of time.

9:48AM V8.00004 Tuning Higher Education , BRADLEY CARROLL, Weber State University — In April 2009, the Lumina Foundation launched its Tuning USA project. Faculty teams in selected disciplines from Indiana, Minnesota, and Utah started pilot Tuning programs at their home institutions. Using Europe's Bologna Process as a guide, Utah physicists worked to reach a consensus about the knowledge and skills that should characterize the 2-year, batchelor's, and master's degree levels. I will share my experience as a member of Utah's physics Tuning team, and describe our progress, frustrations, and evolving understanding of the Tuning project's history, methods, and goals.

10:24AM V8.00005 Shedding light on molecular dynamics: The role of physicists in the age of biomedical science , FU-JEN KAO, Institute of Biophotonics, National Yang-Ming University, Taipei, Taiwan — Fundamental discoveries of the physics of imaging in the areas of microscopy, MRI, and CCD image sensing have produced innovations throughout the 20th century and continuing into the 21st. Not only have these fundamental discoveries received recognition from the Nobel Foundation in 1953, 1986, 1986, 2003, and 2009, but they have also revolutionized basic interdisciplinary research in areas such as biophysics and biomedical physics to the point at which applied physicists, engineers, and medical clinicians are working together to design experiments and develop tools for use in a broad range of areas including clinical diagnosis and pharmaceutical clinical trials. In this presentation, I will describe several innovative approaches in physics combined with engineering that have revolutionized the frontier in the biomedical sciences. Specifically, I will present examples of basic research as well as design, development, and commercialization of photonics research in the biomedical area within the context of biophotonics and molecular imaging. These examples will include the use of optical, photonics, and imaging techniques to (1) understand and elucidate the fundamental physics and chemistry of biological functions; and (2) understand and describe the critical role of these techniques for disease diagnosis, prognosis, prevention, and treatment with novel noninvasive (or minimally invasive) procedures.

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V9 DFD: Self Assembly I D220

8:00AM V9.00001 Effects of cluster diffusion on the island density and size-distribution in submonolayer island growth , YEVGEN KRYUKOV, JACQUES AMAR, University of Toledo — The effects of cluster diffusion on the submonolayer island density and island-size distribution (ISD) $N_s(\theta)$ (where $N_s(\theta)$ is the number of islands of size s at coverage θ) are studied for the case of irreversible submonolayer growth of compact islands on a 2D substrate. In our model, monomers are deposited with deposition rate F while the mobility D_s of an island of size s satisfies $D_s \sim s^{-\mu}$. Results are presented for $\mu = 1/2$ (corresponding to Brownian motion) as well as for higher values of μ. In general, we find that the exponents describing the flux-dependence of the island and monomer densities vary continuously as a function of μ. For $\mu < 1$ we also find that the ISD exhibits power-law behavior up to a cross-over size S_c. However, the values of the corresponding exponents are significantly larger than previous theoretical predictions. A generalized scaling form for the ISD for $\mu < 1$ is also proposed which leads to excellent scaling of the entire distribution. In contrast, for $\mu \geq 1$ we find that, due to a competition between size-scales, neither our generalized scaling form nor the standard scaling form $N_s(\theta) = \theta/S^2\ f(s/S)$ (where S is the average island-size) lead to scaling of the entire ISD. Instead, the scaled ISD becomes more sharply peaked with increasing D_1/F and coverage. This is in contrast to models with limited cluster mobility for which good scaling occurs over a wide range of coverages and D_1/F.

8:12AM V9.00002 Rate-equation approach to irreversible island growth with cluster diffusion , BRADLEY HUBARTT, YEVGEN KRYUKOV, JACQUES AMAR, University of Toledo — A self-consistent rate-equation (RE) approach to irreversible island growth and nucleation is presented which takes into account the effects of cluster mobility. As a first application we consider the irreversible growth of compact islands on a 2D surface in the presence of monomer deposition (with rate F) and monomer diffusion (with rate D_1) while the mobility of an island of size s is assumed to satisfy $D_s = D_1 s^{-\mu}$ where $\mu \geq 0$. For coverages up to the peak island-density, we find excellent agreement between our RE and simulation results for the dependence of the island-density $N(\theta)$ on coverage θ for all values of μ considered, ranging from $\mu = 1/2$ (Brownian motion) to $\mu = \infty$ (immobile clusters). For $\mu \leq 2$, excellent agreement is also found between our simulation and RE results for the island-size distribution (ISD), while for higher values of μ the effects of correlations become important. We also demonstrate that the discrepancies between recent theoretical predictions for the exponents $\tau(\mu)$ and $\zeta(\mu)$ describing the size-dependence of the ISD for $\mu < 1$ and simulations can be explained by the geometry of compact islands. Our self-consistent RE approach may also be generalized to higher dimensions as well as to an arbitrary dependence of the cluster mobility on island-size.

8:24AM V9.00003 Kinetics and Thermodynamics of the Association of DNA Coated Colloids , KUN-TA WU, FENG LANG, Center for Soft Matter Research, New York University, RUOJIE SHA, Chemistry Department, New York University, REMI DREYFUS, Complex Assemblies of Soft Matter, CNRS-Rhodia-UPenn UMI 3254, NADRIAN SEEMAN, Chemistry Department, New York University, PAUL CHAIKIN, Center for Soft Matter Research, New York University — We have investigated the aggregation kinetics and thermodynamics of complementary DNA coated particles as a function of DNA coverage. The streptavidin on our particles can accommodate 69800 biotinalated DNA which has 50 base pair double strands and 11 base sticky ends. For full 100% coverage, the melting temperature, T_m, is 50.3 C. The transition width, ΔT, is 0.8 C, and the characteristic aggregation time, τ, is 4 minutes. For 2.5% (40 times less) coverage $T_m = 22$ C, $\Delta T = 5$ C, and $\tau = 11$ hours. A simple model which takes into account the number of DNA bonds and the multiplicity of their arrangements accounts for the full time and temperature dependence of the particle aggregation.

8:36AM V9.00004 DNA driven 2D Assembly of Nanoparticles on Lipid Surfaces , SUNITA SRIVASTAVA, DMYTRO NYKYPANCHUK, OLEG GANG, Brookhaven National Laboratory, Upton, NY, 11973 — Use of biomolecular linkers such as DNA due to its sequence-specific hybridization properties provides a versatile platform for assembly of nanoscale components. Here we investigated the DNA-based self-assembly of gold nanoparticles in 2D using lipid layer as fluid substrate. We examined the effect of lipid composition by vary the fraction of cationic and zwitterion lipids on formation of a particle monolayer. Using in-situ X -ray reflectivity we observed adsorption of DNA functionalized nanoparticles on charged lipid surfaces. The surface density of the particle monolayer can be tuned by changing the electrostatic interaction between the particles and the lipid surface. The in-situ measured particle desorption from the lipid surface due to a change of a salt concentration provides quantitative information on particle-surface interactions. The ex-situ studies on samples using XPS under similar conditions support our observations. Our studies explore the possibility to form regulated 2D systems, as well as provide basic understanding of interactions of charge nano-objects with lipids, which is important for the biomedical applications.

8:48AM V9.00005 Computational Analysis of DNA-Mediated Crystallization of Binary Colloidal Superlattices , TALID SINNO, RAYNALDO SCARLETT, MARIE UNG, JOHN CROCKER, University of Pennsylvania — Colloidal self-assembly provides a potential avenue for the design of novel devices with unique optical and structural properties. Colloidal systems also provide useful insights into fundamental mechanisms of phase transitions such as crystal nucleation, growth and melting that are otherwise difficult to probe in atomic systems. A promising approach for realizing highly tunable colloidal assembly is to graft single-stranded DNA oligomer brushes onto the surfaces of particles in order to create attractive interactions between them. Using this approach, micro- and nanoscale particles have now been successfully assembled into several crystalline phases, including ordered, binary superlattice structures. Here, we apply Monte Carlo simulations and free energy calculations to generate a detailed picture for the assembly binary superlattice crystals. The interparticle potential used to perform the calculations was generated specifically for DNA-mediated interactions and verified by measurements. We develop a pseudo-phase diagram for the binary superlattice system which includes both thermodynamic and kinetic influences. The predictions of the pseudo-phase diagram are validated using direct simulations of crystal nucleation. Finally, we discuss recent findings related to diffusionless transformations in growing superlattice crystals that may be important in experiments aimed at growing these structures.

9:00AM V9.00006 DNA Linker Mediated Assembly of Gold Nanoparticles Superlattice[1] , HUIMING XIONG, CFN, BNL & Shanghai Jiao Tong University, MATTEW Y. SFEIR, CFN, BNL, DANIEL VAN DER LELIE, Biology Department, BNL, OLEG GANG, CFN, BNL — A BCC (body-centered-cubic) crystalline phase forms when flexible ssDNA linkers are added to the mixture of two types of dispersed, ssDNAs capped gold nanocolloids which are mutually non-complementary but complementary to the respective ends of the linker DNA. The state diagram of DNA linker mediated nanoparticle assemblies has been experimentally investigated and constructed by using in-situ small angle x-ray scattering. The optically active three-dimensional superlattice containing plasmonic particles and DNA-encoded chromophors were further fabricated using this approach. We investigated structural tunability and corresponding optical response of the multicomponent superlattices.

[1]Support from the U. S. DOE Office of Science and Office of Basic Energy Sciences under contract No. DE-AC-02-98CH10886 and Shanghai Pujiang Program (10PJ1405400) is appreciated.

9:12AM V9.00007 Directed Self-Assembly of Colloidal Particles , ZORANA ZERAVCIC, School of Engineering and Applied Sciences, Harvard University, JESSE COLLINS, Department of Physics, Harvard University, VINOTHAN MANOHARAN, School of Engineering and Applied Sciences, Harvard University and Department of Physics, Harvard University, MICHAEL BRENNER, School of Engineering and Applied Sciences, Harvard University — In nature, simple constituents like atoms, molecules and polymer chains, spontaneously organize into larger, higher order structures. Interactions involved in this self-assembly act on a local level. These facts inspire experimental and theoretical engineering of components able to organize into pre-designed complex systems. We perform numerical simulations of collections of DNA coated colloidal particles. We test different design rules for self-assembly with short-range interactions and explore the stability of equilibrium structures.

9:24AM V9.00008 Replication of nanoscale DNA patterns[1] , CORINNA MAASS, TONG WANG, RUOJIE SHA, MIRJAM LEUNISSEN, REMI DREYFUS, NADRIAN SEEMAN, PAUL CHAIKIN — We present an artificial supramolecular system mimicking self- replication and information transmission strategies in nature, but without the aid of enzymes or equivalent biological mechanisms. Using DNA nanotechnology techniques, we can make DNA tiles with selective interactions based on complementary single-strand connections. A linear tile pattern distinguished by their connector sequences is transmitted to a subsequent generation of copies by connector hybridisation. Longitudinal pattern formation and transverse copy attachment are well separated by different melting temperatures. We have achieved a faithful transmission of the pattern information to the second replication generation. We use AFM imaging to test for pattern fidelity and gel electrophoresis for quantitative yield analysis.

[1]supported by a DAAD postdoc grant

9:36AM V9.00009 Designing colloids for alignment , REMI DREYFUS, CNRS, Compass Lab, TYCHO SLEATOR, NYU, KENNY MAYORAL, THOMAS G. MASON, UCLA, PAUL M. CHAIKIN, NYU — Inducing the spontaneous association of microscopic building blocks into macroscopic structures has been a promising way to create new materials for a variety of useful applications. Such fabrication processes typically require interactions between microscopic building blocks. The interactions that govern the assembly of these microscopic building clocks: electrostatic, magnetic, Van der Waals, depletion, and DNA interactions, are all currently being investigated. For all these cases, the attractive energy between the particles is proportional to the overlapping surface between the colloids. Controlling the positions and orientations of the microscopic building blocks is a critical issue in such processes. To date there has been no efficient or reliable process that enables such spontaneous assembly of building blocks. For the successful alignment of any particles that we desire to self-assemble, a shape with unique physical and mathematical properties must be identified. Under the assumption that energy is reduced in proportion to area overlap, we present a geometrical shape which, when encountering a similar shape from any initial configuration, is forced into a single relative orientation maximizing the overlap. The unique minimum of energy in the energy landscape drives the particles to self-assemble in a controlled orientation.

9:48AM V9.00010 Self-assembly of Nanoparticles into Planar Modulated Superstructures , MICHAEL ENGEL, University of Michigan — The advance in the synthesis of nanoparticles and colloids opens up the possibility to use them as building blocks for self-assembling novel materials. Ordered structures are especially interesting because they have unique photonic and electronic properties. Among the most complex ordered phases are commensurately and incommensurately modulated crystals. Although frequently found on the atomic scale in the bulk and as ordered structures of noble gases in adsorbed layers, modulated phases have so far not been known to self-assemble with nanoparticles. Here, we use computer simulations to study a two-dimensional system characterized by a simple isotropic interaction that could be realized in future with building blocks on the nanoscale. We find that the particles arrange themselves into planar hexagonal superstructures whose superlattice vector can be tuned reversibly by changing the temperature. Thermodynamic stability is confirmed by calculating the free energy with a combination of thermodynamic integration and the Frenkel-Ladd method. Different contributions to the free energy difference are discussed.

10:00AM V9.00011 Programmable, directed assembly of micron-scale components , CASPAR FLORYAN, ROBERT WESTERVELT[1], Harvard University — Self assembly is a nascent paradigm for assembling components in the micron to millimeter size range. Such assemblies are often performed by modifying the surface chemistries of the individual components or by creating flow fields directing them into position. We propose a method of directed assembly using dielectric contrast between the components and a surrounding fluid. A hybrid integrated-circuit / microfluidic device[2] will be used to trap and manipulate pieces into pre-defined patterns. The device contains an array of electrically-chargeable pixels on its surface, with a resolution of 10 μm.

[1]PI

[2]Thomas Hunt, David Issadore, Robert Westervelt "Integrated Circuit/Microfluidic Chip to Programmably Trap and Move Cells and Droplets with Dielectrophoresis" *Lab on a Chip 8*, 81-87 (2008)

10:12AM V9.00012 Synthesis and Evaporative Self-Assembly of Polystyrene Nanotubes under Confinement , LU ZHANG, JODIE LUTKENHAUS, Texas A&M University, TEXAS A&M UNIVERSITY TEAM — Synthesis and manipulation of anisotropic building blocks into ordered structures has attracted increasing attention in recent years as nanowires and nanotubes (NWs/NTs) show great potential in many emerging technologies such as novel electric devices, optical units and biosensors. Here we use evaporation to align polystryrene NWs/NTs into distinct and interesting patterns. We synthesized polystyrene (PS) NWs/NTs of varied aspect ratio using anodic aluminum oxide (AAO) templates (200 nm pore size) using a melt-wetting technique. The template was removed, and NWs/NTs of controllable length ranging from several hundred nanometers to a few micrometers were released from the bulk PS film under ultrasonication. We further investigate the evaporative self-assembly of the synthesized polystyrene NTs under confined and "open" geometries and observe the alignment and assembled structures of the polystyrene NTs using scanning electron microscopy. Confocal laser scanning microscopy was also used to monitor the kinetics of the alignment process during evaporation. Results indicate that many factors (solvent, aspect ratio) contribute to the degree of NW/NT alignment relative to the evaporation front.

10:24AM V9.00013 Dynamic self-assembly of chemically-propelled nanoscale building blocks , YANPING CHEN, YUNFENG SHI, Rensselaer Polytechnic Institute — Self-assembly technique offers spontaneous, massively-parallel structure formation from bottom-up. So far, most research efforts have been focused on static self-assembly that is thermally driven towards a thermodynamic equilibrium. Less attention has been paid to dynamic self-assembly that evolves to a non-equilibrium steady state under a dissipative driving force. This project aims to investigate the non-equilibrium self-assembly behaviors of chemically-propelled nanoscale building blocks via molecular dynamics simulations. We utilize a catalytic building block, that has been shown, when isolated, to exhibit self-motile behavior when immersed in a fuel environment. Upon increasing the number density of the building blocks, interesting collective behaviors emerge due to direct interactions between the building blocks or indirect interactions via the fuel environment. The simulation system is also subjected to an artificial operation of converting products back to fuel molecules. The heat generated by the exothermic chemical reaction will also be removed. In this way, a steady-state, as well as the resulting dynamic self-assembly pattern, can be obtained.

10:36AM V9.00014 Dynamic Self-Assembly and Self-Propulsion in Nonequilibrium Magnetic Colloidal Ensembles at a Liquid/Liquid Interface[1] , ALEXEY SNEZHKO, IGOR ARANSON, Argonne National Lab — Ensembles of interacting particles subject to external periodic energy fluxes often develop nontrivial dynamics. Magnetic colloidal particles suspended over an interface of two immiscible liquids and energized by vertical alternating magnetic fields give rise to novel dynamic self-assembled structures ("asters") which are not accessible at the liquid/air interfaces. Ferromagnetically ordered nickel spherical particles have been used in our experiments. Novel structures are attributed to the interplay between surface waves, generated at the liquid/liquid interface by the collective response of magnetic microparticles to the alternating magnetic field, and hydrodynamic fields induced in the boundary layers of *both* liquids forming the interface. Two types of magnetic order is reported. We show that self-assembled aster structures become distorted in the presence of a small in-plane dc magnetic field and develop self-propulsion. The speed of locomotion can be effectively tuned by the amplitude of the dc field.

[1]The research was supported by the U.S. DOE, Office of Basic Energy Sciences, Division of Materials Science and Engineering, under the Contract No. DE AC02-06CH11357

10:48AM V9.00015 A Tunable Terahertz Detector Based On Self Assembled Plasmonic Structure on a GaAs 2DEG , CHE JIN BAE, DEEPU GEORGE, ROHIT SINGH, ANDREA MARKELZ, SUNY at Buffalo — Recently compact frequency sensitive THz detection has been achieved using gated gratings on 2DEG structure. The method is based on the resonant absorption of the 2D plasmon dependence on system dimension and the tunability of that dimension by depletion gating. Here we attempt to improve detector sensitivity, tunability and remove polarization dependence through the development of a gated grid design. The requirement for imaging applications of device dimensions on the order of < 1 micron over a detector area of 4 mm2, suggest that standard lithographic approaches will be too costly for large scale detector production. Here we realize the gated grid plasmonic structure on 2DEG material by using nanosphere self assembly lithography. This fabrication method has not been widely developed for III-V processing but allows us to achieve large area sensitive detectors with tunability in the 1-4 THz range. In this paper we will discuss the fabrication method and characterization of the devices as a function of gate bias and temperature using FTIR and THz time domain measurements.

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V10 DMP: Focus Session: Growth, Structure, Dynamics, and Function of Nanostructured Surfaces and Interfaces – Semiconductors D221

8:00AM V10.00001 In situ x-ray scattering investigation of Ag/Si(111)7x7 , YIYAO CHEN, M.W. GRAMLICH, S.T. HAYDEN, University of Missouri, Columbia, MO, M.C. TRINGIDIES, Ames Lab-USDOE, Iowa State University, Ames, Iowa, P.F. MICELI, University of Missouri, Columbia, MO — We have used in situ synchrotron x-ray scattering to investigate the growth of quantum-size-effect (QSE) Ag nanocrystals on Si(111)-7x7. The experiments explore the buried interface and the wetting layer as well as the interlayer spacings and the height distribution of the islands at different coverage and temperatures. The areal density of the wetting layer is found to be 30% of Ag(111) and it is located above the adatom layer at a sharp interface. As the coverage is varied, all Ag layer heights are observed in the height distribution except for 2 atomic layers (measured from the Si surface), which were negligible. The structure of the islands and wetting layer will be discussed in relation to recent work that questions whether Ag/Si(111) is a QSE system. Research funding is supported by NSF DMR-0706278. The experiments were performed at the Advanced Photon Source Sector 6 beam-line at Argonne National Laboratory, which is supported by the US-DOE through Ames Lab under Contract No. W-7405-Eng-82.

8:12AM V10.00002 Grazing incidence surface scattering in the Pb/Si(111) system using an Area Detector , M.W. GRAMLICH, S.T. HAYDEN, YIYAO CHEN, P.F. MICELI, U. of Missouri — Geometrical effects are considered when using an area detector for in situ x-ray grazing incidence scattering studies of the Pb/Si(111) system. Rod-like scattering and 3D-crystallite diffraction can both occur during in situ studies and these require different geometrical considerations. The Pb/Si(111) system conveniently exhibits different surface phases that provide useful examples, including randomly oriented 3D-crystallites on the surface that form powder diffraction rings. The shape of a diffraction ring depends on the position of the detector in real space. For rod scattering, the length of the image on the detector depends on resolution as well as domain size. We will discuss methods for obtaining reciprocal space information from area detector images in surface diffraction. Research funding is supported by NSF DMR-0706278. The experiments were performed at the Advanced Photon Source Sector 6 beam-line at Argonne National Laboratory, which is supported by the US-DOE through Ames Lab under Contract No. W-7405-Eng-82.

8:24AM V10.00003 Increased structural ordering of the low temperature wetting layer in the Pb/Si(111)-7x7 system , P.F. MICELI, M.W. GRAMLICH, S.T. HAYDEN, YIYAO CHEN, U. of Missouri-Columbia, C. KIM, Kyung Hee U., Korea, E.H. CONRAD, Georgia Inst. Tech., M.C. TRINGIDES, Iowa State U. — The Pb/Si(111)-7x7 system exhibits interesting quantum size effects (QSE) for Pb nano-islands, including anomalously fast island coarsening that is facilitated by the wetting layer between the islands. While it is known that the wetting layer has a disordered 8x8 structure, the exact structure of the layer is still an open question. Our in situ x-ray scattering studies show that the wetting layer structure evolves temporally over a remarkably broad range of temperatures due to *two* physically independent mechanisms. The as grown low temperature wetting layer is found to slowly anneal into a *better-ordered 8x8 structure*, which suggests that it is highly dynamic as it attempts to accommodate the large corrugation of the Si(111)7x7 substrate. This increased order has important implications for the fast atom transport between the QSE-islands. Research funding is supported by NSF DMR-0706278 and the Ministry of Knowledge Economy of Korea 2009-F014-01 (CK). The experiments were performed at the Advanced Photon Source Sector 6 beam-line at Argonne National Laboratory, which is supported by the US-DOE through Ames Lab under Contract No. W-7405-Eng-82.

8:36AM V10.00004 Quantum Growth of a Metal/Insulator System , HAWOONG HONG, Argonne Natinoal Laboratory, AARON GRAY, University of Illinois at Urbana-Champaign, RUQING XU, Argonne National Laboratory, LONGXIANG ZHANG, TAI-C. CHIANG, University of Illinois at Urbana-Champaign — Quantum confinement of electrons in thin metal films can lead to novel effects on the growth, structure, stability, and various other physical and chemical properties, as demonstrated by recent work on metal films grown on semiconductor substrates. We report herein the observation of quantum growth behavior in a metal-on-insulator system; the results show substantial differences. Insulating substrates, with their large band gaps, offer minimal electronic coupling at the interface. This decoupling should maximize quantum confinement effects. Indeed, in a study of Pb film growth and thermal processing on sapphire, we have observed robust preferred island height selection over a wide thickness range – a hallmark of quantum confinement effects – for processing temperatures up to 250 degrees C. By contrast, room temperature is the limit for Pb films prepared on the semiconducting substrate Si(111). These results provide the first evidence connecting the quantum growth behavior of overlayers with the substrate band gap.

8:48AM V10.00005 Electron coherence in Pb/Ag heterostructures epitaxially grown on Si(111)[1] , JISUN KIM, Department of Physics, The University of Texas, Austin, TX 78712, CHENDONG ZHANG, Department of Physics, The University of Texas, Austin; Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, CAS, HONGJUN GAO, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, CAS, CHIH-KANG SHIH, Department of Physics, The University of Texas, Austin, TX 78712 — Along with other metals, Pb and Ag can form globally flat ultra- thin films on the Si(111) surface. Due to electron confinement along the growth direction, such films exhibit distinctive quantum well states (QWS's). Confinement occurs between the vacuum-solid and solid-solid interfaces. It was reported earlier, using angle-resolved photoemission, that quantum confined states existing in Ag thin films can coherently propagate through a Pb overlayer with thickness much thicker than the typical electron mean free path. Here we use scanning tunneling microscopy and spectroscopy to investigate the quantum well states formed in double quantum wells (Pb quantum well and Ag quantum well) formed in Pb/Ag/Si(111) double- heterostructures. Both the growth mechanism and the coherent coupling between the Pb and Ag quantum wells will be reported.

[1]NSF grant DMR-0906025, CMMI-0928664, Welch Foundation F-1672, and Texas Advanced Research Program 003658-0037-2007

9:00AM V10.00006 Surface plasmon excitation in ultrathin Mg films on Si(111) , AO TENG, The University of Tennessee, Knoxville, TN, GEUNSEOP LEE, Inha University, Incheon, Korea, SABAN HUS, The University of Tennessee, Knoxville, TN, HANNO WEITERING, The University of Tennessee, Knoxville, TN & Oak Ridge National Laboratory, Oak Ridge,TN — We investigated the dispersion of the surface plasmon in ultrathin Mg(0001) films, grown on a Si(111)-7×7 surface, as a function of film thickness and parallel momentum ($q_{||}$), using angle-resolved high-resolution electron-energy-loss spectroscopy (HREELS). In Mg films thicker than ~ 3 ML, surface plasmon excitations exhibit negative dispersions for small $q_{||}$(long wavelength limit). In contrast, the surface plasmons of ultrathin Al(111) films are known to exhibit positive dispersions near $q_{||} \sim 0$. The surface plasmon energies of the Mg films increase as the film thickness decreases. The plasmon line widths reveal similar trends, namely, for a given film thickness the line width decreases initially with increasing $q_{||}$ while it increases with film thickness. Possible explanations for the observed thickness dependence of the surface plasmon dispersion and damping will be discussed.

9:12AM V10.00007 Plasmon response of a quantum-confined electron gas probed by core-level photoemission[1] , MUSTAFA M. OZER, Oak Ridge National Laboratory, EUN JU MOON, ADOLFO G. EGUILUZ, HANNO H. WEITERING, University of Tennessee — The emergence of the "bulk" plasmon in *atomically-smooth* ultrathin Mg(0001) films on Si(111) has been determined using x-ray photoelectron spectroscopy (XPS). Plasmons in this quasi two-dimensional (2D) regime turn out to be excited primarily via the sudden creation of the core hole, as the extrinsic loss channel (which is dominant in bulk XPS spectra) is suppressed by electron confinement. The collective plasmon response of the films is remarkably similar to that of a thin slice of *bulk matter*, subject to quantum-size boundary conditions, in spite of the fact that the one-electron degrees of freedom are quantized. The energy-loss spectra of the thinnest films are characterized by a gradual transfer of spectral-weight from the bulk-like collective modes to the low-energy one-electron excitations, and the plasmon ultimately collapses below six monolayers. Our results represent striking manifestations of the role of electronic confinement on plasmon resonances in precisely-controlled nanostructures.

[1]DOE Office of BES, Division of Materials Sciences and Engineering

9:24AM V10.00008 Controlled Surface functionalization via self-selective metal adsorption and pattern transformation on vicinal Si(111) surface[1] , F.K. MEN, A.L. CHIN, Department of Physics, National Chung Cheng University, Chia-Yi 621, Taiwan, ROC, FENG LIU, Department of MSE, University of Utah, Salt Lake City, UT 84112, USA — We demonstrate a self-selective metal adsorption and pattern transformation process on vicinal Si(111) surfaces. When Au atoms are deposited onto the self-organized periodic Si(111) surface patterns, the Au atoms self-select to adsorb predominantly onto one of the two distinct domains, the Si(111) terrace or the step-bunched facet, at different Au coverage. This leads to a systematic transformation of the surface pattern, whose domain population changes while its periodicity remains intact with the increasing Au coverage. A stress-domain model is used to explain the observed phenomenon. Our findings suggest a unique method for controlled functionalization of surfaces at the nanoscale, as illustrated further by domain- selective self-assembly of uniform $CoSi_2$ nanoclusters on the Au-functionalized vicinal Si(111) surface.

[1]Work supported by NSC of Taiwan, ROC (Men) and NSF and DOE-BES of US (Liu).

9:36AM V10.00009 Epitaxial silicene formed on single-crystalline ZrB_2 thin films: structure and electronic properties[1] , ANTOINE FLEURENCE, RAINER FRIEDLEIN, YING WANG, YUKIKO YAMADA-TAKAMURA, School of Materials Science and Research Center for Integrated Science, Japan Advanced Institute of Science and Technology (JAIST) — The experimental realization of extended, two-dimensional sheets of silicene, the silicon counterpart of graphene, has been elusive so far. Here, we demonstrate that such a two-dimensional, epitaxial honeycomb Si layer forms through surface segregation on a metallic zirconium diboride (ZrB_2) film grown itself epitaxially on Si(111). The honeycomb Si layer uniformly covers the ZrB_2(0001) surface forming a (2×2) reconstruction. Surface-sensitive core-level photoelectron spectroscopy performed using a photon energy of 130 eV identifies Si atoms in different chemical states that are either in contact with Zr atoms or not, confirming details of the slightly-buckled honeycomb structure obtained through scanning tunneling microscopy. Angle-resolved ultraviolet photoelectron spectra reflect surface electronic states related to the predicted band structure of slightly-buckled, free standing silicene together with those of the uppermost Zr layer.

[1]Supported by Special Coordination Funds for Promoting Science and Technology, MEXT, and also by KAKENHI (22015008).

9:48AM V10.00010 Endotaxial Si nanolines in Si(001):H[1] , JAMES OWEN, FRANÇOIS BIANCO, SIGRUN A. KÖSTER, DANIEL MAZUR, CHRISTOPH RENNER, University of Geneva, DAVID BOWLER, University College London and London Centre for Nanotechnology — The study of one dimensional wires is of great interest in the area of low-dimensional physics, and these structures also have potential applications in future nanodevices. A perfectly straight nanoline embedded in a H-terminated silicon surface has been fabricated by a process of hydrogenation of a Bi nanoline surface using an atomic H beam source, and comprises a triangular core of Si embedded in the top five layers of the Si substrate. The defect density of this nanoline is extremely low, and being H- terminated, it is stable in air for limited periods of time. Scanning Tunnelling Microscopy experimental data and Density Functional Theory calculations have been used to determine the atomic structure of this nanoline, so-called the Haiku Stripe, and have revealed that there exists a 1D state localised to the nanoline core, lying just above the conduction band minimum.

[1]This work is supported by the Swiss National Science Fundation.

10:00AM V10.00011 Atomic Layer Epitaxy of Si and Ge on Si(100)-(2x1) , JEAN-FRANCOIS VEYAN, HEESUNG CHOI, M.S.E Department, University of Texas at Dallas, Richardson, Texas 75080, USA, JOSHUA BALLARD, Zyvex Labs, Richardson, Texas 75081, USA, STEPHEN MCDONNELL, WILEY P. KIRK, ROBERT M. WALLACE, M.S.E Department, University of Texas at Dallas, Richardson, Texas 75080, USA, JOHN RANDALL, Zyvex Labs, Richardson, Texas 75081, USA, KYEONGJAE CHO, YVES J. CHABAL, M.S.E Department, University of Texas at Dallas, Richardson, Texas 75080, USA — Atomic Layer Epitaxy of Si and Ge on Si(100) surface using disilane (Si_2H_6) and digermane (Ge_2H_6) as precursors is a critical step for constructing 3-D nano-structures, and is indispensable for Atomically Precise Manufacturing of new devices such as quantum dots. Using IRAS and STM together with DFT calculations, we show that Si_2H_6 chemisorbs on clean Si(100)-(2x1) via beta-hydride elimination pathway, involving the intermediate states Si-H and Si-SiH_2-SiH_3. Thermal decomposition of the chemisorbed Si_2H_5 leads to the formation of Si_2H_2 as an added dimer rotated 90 degrees with respect to the initial dimer row. A similar chemisorption pathway is observed for Ge_2H_6 on Si(100)x(2x1). The thermal decomposition of Ge_2H_5 involves the migration of H from Ge to Si, and Ge ad-dimer formation. Evidence for Ge epitaxial growth on Si(100)x(2x1) using Ge_2H_6 will be presented.

10:12AM V10.00012 Kinetics-Limited Composition Profile of Semiconductor Alloy Quantum Dots[1] , XIAOBIN NIU, GERALD STRINGFELLOW, FENG LIU, Department of Materials Science and Engineering, University of Utah — Semiconductor alloy quantum dots (QDs) with controlled composition profile are promising nanoscale building blocks for modern nanophotonic and nanoelectronic devices. The overall composition profile of such low-dimensional nanostructures is usually far from equilibrium, because bulk diffusion is negligible at typical growth conditions. However, local equilibrium may be established in the surface regions via surface diffusion. Consequently, the kinetic growth mode, which dictates the way of surface mass transport and alloy mixing in the growth fronts, becomes a key factor in determining the kinetics-limited composition profile. In this talk, we report our recent discovery of a striking correlation between the composition profiles of the strained semiconductor alloy QDs and their growth modes, based on atomistic-strain-model Monte Carlo simulations of InGaN (GeSi) QDs. The layer-by-layer growth forms core-shell structures with the core-rich unstrained component; while the faceted growth forms the core-rich strained component. Our findings suggest a promising method for the control of composition profile of semiconductor alloy QDs by selecting the growth mode.

[1]This work is supported by DOE and the Cao Group.

10:24AM V10.00013 Coarsening and Saturation of Quantum Dot Evolution during Strained Film Heteroepitaxy , CHAMPIKA GIGIRIWALA GAMAGE, ZHI-FENG HUANG, Department of Physics and Astronomy, Wayne State University, Detroit, MI — Morphological properties of an epitaxially grown film and the self-organization process of coherent strained islands are analyzed via the development of a continuum elasticity model based on the 2nd order perturbation method. Effects of wetting stress due to film-substrate interactions have been incorporated in the resulting nonlinear dynamic equation governing the film morphological profile. We study the formation and evolution of surface strained islands or quantum dots for different film/substrate misfit strains, via analyzing the time-dependent behavior of the structure factor for surface heights, its various moments, and the surface roughness. Three regimes of island array evolution have been identified, including a film instability regime at early stage, a slow power-law-type coarsening at intermediate time, and the crossover to a saturated state, with detailed behavior dependent on misfit strains but not qualitatively on finite system sizes. The results are compared to previous experimental and theoretical efforts on quantum dots coarsening and saturation.

10:36AM V10.00014 Directed Self Assembly and Self-Limiting Growth (SLG) of Mound Formation on Patterned GaAs(001) Surface During MBE Homoepitaxy[1] , CHUAN-FU LIN, University of Maryland, HUNG-CHIH KAN, National Chung-Cheng University, Taiwan, SUBRAMANIAM KANAKARAJU, CHRIS RICHARDSON, Laboratory for Physical Sciences, RAY PHANEUF, University of Maryland — We present the results of molecular beam epitaxial growth experiments on nanopit-patterned GaAs(001) surfaces at temperatures near 500°C. We find that in the initial stage of growth, the pattern directs the spontaneous formation of multilayer islands at 2-fold bridge sites between neighboring nanopits along [110], seemingly due to the presence of an Ehrlich-Schwoebel barrier [1]. However, as growth continues, the height of mounds at 2-fold bridge "self-limits": the mounds cease to grow. Beyond this point an initially less favored 4-fold bridge site for mounds dominates and a different pattern of self assembled mounds begins. We propose that a minimum, "critical terrace size" at the top of each mound is responsible for the observed self-limiting growth.

[1] T. Tadayyon-Eslami, H.C. Kan, L.C. Calhoun & R.J. Phaneuf, *Phys. Rev. Lett.* **97**, 126101 (2006)

[1]Work supported by NSF #DMR0705447 and the UM-MRSEC # DMR0520471.

10:48AM V10.00015 Spontaneous Microfaceting and Pyramid Formation during Si(100) Etching , MELISSA HINES, MARC FAGGIN, ANKUSH GUPTA, Cornell University — The spontaneous, etching-induced transformation of an initially flat Si(100) surface to a completely nanofaceted morphology consisting of overlapping pyramidal hillocks has been observed using a combination of morphological and spectroscopic probes and modeled using a kinetic Monte Carlo (KMC) simulation of Si(100) etching. The morphological transformation is driven by highly anisotropic chemical reactions that generate self-propagating pyramidal features with near-perfect microfacets. The atomic-scale mechanism of this etching-induced transformation will be discussed. In contrast to the more commonly studied Si(111) surface, the reactivity of the (100) face is dominated by interadsorbate strain.

Thursday, March 24, 2011 8:00AM - 11:00AM –
Session V11 FIAP: Electronic Structure: Theory and Spectra II D222

8:00AM V11.00001 First principles study of strained Si/Ge core-shell nanowires along [110] direction , XIHONG PENG, PAUL LOGAN, Arizona State University — First principles density-functional calculations were performed to study the electronic properties of Si/Ge core-shell nanowires along the [110] direction with the diameter of the wires up to 5 nm. It was found the band gap of the core-shell wires is smaller than that of both pure Si and Ge wires, given the same diameter. This reduced band gap is ascribed to the intrinsic strain between Ge and Si layers, which partially counters the quantum confinement effect. External uniaxial strain is further applied to the Si/Ge core-shell nanowires for tuning the band structure. At the Γ point, the energy levels of both conduction and valence bands are significantly altered by applied strain, which results in an evident change of the band gap. In contrast, for the K vectors far away from Γ, the variation of the conduction/valence band with strain is much reduced. In addition, with a sufficient tensile strain ($\sim$1%), the valence band edge shifts away from Γ, which indicates that the band gap of the Si/Ge core-shell nanowires experiences a transition from direct to indirect.

8:12AM V11.00002 Electronic structure of partially hydrogenated graphene superlattices , JOO-HYOUNG LEE, JEFFREY GROSSMAN, Massachusetts Institute of Technology — First-principles calculations based on density functional theory are performed to investigate the electronic structure of graphene-graphane superlattices (GSLs) by varying the widths of both the graphene and graphane regions. For the armchair-type interface between the graphene and graphane strips (AGSLs), the superlattices become semiconducting with a band gap exhibiting a similar dependence on the width of the graphene region as in armchair graphene nanoribbons. In contrast with the nanoribbons, however, the band gap of AGSLs shows both direct and indirect characteristics, depending on the graphane width. On the other hand, GSLs with a zigzag interface (ZGSLs) possess magnetic ground states except for those with a very narrow graphene strip. While an anti-ferromagnetic (AFM) phase is found to be energetically more stable than the ferromagnetic (FM) one, the energy difference between the two phases is so small (< 10 meV) that these two phases become nearly degenerate. These findings point toward an alternative route for graphene-based applications without requiring physical cutting as in graphene nanoribbons.

8:24AM V11.00003 First-Principle Calculations of The Conductivity of Br-Doped Graphite[1] , RASHID HAMDAN, CHAO CAO, ALEXANDER KEMPER, HAI-PING CHENG — First-principles calculations are used to study the enhanced in- plane conductivity that was observed experimentally in Br-doped graphite systems.[2] The band structure near the Fermi surface of the doped systems with different bromine concentrations compared to that of pure graphite, and the charge transfer between carbon and bromine atoms are analyzed to understand the conductivity change in the different directions. In addition, we address the effect of the compression of graphite layers on the stability of the bromine molecule Br_2 between these layers and thus on the conductivity of the system. Our calculations show that for large separation between doped graphite layers bromine is more stable in the molecular form (Br_2) and has a negligible effect on in- plane conductivity. However, with increased compression (decreased layer-layer separations) Br_2 molecule tend to dissociate and exchange charge with the nearby graphite layers causing an increase in hole conductivity.

[1]US/DOE/BES/DE-FG02-02ER45995, computational centers: UF-HPC/ NERSC.
[2]Tongay et al. Phys. Rev. B 81, 115428 (2010)

8:36AM V11.00004 Study of Bulk Modulus in Zincblende Nitrogen-doped Gallium Phosphide Alloys Using Density Functional Theory , BRANDON M. BUTLER, University of Texas at Arlington, JOHN A. TURNER, National Renewable Energy Laboratory, MUHAMMAD N. HUDA, University of Texas at Arlington — The prospect of solar energy as a renewable resource is ever-increasing. Density functional theory (DFT) calculations can elicit reliable behavior predictions in energy conversion materials to achieve higher efficiencies. Chemical stability of the photo-catalysts in aqueous solution is of particular interest for its long term performances. The bulk modulus is a mechanical property that is a good indicator of material stability. GaP has a low band gap and is a good candidate for use as a photocatalyst for hydrogen evolution by splitting water. Unfortunately, it is not stable and highly susceptible to corrosion over a very short time period, making it unfeasible for long-term use. GaN has too high of a band gap but a good stability factor. While these materials both possess desirable qualities, they cannot be used solitarily. We will report electronic properties and bulk moduli from the total energy calculations of the zincblende and wurtzite species using DFT-GGA and DFT+U as a function of doping concentration x. We will also present the density of states and charge density distribution of the alloy materials to study the localization/delocalization effects of N defects levels and their impact on the alloys' stability.

8:48AM V11.00005 Topological Insulators in Ternary Compounds with a Honeycomb Lattice[1] , HAI-JUN ZHANG, Stanford University, STANISLAV CHADOV, LUKAS MUCHLER, Institut fur Anorganische Chemie und Analytische Chemie, Johannes Gutenberg - Universtitat, Germany, BINGHAI YAN, XIAO-LIANG QI, Stanford University, JÜRGEN KÜBLER, Institut für Festkörperphysik, Technische Universit"at Darmstadt, Germany, SHOU-CHENG ZHANG, Stanford University, CLAUDIA FELSER, Institut fur Anorganische Chemie und Analytische Chemie, Johannes Gutenberg - Universtitat, Germany — One of the most exciting subjects in solid state physics is a single layer of graphite which exhibits a variety of unconventional novel properties. The key feature of its electronic structure are linear dispersive bands which cross in a single point at the Fermi energy. This is so-called Dirac cone. The ternary compounds, such as LiAuSe and KHgSb with a honeycomb structure of their Au-Se and Hg-Sb layers feature band inversion very similar to HgTe which is a strong precondition for existence of the topological surface states. These materials exhibit the surface states formed by only a single Dirac cone at the G point together with the small direct band gap opened by a strong spin-orbit coupling (SOC) in the bulk. These materials are centro-symmetric, therefore, it is possible to determine the parity of their wave functions, and hence, their topological character.

[1]The work was supported by the supercomputing center at Stanford Institute Materials and Energy Science. The financial support of the DFG/ASPIMATT project (unit 1.2-A) is gratefully acknowledged.

9:00AM V11.00006 The electronic structures of Cu delafossites nanocrystals for PEC hydrogen production: A density functional theory study[1] , MUHAMMAD N. HUDA, Physics Department, University of Texas at Arlington, YANFA YAN, MOWAFAK M. AL-JASSIM, National Renewable Energy Laboragory — Efficient photo-electrochemical (PEC) splitting of water to hydrogen by sun light usually requires that the semiconductor which will be used as a photoelectrodes will satisfy several electronic criteria. As naturally available semiconductors do not meet all these criteria, a thorough understanding of "band-engineering" for mixed alloys both at bulk and nano phases is necessary to successfully design these photoelectrodes. Recently Cu delafossites, CuMO_2, have received much attentions as photo-catalysts for hydrogen production due to their unique properties such as stability in most aqueous solutions and excellent hole mobility. However, due to their large optical band gap they can absorb sun light only in the ultra-violet region. Hence, it is necessary to tailor their electronic properties to enhance their catalytic activities in the visible light regions. In this presentation density functional study of the Cu-delafossite nanocrystals will be presented. The stability of the nanocrystals will be discussed along with the reactivity of the different crystal faces. It will be shown that O-terminated$M$-O octahedrons play a major role in the stability of these nanocrystals, which also makes these surfaces less reactive. We will discuss the charge (electron-hole) separation problems in these nanocrystals.

[1]Supported by National Renewable Energy Laboratory.

9:12AM V11.00007 Lateral Quantum Well States on Pb Films Grown on Cu Step Surface , PINGHENG ZHOU, Louisiana State University, Baton Rouge LA 70806, USA, YANG LIU, TOM MILLER, TAI-CHANG CHIANG, Department of Physics, University of Illinois at Urbana-Champaign,1110 West Green Street, Urbana, Illinois 61801-3080, USA, PAOLO MORAS, CARLO CARBONE, Istituto di Struttura Materia, Consiglio Nazionale delle Ricerche, Trieste, Italy, LOUISIANA STATE UNIVERSITY, BATON ROUGE LA 70806, USA TEAM, DEPARTMENT OF PHYSICS, UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN, ILLINOIS 61801-3080, USA TEAM, ISTITUTO DI STRUTTURA MATERIA, CONSIGLIO NAZIONALE DELLE RICERCHE, TRIESTE, ITALY TEAM — The highly ordered Pb films were found to grow on Cu step surface as a "magic" heteroepitaxial grown model. The lateral quantum well states in these Pb have been investigated by angle-resolved photoemission. Across the step direction, the quantum well state display a dispersive character, with periodicity in reciprocal space defined by the step superlattice geometry. These observations are compared and analyzed with *ab initio* calculations based on the full-potential linearized augmented plane wave method.

9:24AM V11.00008 Influence of local environment on the characterization of the p-type TCO in silver vanadates[1] , JINO IM, GIANCARLO TRIMARCHI, HAOWEI PENG, KENNETH POEPPELMEIER, ARTHUR FREEMAN, Northwestern University, Evanston, IL 60208, USA — Cu and Ag oxides are often considered as possible candidates for p-type transparent conducting oxides (TCO's) because the d^{10} valence structure usually gives rise to dispersive d-bands at the valence band maximum. Among them, multi-cation oxides of silver and vanadium show various atomic structures such as the $\alpha-$ and the $\beta-$phase of Ag_3VO_4 and $KAg_{11}(VO_4)_4$. Hence, these compounds, especially $KAg_{11}(VO_4)_4$, offer several local environments at Ag sites and it is interesting to assess how they influence the electronic structure. Based on first-principles density functional theory, we point out a relation between the local environment and d-s orbital mixing at the Ag site. In turn, this mixing determines the orbital composition of the band extrema and band gaps. The influence on band gaps of the substitution of Nb and Ta for V in Ag_3VO_4 and of the substitution of alkali metals for K in $KAg_{11}(VO_4)_4$ will also be discussed.

[1]Supported by the DOE EFRC for Inverse Design (Grant No. DE-AC36-08GO28308).

9:36AM V11.00009 Electronic structures of Tl-based materials for γ-ray detectors; First-principles study[1] , JUNG-HWAN SONG, HOSUB JIN, ARTHUR J. FREEMAN, SIMON JOHNSEN, JOHN ANDROULAKIS, PETER SEBASTIAN, ZHIFU LIU, JOHN A. PETER, NAM-KI CHO, BRUCE WESSELS, MERCOURI G. KANATZIDIS, Northwestern University — For Tl-based semiconductors, investigated to find good candidate materials for γ-ray detectors, we performed ab-initio calculations using the full-potential linearized augmented plane wave (FLAPW) method[2] to find their electronic structures and to estimate their physical properties such as band gaps, effective masses, absorption coefficients, dielectric constants, and work functions. Within the LDA scheme, the underestimation of the band gap is well-known and causes serious problems in obtaining optical properties. Therefore, we adopted the screened-exchange LDA (sX-LDA) scheme and acquired correct gap values close to experimental ones. With the sX-LDA, we found that Tl_6I_4S and Tl_6I_4Se have direct band gaps of 2.36 and 1.88 eV, respectively, and they exhibit dispersive bands near the band edges. Based on the calculated and experimental results, we discuss the relationship between atom species/crystal structure and electronic characteristics, and suggest several materials for γ-ray detectors.

[1]Supported by NSF (Grant No. ARI-MA CMMI-0938810).
[2]Wimmer, Krakauer,Weinert, Freeman, Phys. Rev. B, **24**, 864 (1981)

9:48AM V11.00010 Non-equilibrium Fermi-edge Singularity in Mesoscopic Devices , JIN ZHANG, NICHOLAS D'AMBRUMENIL, BORIS MUZYKANTSKII, University of Warwick, DAVID COBDEN, University of Washington — The non-equilibrium Fermi-edge singularity (NFES) was observed as a non-linearity in the random telegraph signal [1] in mesoscopic devices at low temperatures. Based on a modified NFES theory, we found that when a low-frequency ac signal is applied, the Fumi shift and the electron dephasing contribute in an opposite way to the violation of the detailed balance, which is measured in the logarithmic ratio of tunneling rates. In the case of large electron phase shift and weak dephasing, the usually-ignored Fumi shift plays an important role, and manifests itself as an "S"- shape curve in the logarithmic ratio of rates. For stronger dephasing, near the transition threshold, the tunneling spectra are dominated by the increased effective temperature because of the bias voltage, while for energies larger than that of the probing signal, the thermal excitation restores the system to pseudo-equilibrium. The overall shape of the logarithmic ratio of rates shows a "Z"-shape.

[1] D. H. Cobden, and B. A. Muzykantskii, Phys. Rev. Lett. 75, 4274 (1995)

10:00AM V11.00011 Dirac Point Degenerate with Massive Bands at a Topological Quantum Critical Point , SWAPNONIL BANERJEE, UC Davis, WARREN PICKETT, JUSTIN SMITH, VICTOR PARDO, RAJIV SINGH TEAM — In the band structure of the Skutterudite, as the Sb sublattice in the unit cell is moved slightly retaining the crystal symmetry, the small gap at the Fermi energy closes due to a band crossing at Gamma. At this critical point a pair of linear ("Dirac") bands are degenerate with two conventional bands. Because of the crystal symmetry three out of the four bands are degenerate even when one is away from the critical point. Insulators in 3D, as well as in 2D, can be characterized by topological invariants. When inversion symmetry is present (as in the space group 204 of Skutterudite), the Z2 invariant can be obtained from the parities of the occupied states at the invariant momenta, which in the bcc structure consist of Gamma, three H points, and the four P points. Here only the Gamma point requires consideration, since reoccupation occurs only there. The singlet has odd parity at Gamma while for the triplet it is even. As the critical point is crossed, the product of the parities of the occupied bands at Gamma, and hence the Z2 invariant, changes sign due to the reversal of the singlet- triplet position; the signal of a trivial to topological transition.

10:12AM V11.00012 Sixteen-band atomic bond-orbital model for zinc-blende structures , HSIU-FEN KAO, JIH-CHEN CHIANG, W.T. WANG, IKAI LO, Y.C. HSU, C.L. WU, D.J. JANG, Department of Physics, National Sun Yat-sen University, Kaohsiung 80424, Taiwan, MENG-EN LEE, C.Y. REN, YEN-CHIH TSENG, Department of Physics, National Kaohsiung Normal University, Yanchao, Kaohsiung County 82444, Taiwan, CHUN-NAN CHEN, Department of Physics, Tamkang University, Tamsui, Taipei County 25137, Taiwan — We develop a sixteen-band atomic bond-orbital model (16ABOM) which is able to compute the spin splitting induced by bulk inversion asymmetry. This model is derived from the linear combination of atomic orbital (LCAO) scheme such that the characteristics of real atomic orbitals can be preserved for spin-splitting calculations. We derive the Hamiltonian of 16ABOM by performing a similarity transform on the nearest-neighbor LCAO Hamiltonian, followed by taking a second-order Taylor series expansion over k-vector at the Γ point. The spin-splitting energies in bulk zinc-blendes are calculated using this model, and the results are in good agreement with LCAO and first-principles calculations. In addition, it is found the spin-orbit coupling between anti-bonding and bonding p-like states, which can be evaluated directly by this 16ABOM, dominates the magnitude of the spin splitting of the lowest conduction bands in middle-bandgap and wide-bandgap materials.

10:24AM V11.00013 Real-space Green's Function Calculations including Hubbard Contributions[1] , TOWFIQ AHMED, J. J. KAS, J. J. REHR, U. Washington — Hubbard model contributions are introduced into the real space Green's function formalism in terms of an effective self-energy, based on the LDA+U method of Anisimov et al.[2] The effective self-energy is then applied to localized d-states in a material, e.g. at the metal sites of transition metal oxides. The approach is implemented in an extension of the FEFF9 spectroscopy code and leads to an efficient procedure for including strong correlation effects in the electronic structure and x-ray spectra of d-electron materials, such as transition metal oxides and high T_c cuprates. Calculations are presented for the angular momentum projected density of states of MnO, NiO and $La_{(2-x)}Sr_xCuO_4$ and for the K-edge x-ray absorption and emission spectra of the O atoms in these materials, and the results are found to be in reasonable agreement with experiment.

[1]Supported by DOE BES DMSE Grant DE-FG03-97ER45623 and the DOE CMCSN

[2]V. I. Anisimov, F. Aryasetiawan, and A. I. Lichtenstein, J. Phys.: Condens Matter 9, 767 (1997)

10:36AM V11.00014 A Plane-Wave Implementation of Quasiparticle Self-Consistent GW (QSGW)[1] , DEREK VIGIL CURREY, JACK DESLIPPE, STEVEN G. LOUIE, University of California-Berkeley and Lawrence Berkeley National Lab — The use of GW techniques in calculating the quasiparticle properties of certain classes of materials, e.g. complex oxides, is sometimes hindered by the poor mean-field starting point that density functional theory (DFT) within standard Kohn-Sham implementations provides. There has been considerable effort in the community to improve upon the mean-field starting point for a broad range of materials. A recently proposed method, the quasiparticle self-consistent GW (QSGW) method, employs a process in which a mean-field exchange-correlation potential is approximated from and updated self-consistently using the self-energy operator from previous iteration GW calculations. We present an implementation of this method in a plane-wave basis, and discuss its accuracy, computational cost, and physical implications for a variety of semiconducting materials.

[1]This work was supported by NSF Grant No. DMR10-1006184 and U.S. DOE Contract No. DE-AC02-05CH11231. Computational resources were provided by NERSC. Derek Vigil Currey acknowledges funding from UC-Berkeley through the Chancellor's Fellowship.

10:48AM V11.00015 Assessment of dispersion-corrected density functional approaches for extended systems , WISSAM AL-SAIDI, University of Pittsburgh, Chemical and Petroleum Engineering, VAMSEE VOORA, KEN JORDAN, University of Pittsburgh, Department of Chemistry — Standard density functional (DFT) methods are known to fail in describing the long range van der Waals interactions, and currently, there is a great interest in incorporating dispersion corrections in density functionals. Recently, Tkatchenko and Scheffler introduced a new scheme where dispersion corrections are included by a summation of damped interatomic C_6/R^6 terms. However, contrary to the DFT-D2 approach of Grimme, the C_6 coefficients depend on the electron density through a Hirshfeld atom-in-a-molecule decomposition scheme. We have implemented the vdW-TS approach in VASP and applied it to the study of a series of prototype dispersion-dominated systems including layered materials, noble-gas solids and molecular crystals. Full optimization of all degrees of freedom is possible in our implementation because dispersion corrections are computed for the forces acting on the atoms, and also the stresses on the unitcell. Our results show that the vdW-TS method yield good structure, bulk moduli, and cohesive energies of weakly bonded systems in much better agreement with experiment than those obtained with standard DFT approaches.

Thursday, March 24, 2011 8:00AM - 11:00AM –
Session V12 FIAP: Transport in 2-D Systems D223/224

8:00AM V12.00001 In-Plane Field Magneto-transport in a Six-fold Degenerate Si-(111) 2DEG , TOMASZ M. KOTT, BINHUI HU, ROBERT N. MCFARLAND, STEPHEN H. BROWN, BRUCE E. KANE, University of Maryland, College Park — In-plane magneto-transport is an effective tool for measuring sub-band occupancy and differentiating between effects such as the so-called "reentrant Metal-Insulator Transition" or a ferromagnetic to paramagnetic phase transition. Using a two-dimensional electron gas (2DEG) on high mobility (up to $100,000$ cm^2/Vs) hydrogen terminated Si-(111) surfaces [1], we have studied the magneto-resistance due to in-plane magnetic fields of this six-fold degenerate system. While high perpendicular field (up to 12 T) measurements indicate field-dependent valley splitting, parallel field data helps differentiate this dependence from spin dynamics. The application of an in-plane field polarizes the 2DEG into distinct sub-bands. I will present measurements of both spin and valley sub-band polarization in parallel magnetic fields from samples of various mobility ($10,000 - 100,000$ cm^2/Vs) and discuss these results in the context of the broader question of field-dependent valley splitting. In a simple picture of valley splitting on Si-(111) surfaces, one would expect two valley polarization fields in addition to the spin polarization. I will discuss how this interaction-free model fits with the perpendicular field measurements, and what we can learn about the six-fold degenerate system.
[1] R. N. McFarland et al., *Phys. Rev. B* **80** 161310R (2009)

8:12AM V12.00002 Zero Differential Resistance State in double GaAs quantum wells at high filling factors[1] , ALEXEY BYKOV, E.G. MOSULEV, Institute of Semiconductor Physics, 630090 Novosibirsk, Russia, S.A. VITKALOV, The City College of New York, New York, NY 10031, USA — Differential resistance r_{xx} of 2D electrons was investigated in double GaAs quantum wells placed in magnetic fields $B < 0.5$ (T) at temperatures $T = 1.6 - 4.2$ (K). Electron state with Zero Differential Resistance (ZDR) is found in finite current range at maximums of inter-subband quantum oscillations. The experiment shows that the ZDR state exists at $2R_cE_H/\hbar\omega_c < 1/2$, where R_c is electron cyclotron radius at Fermi level, E_H is Hall electric field, induced by the dc bias, and ω_c is cyclotron frequency.

[1] A.A. Bykov, E. G. Mosulev and S. A. Vitkalov, JETP Letters v92, (2010) to be published

[1]Support: NSF DMR 0349049 and RFBR Projects No. 10-02-00285

8:24AM V12.00003 Degenerate versus semi-degenerate transport in a correlated 2D hole system[1] , RICHARD L.J. QIU, XUAN P.A. GAO, Dept. of Physics, Case Western Reserve University, LOREN N. PFEIFFER, KEN W. WEST, Dept. of Electrical Engineering, Princeton University — It has been puzzling that the resistivity of high mobility two-dimensional (2D) carrier systems in semiconductors with low carrier density often exhibits a large increase followed by a decrease when the temperature (T) is raised above a characteristic temperature comparable with the Fermi temperature (T_F). We find that the metallic 2D hole system (2DHS) in GaAs quantum well (QW) has a linear density (p) dependent conductivity, $\sigma \approx e\mu^*(p - p_0)$, in both the degenerate ($T << T_F$) and semi-degenerate ($T \sim T_F$) regimes. The T-dependence of $\sigma(p)$ suggests that the metallic conduction (dσ/dT <0) at low T is associated with the increase in μ^*, the effective mobility of itinerant carriers. However, the resistivity decrease in the semi-degenerate regime ($T > T_F$) is originated from the reduced p_0, the density of immobile carriers in a two-phase picture. Quantum oscillations in the magneto-resistivity are also found to persist into the semi-degenerate regime in our strongly correlated 2DHS.

[1]Supported by NSF grant (DMR-0906415)

8:36AM V12.00004 Nonlinear transport in very high Landau levels of a high mobility quantum Hall systems[1] , M.A. ZUDOV, H.-S. CHIANG, A.T. HATKE, University of Minnesota, M. KHODAS, University of Iowa, L.N. PFEIFFER, K.W. WEST, Princeton University — When a dc current is passed through a high-mobility two-dimensional electron system its differential resistivity exhibits oscillations with the applied magnetic field. The minima of these oscillations can extend all the way to zero leading to states with zero-differential resistance. This talk will discuss our recent experiments studying the evolution of the differential resistivity with temperature and with perpendicular and in-plane magnetic fields.

[1]This work is supported by NSF DMR-0548014.

8:48AM V12.00005 Charge carrier velocity distribution in amorphous oxide field-effect transistors , CHEN-GUAN LEE, BRIAN COBB, ANANTH DODABALAPUR, University of Texas at Austin — Charge transport in field-effect transistors (FETs) and the underlying physical mechanisms have been the subjects of numerous studies. Many types of transistors have been studied utilizing organic/polymer, amorphous silicon, and thin-film inorganic active layers. Most of these studies involve the evaluation of charge carrier mobility from steady-state characteristics as a function of temperature, electric field, channel dimensions, etc. In this study, we describe a technique to measure the velocity distribution of charge carriers in a thin-film transistor. We use this technique to evaluate velocity distributions in zinc-tin oxide (ZTO) thin-film transistors at various temperatures. In ZTO FETs, we observe multiple distinct transport pathways, each with a distinct activation energy. In contrast, steady state measurements yield a single activation energy. This shows that new insights into charge transport mechanisms and phenomena can be obtained with such time-resolved transport measurements which are not possible with steady-state approaches.

9:00AM V12.00006 Electronic Transport Properties of Epitaxial ZnO Films by Electron Dephasing and Mobility Spectrum Analysis , KUI ZHANG, WEI GUO, MICHAEL KATZ, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI 48109, TASSILO HEEG, DARRELL SCHLOM, Department of Materials Science and Engineering, Cornell University, Ithaca, NY 14853, MINGRUI HAO, WENZHONG SHEN, Department of Physics, Shanghai Jiao Tong University, Shanghai 200240, China, XIAOQING PAN, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI 48109 — Epitaxial ZnO films were grown by pulsed laser deposition on (111) Si substrates with bixbyite oxide buffers. Carrier transport properties were investigated using Hall measurements (4–300 K) under magnetic fields of 0–10 T, indicating mobility up to 113 cm^2/Vs. A diffusive Fermi surface (DFS) model incorporating electron dephasing theories was used to fit the abnormally positive magneto-conductivity observed below 150 K. Quantitative mobility spectrum analysis revealed the presence of a hole group at lower mobility accompanying the major electron group. Geometric distribution of the conducting groups was examined by capacitance-frequency experiments, while both temperature-dependent photoluminescence and mobility fitting confirmed a donor binding energy of ∼60 meV.

9:12AM V12.00007 Response of the Cyclotron Harmonic Spike to an In-Plane Magnetic Field[1] , YANHUA DAI, R.R. DU, Rice University, L.N. PFEIFFER, K.W. WEST, Princeton University — Microwave-induced resistance oscillations (MIRO) have been commonly observed in high- mobility GaAs/AlGaAs two-dimensional electrons systems (2DES) under microwave irradiations. In ultraclean GaAs/AlGaAs quantum wells (mobility $\sim 3.0 \times 10^7 cm^2/Vs$) we have recently observed an extraordinary resistance spike at the second harmonic of cyclotron resonance. In order to elucidate its origin, we have studied the response of microwave photoresistances in a two-axis magnetic field configuration, where the perpendicular (B_{perp}) and the in-plane ($B_{//}$) components can be independently applied to the sample. The experiments reveal a distinctive response of the spike to the $B_{//}$ as compared with that of the MIRO. While the major MIRO peaks show an increasing phase-shift towards 0.25 in increasing $B_{//}$, the spike position shows an essentially zero shift. This finding lends additional support for the notion that the spike is a new effect in the microwave-driven 2DES.

[1]The work at Rice was supported by NSF DMR-0706634.

9:24AM V12.00008 Conductivity kinks in the transport of ultra-dilute GaAs two-dimensional hole systems in zero field , JIAN HUANG, Wayne State University, L.N. PFEIFFER, K.N. WEST, Princeton University — Though Wigner crystal was first observed for electrons on helium in 1979, a Fermi Liquid-to-Wigner crystal transition has never been demonstrated. Important questions on how interaction drives such a transition and the nature of the transition remain unanswered. Apart from the complexity associated with the disorder which competes with or even dominates interaction by rendering the system into an Anderson insulator, an important question is whether there exists intermediate phases that hinder a direct first order transition. We report findings obtained via measuring ultra-high-purity GaAs two-dimensional hole systems with dilute charge concentrations down to 8x10^8 cm^{-2}. For fixed charge densities below 4x10^{9}cm^{-2}, a conductivity (σ) kink is observed while sweeping the temperature across some characteristic value where the derivative dσ/dT exhibits a discontinuous step. For charge densities above 4x10^{9}cm^{-2}, the kink evolves into a dip which diminishes for charge densities beyond 7x10^{9}cm^{-2}. A possible first order phase transition will be discussed.

9:36AM V12.00009 The Zero-Resistance States in InN Films , XIAOWEI HE, IVAN KNEZ, YANHUA DAI, RUIRUI DU, Rice University, XINQIANG WANG, BO SHEN, Peking University, RICE UNIVERSITY COLLABORATION, PEKING UNIVERSITY COLLABORATION — InN is a narrow gap semiconductor which possesses interesting transport properties. Besides the 2D electron accumulation layer on the surface, low temperature zero-resistance states have been observed in InN thin films and attributed to superconductivity. In order to elucidate the origin of superconductivity, we have studied systematically the temperature and magnetic field dependences of resistance in InN films of various thicknesses. High quality InN film samples of thickness between 50 nm and 5 μm were grown by molecular beam epitaxy on Al_2O_3 substrate with a GaN buffer layer. Typically these films have an electron density of 3x10^{17}- 6 x10^{18} cm^{-3}, and the mobility between 1000-2400 cm^2/Vs at 300 mK. Zero-resistance states were observed in films of thickness above 1 μm with the transition temperature of $\sim$ 1K, along with marked nonlinear I-V characteristics suggesting the presence of supercurrent. We observed anisotropic dependences of resistance on in-plane magnetic fields with respect to the direction of applied current. This work in Rice was supported by NSF DMR-0706634 and Welch Foundation C-1682, in Peking University was supported by the NSFC of China (Nos. 60990313, 10774001), and RFDP (No. 20090001120008).

9:48AM V12.00010 Electron interaction effects on Aharonov-Bohm resonances in an antidot-based quantum Hall interferometer , WOO-RAM LEE, Korea Institute for Advanced Study, HEUNG-SUN SIM, Korea Advanced Institue of Science and Technology — We theoretically study the electron interaction effects on Aharonov-Bohm resonances in an antidot-based quantum Hall interferometer in the integer quantum Hall regime. We introduce a general capacitive interaction model for an antidot with multiple bound modes of edge states, and find that the pattern of Aharonov-Bohm resonances is governed by the spectator behavior: The resonances of some modes disappear and instead are replaced by those of the other modes, due to charge relaxation between bound modes in the cotunneling regime. This behavior gives a reasonable understanding on the nontrivial features of previous experimental data, e.g., spectator behavior in an antidot molecule and resonance peaks in a single antidot with two, three, or four modes.
References:

[1] W.-R. Lee and H.-S. Sim, Phys. Rev. Lett. 104, 196802 (2010);
[2] W.-R. Lee and H.-S. Sim, arXiv: 1009.1004.

10:00AM V12.00011 Effective interlayer charge transfer in an electron bilayer system , VICTOR SOLOVYEV, Russian Academy of Sciences, Chernogolovka, STEFAN SCHMULT, WERNER DIETSCHE, Max-Planck-Institute for Solid State Research, Stuttgart, IGOR KUKUSHKIN, Russian Academy of Sciences, Chernogolovka — An electron bilayer system is realized in a wide GaAs quantum well. The chemical potentials of both layers can be tuned by intrinsic back and top gates. The Landau level spectrum for various charge distributions is probed by photoluminescence (PL), able to discriminate between both layers independently. The PL spectra show unambiguously how the system spontaneously deforms itself in strong magnetic fields as a consequence of energy minimization under Landau quantization and huge SAS energy gaps, reaching up to the cyclotron energy, become visible in the PL spectra [1].

[1] V.V. Solovyev, S. Schmult, W. Dietsche, I.V. Kukushkin, PRB 80, 241310, 2009.

10:12AM V12.00012 Exciton condensates in Pfaffian Quantum Hall states[1] , HANS HANSSON, Stockholm University — We apply recently developed (arXiv:1004.3657) conformal field theory techniques to describe exciton condensates in non-abeliann quantum Hall states of the Pfaffian type.

[1]Work supported by the Swedish Reserach Council.

10:24AM V12.00013 Spin-full quantum Hall states: squeezing techniques , EDDY ARDONNE, Nordita, Stockholm, MARIA HERMANNS, B. ANDREI BERNEVIG, Department of Physics, Princeton University, NICOLAS REGNAULT, Laboratoire Pierre Aigrain, ENS and CNRS, Paris — Despite the high magnetic field does the spin of the electron play an important role in the quantum Hall effect. Various spin (singlet) quantum Hall states have been proposed to explain various observed quantum Hall plateaux. In this talk, we present a method to generate spin-full quantum Hall states, by employing a squeezing procedure, as is used in the polarized state. This squeezing procedure also sheds additional light on the underlying (topological) structure of such states. By using connections between polarized and un-polarized states, one gains insight in the polarized state, as is the case for the Haffnian and Haldane-Rezayi states.

10:36AM V12.00014 Spin polarization measurement of the $\nu = 5/2$ fractional quantum Hall state via NMR , LARS TIEMANN, NTT and ERATO-JST, GERARDO GAMEZ, NORIO KUMADA, NTT, KOJI MURAKI, NTT and ERATO-JST — The $\nu = 5/2$ fractional quantum Hall state has attracted much interest due to its possible non-Abelian statistics, which are expected for the *Pfaffian* state. While the *Pfaffian* model assumes full spin polarization, recent optical experiments suggest a spin-unpolarized ground state at $\nu = 5/2$ instead [1, 2], and have thus posed a new challenge for understanding the true nature of the 5/2 state. Here, we report a spin polarization measurement of the $\nu = 5/2$ state using resistively-detected NMR and demonstrate its full polarization. The measurements were performed at $T = 10$ mK on a gated 30-nm quantum well at 4.4 T. For the resistive read-out of the nuclear resonance frequencies, we used the $\nu = 2/3$ spin transition by comparing its R_{xx} prior to and after the application of an *rf* pulse at $\nu = 5/2$. The NMR spectrum at $\nu = 5/2$ is shifted to lower frequencies from the one at $\nu = 2$, where the system is unpolarized, indicating a nonzero polarization at $\nu = 5/2$. Our analysis, which considers the changes of the sub-band wave function under a gate bias, indicates that the polarization at $\nu = 5/2$ is very close to its maximal value. This, in turn, gives support for the Pfaffian state.
[1] T. D. Rhone, APS March Meeting 2010, Y2.00003 [2], M. Stern *et al.*, Phys. Rev. Lett. **105**, 096801 (2010).

10:48AM V12.00015 Observation of a Well-Developed $\nu = 5/2$ Fractional Quantum Hall State in Low-Mobility Electron Systems , GERARDO GAMEZ, KOJI MURAKI, NTT Basic Research Labs — The fractional quantum Hall (FQH) state at filling factor 5/2 is currently one of the hottest issues in FQH physics. This is mainly due to the predicted non-Abelian statistics of its quasiparticles and their possible implementation in quantum computation. However, experimental efforts to explore the 5/2 FQH state are severely hampered by the extremely high sample quality required for its emergence. Indeed, well-developed 5/2 FQH states have been reported only in samples with an ultra high mobility in excess of 1x10^7 cm^2/Vs. Here, we report the observation of a fully developed 5/2 FQH state in a GaAs/Al_xGa_{1-x}As quantum well with a mobility of 4.8x10^6 cm^2/Vs, which was established after illumination at low temperatures by a red LED. To clarify the mechanism underlying the emergence of the 5/2 state, we carried out a systematic study on a series of samples with different parameters. Our study unveils that the screening of the remote impurity (RI) potential by the nearby neutral donors in the modulation doping layer plays the essential role. We also find that while the emergence of the 5/2 state is governed by the RI potential, once this state has emerged, the energy gap at 5/2 is still limited by the background impurity potential. Based on the analysis of the transport and quantum lifetimes, the relation between the 5/2 gap and these parameters will be discussed.

Thursday, March 24, 2011 8:00AM - 10:48AM –
Session V13 GSNP DFD: Glassy Systems and Jamming II D225/226

8:00AM V13.00001 Phonon Spectra in Disordered Clusters of Colloidal Particles with Attractive Interactions[1] , ARJUN G. YODH, PETER J. YUNKER, KE CHEN, University of Pennsylvania, ZEXIN ZHANG, Soochow University — The influence of size and morphology on the vibrational properties of disordered clusters of colloidal particles with attractive interactions is studied experimentally. Water- lutidine mixtures induce fluid mediated attraction between micron-sized polystyrene particles, leading to the formation of attractive glasses with high local packing fractions. By measuring displacement correlations between particles, we extract the vibrational properties of these disordered clusters. Surprisingly, the spectra and character of vibrational modes did not depend on the number of particles involved. Rather, it depended strongly on the average number of nearest neighbors. An increase in the number of nearest neighbors shifted the phonon spectrum to higher frequencies, independent of the total number of particles in in the cluster. Simulations of structureless random networks of springs support these results, and further suggest that the dependence of phonon spectrum on number of nearest neighbors is a generic property of disordered networks.

[1]We acknowledge financial support from the NSF through DMR-0804881, the PENN MRSEC DMR-0520020, and NASA NNX08AO0G.

8:12AM V13.00002 Dynamics of Small-Molecule Glass Formers Confined in Nanopores[1] , TIMOTHY PRISK, Indiana University Department of Physics, MADHUSUDAN TYAGI, NIST Center for Neutron Research, PAUL SOKOL, Indiana University Department of Physics — We report a comparative neutron scattering study of the molecular mobility and non-exponential relaxation of three structurally similar glass-forming liquids (isopropanol, propylene glycol, and glycerol) in bulk and confined in porous Vycor glass. Confinement reduces molecular mobility in all three liquids, and suppresses crystallization in isopropanol. High-resolution quasi-elastic neutron scattering spectra were fit to Fourier transformed Kohlrausch functions $\exp[-(t/\tau)^{\beta}]$, describing α-relaxation. The stretching parameter β is roughly constant with wavevector Q and temperature. Average relaxation times $\langle\tau(Q)\rangle$ are longer at lower temperatures and in confinement. They obey a power law $\langle\tau(Q)\rangle \propto Q^{-\gamma}$, where the exponent γ is modified by both temperature and confinement. Comparison of the bulk and confined liquids lends support to the idea that structural and/or dynamical heterogeneity underlies the non-exponential relaxation of glass- formers, as widely hypothesized in the literature.

[1]This work was prepared under award 70NANB5H1163 from NIST, U.S. Department of Commerce. We acknowledge the support of NIST in providing the neutron research facilities used in this work.

8:24AM V13.00003 ABSTRACT WITHDRAWN –

8:36AM V13.00004 Emergence of rigidity at the dynamic glass transition: a replica approach calculation[1] , GRZEGORZ SZAMEL, ELIJAH FLENNER, Department of Chemistry, Colorado State University — According to the mean-field replica theory of the glass transition, at the so-called dynamic transition the relaxation stops and the liquid freezes into one of many metastable states. We identify Goldstone modes of the resulting amorphous solid and derive a formal expression for its shear modulus. This expression is complementary to the formula used by Yoshino and Mezard [Phys. Rev. Lett. **105**, 015504 (2010)]. We combine our formal expression with the recently proposed version of the replica approach [G. Szamel, Europhys. Lett. **91**, 56004 (2010)] to calculate the shear modulus.

[1]We gratefully acknowledge the support of NSF Grant CHE 0909676.

8:48AM V13.00005 Experimental study of dynamic rearrangements in repulsive and attractive glasses , ZEXIN ZHANG, Soochow University, PETER YUNKER, University of Pennsylvania, PIOTR HABDAS, Saint Joseph's University, ARJUN YODH, University of Pennsylvania — The influence of interparticle attraction versus repulsion on heterogeneous glass dynamics is explored with colloidal particles suspended in water-lutidine mixtures. The mixtures permit interparticle potentials to be tuned in situ from short-range repulsive to short-range attractive. Thus, a direct comparison of colloidal glass dynamics in samples composed of the same particles at the same volume fraction is possible. In both types of glasses, dynamics are found to be heterogeneous, and particles rearrange in a cooperative manner. By comparison to repulsive glasses, attractive glasses exhibit dynamics that are heterogeneous over a wider range of time and length scales, and involve more particles. Clusters of rearranging particles form string-like structures in repulsive glasses, and more compact clusters in attractive glasses. The experiments demonstrate explicitly that interparticle interactions affect glass dynamics.

9:00AM V13.00006 A family of systematically softened glass-formers , ZANE SHI, PABLO DEBENEDETTI, FRANK STILLINGER, Princeton University — We present a computational study of a family of binary glass-forming mixtures that interact via the generic $U = 4\epsilon[\lambda(\sigma/r)^n - \alpha(\sigma/r)^6]$, where $n = 7, 8, 9, 10, 11, 12$. λ and α are chosen such that the location and depth of the potential minimum are constant across all members of the family. We investigate the effects of softening on thermodynamic quantities such as energy and entropy, as well as dynamic properties such as diffusion and scattering. We also investigate the effects of softening on the energy landscape. In spite of the imposed constraint on well depth and location, we find profound effects of softening on all aspects of liquid and glassy behavior. The stability of the glasses is greatly enhanced by softening (soft liquids make hard glasses), and the relaxation rates in the corresponding liquids increase markedly upon softening. We present a comprehensive analysis of kinetic and thermodynamic fragilities in this family of glass-formers.

9:12AM V13.00007 Low-Frequency Vibrational Modes and Rearrangements in a Colloidal Glass Subject to Point Expansion[1] , KEVIN APTOWICZ, MATTHEW COLAGRECO, RYAN MARGOLIS, West Chester University, PETER YUNKER, KE CHEN, ARJUN YODH, University of Pennsylvania — We conduct experiments on two-dimensional packings of colloidal thermosensitive hydrogel particles. The packing fraction of the colloidal suspension is tunable from liquid to deeply jammed by varying the global temperature of the sample. In addition, by tightly focusing an infrared laser on the sample, point expansion of the colloidal glass is induced via thermophoretic forces. We utilize displacement correlation matrix techniques employed in recent papers, and we employ video microscopy to derive the vibrational modes. The response of the sample to induced point expansion is analyzed over a range of packing fractions, with particular focus on the correlation between quasi-localized low-frequency vibrational modes and regions of rearrangements.

[1]This research is supported by an award from Research Corporation (KBA), MRSEC grant DMR-0520020 (AGY), NSF grant DMR-0804881 (AGY), and NASA grant NNX08AO0G (AGY).

9:24AM V13.00008 Crystallization of the Lewis-Wahnström ortho-terphenyl model , ULF PEDERSEN, UC Berkeley, TOBY HUDSON, PETER HARROWELL, School of Chemistry, University of Sydney — Crystallization is observed during long molecular dynamics simulations of bent trimer molecules - one of the standard models in computational studies of viscous supercooled liquids. The crystal was not anticipated, but is surprisingly simple: the three spheres that make up the rigid molecule sit near the sites of a body centered cubic lattice (the trimer bond angle being almost optimal for this structure). Interestingly, the crystal exhibits orientational disorder with molecules aligned randomly along the three Cartesian axis (an example of cubatic orientational order). While crystallization does not disqualify this model for viscous dynamics studies (it may even be valuable that the crystal is known), it illustrates the stubborn ingenuity of molecules to pack in periodic structures and questions our intuition to predict such structures. Finally, this is a rare example of crystallization of a molecular model from melt.

9:36AM V13.00009 Vitrification of a monatomic simple liquid in two dimensions[1] , TAKASHI ODAGAKI, Tokyo Denki University, TOMOKO MIZUGUCHI, Kyushu University — We investigate vitrification and crystallization process of a monatomic system by molecular dynamics simulation, where atoms interact via Lennard-Jones-Gauss potential. We first determine the time-temperature-transformation diagram by observing the crystallization time of the rapidly quenched state from the melt. The crystallization time becomes shortest at a certain temperature T*. The glassy state at low temperatures is shown to be fairly long-lived. In order to examine atomic mechanism of the crystallization, we introduce a modified incoherent intermediate scattering function which measures the structural correlation to a target structure. We show that the crystallization above and below T* take different paths. We also determine the free energy landscape (FEL) and show that the atomic dynamics is consistent with the FEL picture of the glass transition.

[1]This work was partially supported by a Grant-in-Aid for Scientific Research from the Ministry of Education, Science, Sports and Culture.

9:48AM V13.00010 Time reparametrization symmetry in a structural glass model , GCINA MAVIMBELA, HORACIO E. CASTILLO, Ohio University, CLAUDIO CHAMON, Boston University, LETICIA CUGLIANDOLO, Université Pierre et Marie Curie - Paris VI — We explore the existence of time reparametrization symmetry in a particle system with quenched disorder. The system's density fluctuations are described by a stochastic equation (D. S. Dean, J. Phys. A:Math. Gen **29**, L613 (1996)). Using the Renormalization Group (RG) on the Martin-Siggia-Rose generating functional, we analytically probe the long time dynamics by systematically integrating over short time scale fluctuations. We find that the RG flow converges to a fixed point that is invariant under reparametrizations of the time variable.

10:00AM V13.00011 Viscosity, Shear Waves and Atomic Level Stress Correlations[1] , VALENTIN LEVASHOV, JAMES MORRIS, TAKESHI EGAMI, University of Tennessee and Oak Ridge National Laboratory — The Green-Kubo equation relates the macroscopic stress-stress correlation function to a liquid's viscosity. The concept of the atomic level stresses allows the macroscopic stress-stress correlation function in the equation to be expressed in terms of the space/time correlations between the atomic level stress-stress correlation functions. Molecular dynamics studies show surprisingly long spatial extension of stress-stress correlations and also longitudinal and transverse waves propagating in liquids over ranges exceeding the system size. The results reveal that the range of propagation of shear waves corresponds to the range of distances relevant for viscosity. Thus our results show that viscosity is a fundamentally non-local quantity. We also show that periodic boundary conditions play very non-trivial, previously undiscussed, role in molecular dynamics simulations effectively masking the long range nature of viscosity.

[1]This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences.

10:12AM V13.00012 Study of the de Almeida-Thouless line using power-law diluted one-dimensional Heisenberg spin glasses[1] , AUDITYA SHARMA, PETER YOUNG, University of California at Santa Cruz — In a recent study, we showed that in mean-field theory, there is a de Almeida-Thouless (AT) line, that separates the low-temperature, low-field spin-glass phase from a high-temperature, high-field paramagnetic phase, for arbitrary m-component vector spin glasses, provided one applies a magnetic field that is *random in direction*. Building on this piece of work, here, we investigate whether or not there is an AT line beyond mean-field theory for Heisenberg spin glasses by performing Monte Carlo simulations on a power-law diluted one-dimensional Heisenberg spin glass for very large system sizes.

[1]NSF

10:24AM V13.00013 Renormalization group analysis of the random first order transition , CHIARA CAMMAROTA, GIULIO BIROLI, IPhT, CEA/DSM-CNRS/URA 2306, CEA, Saclay France, MARCO TARZIA, GILLES TARJUS, LPTMC, CNRS-UMR 7600, Universite Pierre et Marie Curie, Paris — We consider the approach describing glass formation in liquids as a progressive trapping in an exponentially large number of metastable states. To go beyond the mean-field setting, we provide a real-space renormalization group (RG) analysis of the associated replica free-energy functional. The present approximation yields in finite dimensions an ideal glass transition similar to that found in mean field. However, we find that along the RG flow the properties associated with metastable glassy states, such as the configurational entropy, are only defined up to a characteristic length scale that diverges as one approaches the ideal glass transition. The critical exponents characterizing the vicinity of the transition are the usual ones associated with a first-order discontinuity fixed point.

10:36AM V13.00014 Influence of pressure on fast relaxation in glass-forming materials , VLADIMIR NOVIKOV, University of Tennessee, Chemical Department, 1420 Circle Dr., TN, 37996, LIANG HONG, ALEXANDER KISLIUK, Oak Ridge National Laboratory, Oak Ridge, TN 37831, ALEXEI SOKOLOV, University of Tennessee, Chemical Department, 1420 Circle Dr., Knoxville, TN, 37996 — The spectra of GHz-THz dynamics in glass forming materials have two main contributions: the boson peak and the fast relaxation that overlaps with the low-frequency flank of the boson peak. The nature of both contributions remains a subject of active discussions. Applying pressure helps to separate the temperature and volume effects on the fast dynamics. Although the boson peak under pressure was investigated recently by several groups, less attention was devoted to the fast relaxation. In this work we present the study of the fast relaxation measured in some molecular and polymeric glass formers under pressure by light (Raman and Brillouin) scattering. Different experimental conditions were applied: isothermal, isobaric, isokinetic, and isochoric. The results are analyzed within the frames of various theoretical models. In particular, we check in detail the predictions of the soft-potential model of glassy dynamics.

Thursday, March 24, 2011 8:00AM - 11:00AM –
Session V14 GSNP: Focus Session: Statistical Mechanics of Complex Networks I D227

8:00AM V14.00001 Sensitive Dependence on Network Structure , ADILSON MOTTER, Northwestern University — Much of the recent research in complex networks has been focused on establishing relations between network structure and dynamics and on exploiting these relations to optimize network processes. Using diffusion, consensus, and synchronization dynamics as model processes of broad significance, I will show that optimization can often lead to sensitive dependence of the dynamics on the structure of the network. This sensitivity, which is characterized by cuspy or discontinuous dependence of the fitness function on network structural parameters, is shown to be determined by transitions in the complement graph that are reminiscent of explosive percolation. I will also discuss the prevalence of sensitive dependence. I will argue that this phenomenon is not limited to optimized systems, and may in fact be observed under rather general conditions in systems as diverse as power-grid and laser networks. This phenomenon sets experimental limits but also leads to improved controllability, in which the dynamics can be enhanced by exploiting antagonistic interactions between different fitness-inhibiting network structures.

8:36AM V14.00002 Critical percolation phase, geometric phase transitions with continuously varying exponents, and thermal Berezinskii-Kosterlitz-Thouless transition in a scale-free network with short-range and long-range random bonds , A. NIHAT BERKER, Sabanci University, MICHAEL HINCZEWSKI, University of Maryland, ROLAND R. NETZ, Technical University of Munich — Percolation in a scale-free hierarchical network is solved exactly by renormalization-group theory in terms of the different probabilities of short-range and long-range bonds [1]. A phase of critical percolation, with algebraic [Berezinskii-Kosterlitz-Thouless (BKT)] geometric order, occurs in the phase diagram in addition to the ordinary (compact) percolating phase and the nonpercolating phase. The algebraically ordered phase is underpinned by a renormalization-group fixed line along which the flows reverse stability, thus also leading to geometric phase transitions with continuously varying exponents. It is found that no connection exists between, on the one hand, the onset of the geometric BKT behavior and, on the other hand, the onsets of the highly clustered small-world character of the network and of the thermal BKT transition of the Ising model on this network. Nevertheless, both geometric and thermal BKT behaviors have inverted characters, occurring where disorder is expected, namely, at low bond probability and high temperature, respectively. This may be a general property of long-range networks. [1] A.N. Berker, M. Hinczewski, and R.R. Netz, Phys. Rev. E 80, 041118 (2009).

8:48AM V14.00003 Renormalization Group Classification of Critical Phenomena in Complex Networks[1]

, STEFAN BOETTCHER, TRENT BRUNSON, Physics Dept, Emory University — We discuss critical phenomena for a variety equilibrium statistical models on hierarchical networks with long-range bonds. An exact renormalization group (RG) study reveals that the observed critical behavior, albeit non-universal, can be classified into three generic categories. The non-universality is a direct result of the existence of long-range bonds, while the categories derive from their relative coupling strength. One of these categories is characterized by an infinite-order transition similar in appearance to the Kosterlitz-Thouless type, which has been observed recently in a number of network problems. Our result, if applicable to a wider set of networks, may explain the prevalence of such transitions, and may provide the basis for a generalized RG classification of criticality in complex networks.

[1]We thank the NSF-DMR for its support under grant #0812204.

9:00AM V14.00004 Contact process on static and adaptive preferred degree networks[1]

, SHIVAKUMAR JOLAD, WENJIA LIU, BEATE SCHMITTMANN, R.K.P. ZIA, Virginia Polytechnic Institute and State University — We consider epidemic spreading on an adaptive network where individuals have a fluctuating number of connections around some preferred degree κ. Using very simple rules for forming such a network, we find some unusual statistical properties which provide an excellent platform to study adaptive contact processes. For example, by letting κ depend on the fraction of infected individuals, we can model behavioral changes in response to how the extent of the epidemic is perceived. Specifically, we explore how various simple feedback mechanisms affect transitions between active and inactive states. In addition, we investigate the effects of two interacting networks, e.g., with a variety of κ's and cross links.

[1]Supported in part by NSF-DMR-0705152 and 1005417.

9:12AM V14.00005 Synchronization with Time Delays in a Noisy Environment[1]

, D. HUNT, G. KORNISS, B.K. SZYMANSKI, Rensselaer Polytechnic Institute — We study the effects of nonzero time delays in stochastic synchronization problems with linear couplings in an arbitrary network. We provide the synchronizability threshold using the known exact threshold value from the theory of differential equations with uniform delays and establish the limit of synchronization efficiency by constructing the scaling theory of the underlying fluctuations [2]. Nonzero delays lead to a scaling function for each fluctuation mode that does not vary monotonically as communication is improved (i.e., increasing strength or frequency). The strength and/or frequency of communication can then be tuned in order to subdue the stresses caused by growing the network to larger sizes, the presence of hubs, or lengthening delays. The implications can be counterintuitive: Improving communication is not always beneficial. In fact, making communication worse may salvage an otherwise unsynchronizable network. Insights into these trade-offs allow one to maintain and optimize the synchronization of the networks.

[1]Supported in part by DTRA and ARL.
[2]Hunt, Korniss, Szymanski, Phys. Rev. Lett. **105**, 068701 (2010)

9:24AM V14.00006 A simple model for studying interacting networks[1]

, WENJIA LIU, SHIVAKUMAR JOLAD, BEATE SCHMITTMANN, R.K.P. ZIA, Virginia Tech — Many specific physical networks (e.g., internet, power grid, interstates), have been characterized in considerable detail, but in isolation from each other. Yet, each of these networks supports the functions of the others, and so far, little is known about how their interactions affect their structure and functionality. To address this issue, we consider two coupled model networks. Each network is relatively simple, with a fixed set of nodes, but dynamically generated set of links which has a preferred degree, κ. In the stationary state, the degree distribution has exponential tails (far from κ), an attribute which we can explain. Next, we consider two such networks with different κ's, reminiscent of two social groups, e.g., extroverts and introverts. Finally, we let these networks interact by establishing a controllable fraction of cross links. The resulting distribution of links, both within and across the two model networks, is investigated and discussed, along with some potential consequences for real networks.

[1]Supported in part by NSF-DMR-0705152 and 1005417.

9:36AM V14.00007 Controllability of Complex Networks

, YANG LIU, Northeastern University, JEAN-JACQUES SLOTINE, Massachusetts Institute of Technology, ALBERT-LASZLO BARABASI, Northeastern University — The ultimate proof of our understanding of natural or technological systems is reflected in our ability to control them. While control theory offers mathematical tools to steer engineered systems towards a desired state, we lack a general framework to control complex self-organized systems, like the regulatory network of a cell or the Internet. Here we develop analytical tools to study the controllability of an arbitrary complex directed network, identifying the set of driver nodes whose time-dependent control can guide the system's dynamics. We apply these tools to real and model networks, finding that sparse inhomogeneous networks, which emerge in many real complex systems, are the most difficult to control. In contrast, dense and homogeneous networks can be controlled via a few driver nodes. Counterintuitively, we find that in both model and real systems the driver nodes tend to avoid the hubs. We show that the robustness of control to link failure is determined by a core percolation problem, helping us understand why many complex systems are relatively insensitive to link deletion. The developed approach offers a framework to address the controllability of an arbitrary network, representing a key step towards the eventual control of complex systems.

9:48AM V14.00008 Optimization of flow and cascading effects in weighted complex networks[1]

, ANDREA ASZTALOS, SAMEET SREENIVASAN, Dept. of Physics and Dept. of Computer Science, Rensselaer Polytechnic Institute, Troy NY, BOLESLAW SZYMANSKI, Dep. of Computer Science, Rensselaer Polytechnic Institute, Troy NY, GYORGY KORNISS, Dept. of Physics, Rensselaer Polytechnic Institute, Troy NY — We investigate the effect of edge weighting scheme $\sim(k_i.k_j)^\beta$ on the optimality of flow efficiency and robustness in complex networks. We achieve this by analyzing a simple distributed flow model: current flow in resistor networks. In this scenario the centrality measure of a node (edge) is given by the current-flow betweenness, that is the amount of current flowing through the node (edge), averaged over all source-target pairs, when unit current enters simultaneously at each node and flows towards a randomly chosen target. The largest loads formed on either the nodes or the edges set the maximum amount of input current for which the network is still congestion free. These two optimal values do not occur for the same value of β. As congestion may appear on nodes as well as on edges, we also study the cascading behavior of networks, triggered by the removal of one or more entities.

[1]Supported in part by DTRA

10:00AM V14.00009 Winning consensus on social networks[1] , SAMEET SREENIVASAN, Dept. of Physics and Dept. of Computer Science, Rensselaer Polytechnic Institute, NY, J. XIE, Dept. of Computer Science, Rensselaer Polytechnic Institute, NY, G. KORNISS, Dept. of Physics, Rensselaer Polytechnic Institute, NY, BOLESLAW SZYMANSKI, Dept. of Computer Science, Rensselaer Polytechnic Institute, NY — The adoption of a specific behavior (opinion) by a population of individuals is influenced dramatically by the social network through which the individuals interact. Here, we show the conditions under which a randomly distributed sub-population of committed agents – nodes on the network that consistently profess a unique opinion and are not influenceable to change – can win over an entire population of individuals initially opposed to that opinion. We model the opinion dynamics by a variant of the Naming Game (Baronchelli et al. (2006)), which effectively captures the persistence of dominant opinions. Given this model, we demonstrate that in the asymptotic network size limit, there exists a critical value p_c of the fraction of committed agents, above which the network-state attains consensus, and below which the network-state converges to a non-consensus fixed point. We also discuss finite size corrections to p_c and the scaling of consensus times for finite networks.

[1]Support by ARL, ONR

10:12AM V14.00010 Eigenvalue Spectra of Random Geometric Graphs[1] , AMY NYBERG, KEVIN E. BASSLER, University of Houston — The spectra of the adjacency matrix and the graph Laplacian of networks are important for characterizing both their structural and dynamical properties. We investigate both spectra of random geometric graphs, which describe networks whose nodes have a random physical location and are connected to other nodes that are within a threshold distance. Random geometric graphs model transportation grids, wireless networks, as well as biological processes. Using numerical and analytical methods we investigate the dependence of the spectra on the connectivity threshold. As a function of the number of nodes we consider cases where the average degree is held constant and where the connectivity threshold is kept at a fixed multiple of the critical radius for which the graph is almost surely connected. We find that there exists an eigenvalue separation phenomenon causing the distribution to change form as the graph moves from well connected to sparsely connected. For example, the Laplacian spectra of well connected graphs exhibit a Gaussian envelope of integer values centered about the mean connectivity and superimposed on a real valued distribution. As connectivity decreases, the distribution shifts and includes an accumulation of eigenvalues near zero.

[1]This work is supported by NSF Grant No. DMR - 0908286

10:24AM V14.00011 Renormalization group fixed point analysis on small-world Hanoi networks[1] , TRENT BRUNSON, STEFAN BOETTCHER, Emory University — The Hanoi networks (HN) are a class of small-world hierarchical networks with varying degree distributions. Because of their unique self-similar structure, the renormalization group (RG) can be solved exactly on these networks.[2] The real-space RG framework is used to study the Ising model phase diagrams on HNs and to interpolate between different types of networks using a tunable parameter in the recursion equations. This interpolation between different HNs reveals tunable transitions and critical behavior including the inverted Berezinskii-Kosterlitz-Thouless transition. The fixed point analysis of the RG in HNs explains the behavior of the divergence of the correlation length at critical temperatures as well as other critical phenomena observables.[3,4]

[1]With support from the NSF through grant DMR-0812204.
[2]S. Boettcher, C.T. Brunson, http://arxiv.org/abs/1011.1603
[3]See also http://www.physics.emory.edu/faculty/boettcher/.
[4]See also http://www.physics.emory.edu/students/tbrunson/.

10:36AM V14.00012 Quantum Transport through Hanoi Networks , M.A. NOVOTNY, CHRIS VARGHESE, Mississippi State U., STEFAN BOETTCHER, Emory U. — We present a renormalization group (RG) method to calculate the transmission of quantum particles through networks. The RG method is based on finite-dimensional matrix algebra for a tight-binding Hamiltonian [1], not a Green's function method [2]. The RG method is particularly well suited to application to hierarchical lattices. We apply the RG to obtain the quantum transmission T for Hanoi networks [3] HN3 (three bonds per site) and HN5 (on average 5 bonds per site). We give the transmission T as a function of the energy E of the incoming particle and the tight-binding parameters (on-site energy ϵ and hopping parameters t) for both linear and ring geometries. We have obtained T for up to 2^{200} sites, and have analyzed the RG equations to obtain asymptotic expressions. We find that the HN3 lattice exhibits band gaps, while no such band gaps exist in linear networks or in HN5.

[1] D. Daboul, I. Chang, and A. Aharony, Eur. Phys. J. B **16**, 303 (2000).
[2] S. Datta, *Electronic Transport in Mesoscopic Systems* (Cambridge U. Press, Cambridge UK, 1997), and references therein.
[3] S. Boettcher and B. Goncalves, Europhysics Lett. **84** 30002 (2008).

10:48AM V14.00013 ABSTRACT WITHDRAWN –

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V15 GMAG DMP FIAP: Focus Session: Spins in Semiconductors - Spin Currents III

D171

8:00AM V15.00001 Temperature Dependent Spin Transport in Silicon Controlled by an Electrostatic Gate[1] , JING LI, IAN APPELBAUM, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park, MD 20742 — Long-distance ($\sim$500μm) lateral spin polarized electron transport in undoped silicon under the control of an electrostatic gate is studied from 40K to 120K. The temperature dependence of average spin polarization, transport time, and spin dephasing during coherent precession can be largely attributed to reduction of finite spin lifetime at higher temperatures. Measurements on devices with different transport lengths are shown to modify the effect of electrostatic gating.

[1]Support from ONR is acknowledged

8:12AM V15.00002 Electrical detection of spin accumulation at 500K at FM/SiO2/Si(001) contacts via the Hanle effect[1]

, CONNIE H. LI, OLAF M. J. VAN 'T ERVE, EUGENE A. IMHOFF, BERRY T. JONKER, Naval Research Lab — We demonstrate the electrical detection of spin accumulation in Si (doped n-type 3E18 and 3E19/cm3) via injection from a ferromagnetic contact through a SiO2 tunnel barrier formed by plasma oxidation. The injection of spin-polarized carriers produces a net spin accumulation described by the splitting of the spin-dependent electrochemical potential, and is detected as a voltage. The decrease of this voltage with increasing out-of-plane magnetic field due to spin dephasing, i.e., Hanle precession of the electron spin, is observed at temperatures up to 500K. Lorentzian fits to the Hanle curves yield a spin lifetime of 100 and 320ps for the high and lower doped Si. The direct correlation between spin lifetime and carrier concentration in the Si, and that the magnitude of the Hanle signal agrees well with that expected from theory [1], provide clear evidence that the spin accumulation indeed occurs in the Si and not interface states. These results demonstrate that spin accumulation in Si can be a viable basis for spin-based devices. Supported by ONR.

[1]Fert et al., PRB 64, 184420 (2001), IEEE Elect. Dev. 54, 921 (2007).

8:24AM V15.00003 Quantifying Electron Spin Polarization from Polarized EL in Si spin-LEDs

, G. KIOSEOGLOU, University of Crete, P. LI, H. DERY, University of Rochester, A.T. HANBICKI, C.H. LI, O.M.J. VAN 'T ERVE, P.E. THOMPSON, B.T. JONKER, NRL — We analyze the circular polarization (P_{circ}) of the electroluminescence (EL) from Si-based spin-LEDs using a recent theory [1] which provides a quantitative relation between the polarization of phonon-assisted optical transitions measured in the EL, and the electron spin polarization electrically injected from Fe/Al2O3 and Fe/SiO2 tunnel barrier contacts [2,3]. EL spectra include features due to transverse acoustic (TA) and transverse optical (TO) phonon-mediated recombination occurring in the p-doped (p$\sim 10^{19}$cm-3) substrate. P_{circ} of 3.5% is typical for the TA at 5K, and is systematically higher than that of the TO by a factor $\sim$1.7, consistent with theory. The maximum polarization predicted for the TA is 13% for recombination of 100% polarized electrons in p-type Si (10^{19}cm-3). Thus the measured P_{circ} 3.5% corresponds to an electron spin polarization (P_{spin}) of 27% produced by electrical injection from our tunnel barrier contacts. A similar analysis applied to the TO phonon at 80K yields P_{spin} of 25%. Thus the theory enables quantitative interpretation of optical polarization in indirect gap semiconductors, facilitating future studies of spin injection. [1] P. Li and H. Dery, Phys. Rev. Lett. 105, 037204 (2010). [2] B.T. Jonker, et al., Nature Physics 3, 542 (2007). [3] C.H. Li, et al, Appl. Phys. Lett. 95, 172102 (2009).

8:36AM V15.00004 Electrical spin injection to Germanium using a single crystalline Fe/MgO/Ge tunneling junction

, YI ZHOU, LI-TE CHANG, University of California, Los Angeles, WEI HAN, University of California, Riverside, FAXIAN XIU, MINSHENG WANG, University of California, Los Angeles, MICHAEL OEHME, JOERG SCHULZE, Universitaet Stuttgart, ALEXANDROS SHAILOS, California Nano System Institute, ROLAND KAWAKAMI, University of California, Riverside, KANG WANG, University of California, Los Angeles — Germanium has long been predicted a superior candidate for spintronics with enhanced spin lifetime and transport length due to low spin–orbit interaction and lattice inversion symmetry. One of the critical challenges, however, is to electrically create spin accumulation in otherwise non-magnetic Ge. In this work, we report electrical spin injection to bulk n-type Ge using a single crystalline Fe/MgO/Ge tunneling junction. The spin lifetime and diffusion length are extracted from both 3-terminal Hanle measurement and non-local spin valve measurement. The spin relaxation mechanism in n-type Ge has also been explicitly analyzed from the bias and temperature dependence of the spin relaxation rate.

8:48AM V15.00005 Spin accumulation in Fe/MgO/Si heterostructures[1]

, A.T. HANBICKI, O.M.J. VAN 'T ERVE, S.-F. CHENG, R. GOSWAMI, C.H. LI, G. KIOSEOGLOU, P.E. THOMPSON, B.T. JONKER, Naval Research Laboratory — We report on spin injection experiments at Fe/MgO/Si interfaces using all electrical injection and detection. MgO is a promising magnetic tunnel junction material, and its incorporation with Si-based spintronics has only recently been reported in degenerately doped Si (n $\sim 10^{20} cm^{-3}$) [1]. We focus here on spin accumulation under the injecting contact for much lower n-doping levels by measuring the Hanle effect in a standard 3-terminal scheme where injection and detection are done using the same contact. The Fe/MgO spin injector was sputter deposited onto various n-doped Si bulk substrates using a variety of different substrate temperatures. The best tunnel barriers were obtained when the MgO was deposited at 70°C and annealed $in-situ$ before Fe deposition. Fits to Hanle curves using the drift-diffusion model for Si samples with n=$4x10^{18} cm^{-3}$ yield spin lifetimes τ_s = 0.28 ns up to 30 K and a spin diffusion length $L_s=\sqrt{D\tau_s}$ of 0.65 μm (the diffusion constant D is obtained from the mobility assuming degenerate statistics). We determine the dependence on n, and comment on the potential differences between SOI and bulk Si wafer transport channels. [1] T. Sasaki, et al., Appl. Phys. Exp. 2 (2009).

[1]This work was supported by ONR and core programs at NRL.

9:00AM V15.00006 Electrical spin injection and detection in Si[1]

, YONG PU, Center for Emergent Materials/Department of Physics, Ohio State University, ADRIAN SWARTZ, Department of Physics and Astronomy, University of California-Riverside, JONAS BEARDSLEY, VYDIA BHALLAMUDI, CHRIS HAMMEL, ROLAND KAWAKAMI, EZEKIEL JOHNSTON-HALPERIN, JON PELZ, Center for Emergent Materials/Department of Physics, Ohio State University — We report electrical spin injection from Fe into Si in a Fe/MgO/Si tunnel diode grown by molecular beam epitaxy. Incorporating the spin-degree of freedom into Si adds significant new functionality in a system with established utility. In addition, the use of spin as an intrinsically quantum mechanical degree of freedom may enable more speculative computing paradigms such as spin-based quantum computation. In this work, we investigate spin injection and spin detection and spin-related transport properties in Si. This work also lays the foundation for ongoing studies correlating structural, electronic and magnetic device properties with spin injection efficiency, spin transport mechanism and real-space imaging of spin transport.

[1]Funding for this research was provided by the Center for Emergent Materials at the Ohio State University, an NSF MRSEC (Award Number DMR-0820414).

9:12AM V15.00007 Spin injection into Silicon using Al_2O_3, SiO_2 and MgO tunnel barriers

, OLAF VAN T ERVE, CONNIE LI, AUBREY HANBICKI, GEORGE KIOSEOGLOU, BEREND JONKER, Naval Research Laboratory — We recently demonstrated injection of spin-polarized electrons from an Fe film into Si.[1] The tunnel barrier is the key component in achieving a large spin accumulation in the semiconductor. Here we will compare three different tunnel barriers, Al_2O_3, SiO_2 and MgO, on highly doped Si using three terminal Hanle measurements. Hanle measurements give insight in the spin-accumulation directly underneath the spin injecting contact. We will compare temperature dependence and bias dependence as well as the tunnel barrier properties such as density of interface states based on I-V and C-V measurements. We will compare spin-injection properties, such as spin lifetimes and spin injection efficiency with the oxide/Silicon interface. A spin lifetime of 120ps was obtained for 3e19 n-doped Silicon for both the Al_2O_3 and SiO_2 tunnel barrier, indicating that the spin accumulation occurs in the Si rather than in surface states. Support by ONR.

[1]B. T. Jonker et al., Nature Phys. 3, 542 (2007), O.M.J. van 't Erve et al., App. Phys. Lett. 91, 212109, (2007)

9:24AM V15.00008 Spin injection studies on thin film Fe/MgO/Si tunneling devices , JONAS BEARDSLEY, YONG PU, Ohio State University, ADRIAN SWARTZ, University of California Riverside, VIDYA BHALLAMUDI, Ohio State University, ROLAND KAWAKAMI, University of California Riverside, EZEKIEL JOHNSTON-HALPERIN, CHRIS HAMMEL, JON PELZ, Ohio State University — We report progress on the injection of spin polarized electrons into 35 nm thick Si films, using Fe/MgO injector/tunnel barrier structures grown by molecular beam epitaxy on SIMOX silicon-on-insulator substrates. The device requires heavy top-surface n-type doping of the Si film to produce a suitable tunnel barrier, accomplished by diffusion from a spin-on phosphorous-doped glass. Measurements indicate a roughly exponential doping profile with 7E20 per cubic cm at the top surface and a 2 nm decay length. Three terminal measurements showed evidence of spin injection similar to reports of Jansen et al. [1], while injection with a thinner MgO barrier shows more complicated behavior. On-going measurements and modeling will be discussed.

[1] R. Jansen et al.; Nature 462; 491 (2009) Funding for this research was provided by the Center for Emergent Materials at the Ohio State University, an NSF MRSEC (Award Number DMR-0820414).

9:36AM V15.00009 Room-temperature magnetocurrent in antiferromagnetically coupled Fe/Si/Fe[1] , RASHID GAREEV, MAXIMILIAN SCHMID, JOHANN VANCEA, CHRISTIAN BACK, University of Regensburg, REINERT SCHREIBER, DANIEL BUERGLER, CLAUS SCHNEIDER, Forschungszentrum Juelich, FRANK STROMBERG, HEIKO WENDE, University of Duisburg-Essen — Epitaxial Si-based ferromagnet/semiconductor structures demonstrate strong antiferromagnetic coupling (AFC) as well as resonant-type tunneling magnetoresistance, which vanishes at temperatures above T∼50K [1]. Magnetoresistance effects in Fe/Si/Fe close to room temperature (RT) were not established yet. By using the ballistic electron magnetomicroscopy (BEMM) techniques, with its nanometer-scaled locality [2] we observed for the first time a spin-dependent ballistic magnetotransport in AFC structures. We found that the hot-electron collector current with energies above the Fe/GaAsP Schottky barrier reflects magnetization alignment and changes from I_{cAP} ∼50fA for antiparallel alignment to I_{cP} ∼150fA for the parallel one. Thus, the magnetocurrent [(I_{cP}-I_{cAP})/ I_{cAP}]*100% is near 200 % at RT. The measured BEMM hysteresis loops match nicely with the magnetic MOKE data.
[1]. R.R. Gareev, M.Weides, R. Schreiber, U. Poppe, Appl. Phys. Letts **88**, 172105 (2006); [2]. E. Heindl, J. Vancea, C.H. Back, Phys. Rev.**B75**, 073307 (2007).

[1]This work is supported by the project DFG 9209379.

9:48AM V15.00010 Theory of spin-dependent phonon-assisted optical transitions in Si and quantifying spin polarization in Si[1] , HANAN DERY, University of Rochester — The spin polarization of conduction electrons in a direct-gap semiconductor is readily quantified by measuring the circular polarization of the recombination light luminescence. However, in silicon, owing to its indirect band-gap, such a direct connection between spin polarization and luminescence has been conspicuously absent. This missing link is established with a theory that provides concise relations between the degrees of spin polarization and measured circular polarization for each of the dominant phonon-assisted optical transitions [1]. This theory has two important applications. First, it allows one to determine in a parameter-free manner the spin polarization of electrons from the measured circular polarization of the luminescence. Second, it provides a means to extract the spin relaxation time or the spin injection efficiency across ferromagnet/silicon interfaces. In the first part of the talk, by invoking symmetry arguments, I will derive concise optical selection rules for each of the phonon-assisted optical transitions in unstrained bulk silicon. It will be shown that phonon symmetries play a key role in determining the circular polarization degrees of the various phonon-assisted luminescence peaks. In the second part, the optical selection rules will be used to analyze the polarized luminescence spectrum that is calculated by a comprehensive rigid-ion model for doped silicon. The analysis is used to elucidate results of recent spin injection experiments in silicon [2]. The effect of the (weak) spin-orbit coupling in silicon on the luminescence turns out to be unique due to the proximity of the split-off band to the heavy and light hole bands in unstrained bulk silicon (44 meV). This proximity gives rise to a fast reduction in the circular polarization degree of the luminescence in p- type silicon.

[1] P. Li and H. Dery, Phys. Rev. Lett. 105, 037204 (2010).
[2] B. T. Jonker et al., Nature Phys. 3, 542 (2007).

[1]This work is supported by AFOSR Contract No. FA9550-09-1-0493 and by NSF Contract No. ECCS-0824075.

10:24AM V15.00011 Tunability of spin lifetimes in strained silicon and germanium , JIAN-MING TANG, BRIAN T. COLLINS, University of New Hampshire, MICHAEL E. FLATTE, University of Iowa — The spin lifetimes due to electron-phonon interactions in silicon and germanium are calculated using a sp^3 tight-binding model. Despite of the strong spin-orbit interaction in germanium, the spin lifetime in germanium is only about one order of magnitude shorter than what is in silicon. Near room temperature, the spin-flip scattering is dominated by the inter-valley f processes in silicon and by the inter-valley X processes in germanium. The inter-valley scattering processes can be suppressed by shifting the valley minima with strain. We show that the spin lifetimes can be enhanced by about an order of magnitude in both materials.

10:36AM V15.00012 Theory of optical spin orientation in silicon , JINLUO CHENG, J. RIOUX, Department of Physics and Institute for Optical Sciences, University of Toronto, 60 St. George Street, Toronto, Ontario, Canada M5S 1A7, J. FABIAN, Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany, J.E. SIPE, Department of Physics and Institute for Optical Sciences, University of Toronto, 60 St. George Street, Toronto, Ontario, Canada M5S 1A7 — Despite weak spin-orbit coupling and an indirect band gap, significant optical spin orientation is possible in silicon. We show this by performing full band-structure calculations of the phonon-assisted absorption of circularly polarized light in bulk silicon. At 4 K a maximum spin polarization of 25% is found at the band edge; at room temperature the polarization is still 15%. We present the selection rules and give the contributions from the individual phonon branches, valence bands, and conduction band valleys. Dominant are the TO/LO phonon-assisted transitions from the heavy-hole to the conduction band.

10:48AM V15.00013 Spin-Dependent Phonon-Assisted Optical Transitions in Germanium , DHARA TRIVEDI, Department of Physics, University Of Rochester, PENGKE LI, Department of Electrical and Computer Engineering, University of Rochester, HANAN DERY, Department of Physics & Department of Electrical and Computer Engineering, University Of Rochester — We study the circular polarization of the photoluminescence due to phonon-assisted indirect optical transitions in Germanium. The band structure is calculated by empirical pseudopotential method with the spin-orbit interaction. Phonon modes are obtained by the adiabatic bond charge model and the L - Γ electron-phonon matrix elements are calculated within the rigid-ion approximation. We have used group theory extensively to account for all possible transitions. We quantify the circular polarization of various phonon-assisted optical transitions.

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V16 DMP GMAG: Focus Session: Magnetic Nanostructures, Exchange Coupled System

8:00AM V16.00001 Mu metal exchage bias[1] , PRIYANGA JAYATHILAKA, SCOTT CAMPBELL, CASEY MILLER — The exchange bias of the soft ferromagnet mu-metal, Ni77Fe14Cu5Mo4, with the metallic antiferromagnet Fe50Mn50 has been studied. Two series of multilayer heterostructures were grown with (111) texture induced by different buffer layer materials: Cu(300 A)/Ni77Fe14Cu5Mo4(200 or 400 A)/Fe50Mn50 (100 A)/Cu(300 A) and Ta(50 A)/Ni77Fe14Cu5Mo4(60–400 A)/Fe50Mn50(150 A); control samples were grown without Fe50Mn50. The samples have a clear unidirectional anisotropy induced by depositing in a magnetic field, the exchange bias magnitude is inversely proportional to the mu-metal thickness, and the interfacial coupling energy of 0.045 erg/cm2 agrees with previous results for FeMn antiferromagnets. While the Cu-buffered samples reveal a significant increase in coercivity and saturation field when exchange biased, the Ta-buffered samples retain the soft magnetic properties of the mu-metal simultaneously with the exchange bias. The ability to preserve soft ferromagnetic behavior in an exchange biased heterostructure may be useful for device and sensing applications.

[1]Supported by NSF ECCS

8:12AM V16.00002 Intrinsic Exchange Bias and Origin of Uncompensated Magnetization in FeF_2[1] , IGOR V. ROSHCHIN, KARIE E. BADGLEY, Texas A&M University, K.D. BELASHCHENKO, University of Nebraska-Lincoln, M. ZHERNENKOV, M.R. FITZSIMMONS, LANL, IVAN K. SCHULLER, University of California - San Diego — After more than 50 years since the discovery of Exchange Bias, its microscopic mechanism remains unknown. Several experimental findings demonstrate and many models agree that uncompensated magnetization (UM) in the antiferromagnet (AF) plays an important role in exchange bias. However, the origin of the UM is unknown. Magnetometry and polarized neutron reflectometry (PNR) measurements indicate that the UM is present even in the AF-only, (110)-FeF_2 grown on MgF_2, samples, and the PNR reveals the spatial distribution of the UM. Exchange bias in the AF-only sample is reported. Coupling of the UM to the bulk antiferromagnetic order parameter is supported by several experimental results, including high value of exchange bias field, its temperature dependence and the absence of training effect. We will discuss the origin of the UM based on general symmetry arguments.

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

8:24AM V16.00003 Tuning the Magnetic Properties in Exchange Coupled FeO/Fe_3O_4Core-Shell Nanoparticles , NATALIE FREY HULS, NIST, XIAOLIAN SUN, SHOUHENG SUN, Brown University, NIST COLLABORATION, BROWN UNIVERSITY COLLABORATION — Chemically synthesized FeO with a native oxide shell has recently received attention due to the large exchange bias effects observed in this system. The magnetic properties reported thus far have been highly dependent upon the aging affects of the system given the vulnerability of FeO to further oxidation resulting in degradation of the exchange bias effects. We report on the magnetic properties of FeO nanoparticles chemically synthesized to form several base diameters (10 nm, 20 nm, and 30 nm) which have each been annealed at various temperatures to obtain a variety of core/shell FeO/Fe_3O_4 size ratios. This controlled oxidation method has also given excellent chemical stability to the particles. XRD analysis confirms the existence of polycrystalline phases of FeO and Fe_3O_4, and magnetometry experiments reveal the existence of large exchange bias (up to 230 mT) as well as coercivity enhancements (up of 250 mT) which persist up the Néel temperature (which scales with core size). Other exchange coupling effects such as a large vertical shift in the field cooled hysteresis loops and asymmetric magnetization reversal are observed. Our results further advance the understanding of this exchange coupled system and imply that the properties can be chosen utilizing as-synthesized particle size and annealing temperatures.

8:36AM V16.00004 Tuning exchange bias in Ni/FeF_2 heterostructures using antidot arrays , XAVIER BATLLE, M. KOVYLINA, A. LABARTA, Dept. Física Fonamental, Universitat de Barcelona, 08028 Barcelona, Catalonia, Spain, R. MORALES, Basque Foundation for Science, IKERBASQUE, 48011 Bilbao, Spain, J.E. VILLEGAS, CNRS/Thales, Université Paris Sud, 91405 Orsay, France, M. EREKHINSKY, IVAN K. SCHULLER, Physics Department, University of California San Diego, La Jolla 92093 CA, USA — The transition from positive to negative exchange bias can be systematically tuned with antidot arrays artificially introduced into Ni/FeF_2 ferromagnetic (FM)/antiferromagnetic (AF) heterostructures. This is a consequence of the energy balance between the Zeeman coupling of the AF spins to the cooling field, and the AF exchange coupling at the FM/AF interface. The nanostructure plays a key role in the formation of pinned uncompensated spins in the AF: the antidot carving produces regions of locally pinned uncompensated spins throughout the antidot faces of the FeF_2 and these *non* interfacial magnetic moments favor the onset of positive exchange bias at lower cooling fields, by increasing the Zeeman energy of AF domains and favoring the alignment with the latter. Those *non* interfacial AF spins, and the pinned uncompensated interfacial AF spins responsible for the exchange bias (loop shift), align simultaneously with the cooling field since they belong to the same AF domain and become pinned below the Néel temperature.

8:48AM V16.00005 Depth Profiles of Exchange Stiffness and Anisotropy in a Spring Magnet with Intermixed Interfaces[1] , YAOHUA LIU, S.G.E. TE VELTHUIS, J.S. JIANG, Y. CHOI, S.D. BADER, Argonne National Laboratory, A.A. PARIZZI, H. AMBAYE, V. LAUTER, Oak Ridge National Laboratory — With complementary studies of Polarized Neutron Reflectometry (PNR) and micromagnetic simulations, we determined the depth profiles of the intrinsic magnetic properties in an Fe/Sm-Co spring magnet with intermixed interfaces, including saturated magnetiztion, exchange Stiffness and magnetic anisotropy. We found that intermixed region at the Fe/Sm-Co interface is about 8 nm wide, where the magnetic properties change gradually. We compared the results to a model based on a simple mixture of the Fe phase and the Sm-Co phase, as determined from the chemical depth profile using x-ray and neutron reflectivities. In the intermixed region, the saturation magnetization is slightly lower than the value estimated from the model but the exchange stiffness is higher. The magnetic anisotropy is also lower than the expected value from the model. Therefore the intermixed interface yields superior exchange coupling between the Fe and the Sm-Co layers but at the cost of total magnetization.

[1]Work supported by US-DOE, Office of Science, BES, contract No. DE-AC02-06CH11357.

9:00AM V16.00006 Geometric Structure of Magnetic Domains in CoPd/IrMn Multilayer Films[1] , RUN SU, Physics Department, University of Oregon, SUJOY ROY, Advanced Light Source, Lawrence Berkeley National Laboratory, KEOKI SEU, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, DANIEL PARKS, Physics Department, University of Oregon, JIMMY KAN, ERIC FULLERTON, Department of Electrical and Computer Engineering, University of California, San Diego, STEPHEN KEVAN, Physics Department, University of Oregon — Using coherent x-ray resonant scattering in a transmission geometry, we collected magnetic scattering signal from CoPd/IrMn exchange biased multilayer films. The incident photon energy was tuned to the Co L3 edge allowing the magnetic domain configuration in Q space to be probed. Rotational autocorrelation functions of the resulting speckle diffraction patterns manifest the local geometric character of domain structure in Q-dependent fashion. These results are compared to microscopic magnetic domain memory probed by cross correlating different patterns. The memory under two different cooling conditions, with saturating field or with zero field was investigated, as well as the dependence of memory on external parameters, such as applied magnetic field and temperature.

[1]This research used the Lawrencium computational cluster resource provided by the IT Division at the Lawrence Berkeley National Laboratory.

9:12AM V16.00007 Correlation between bias fields and magnetoresistance in CoPt biased NiFe/Ta/NiFe heterosystems , YI WANG, XI HE, TATHAGATA MUKHERJEE, Department of Physics and Astronomy, University of Nebraska-Lincoln, SARBESWAR SAHOO, Seagate Technology, MICHAEL FITZSIMMONS, Los Alamos National Laboratory, CHRISTIAN BINEK, Department of Physics and Astronomy, University of Nebraska-Lincoln — Exchange coupled magnetic hard layer/soft layer (SL) thin films show SL biasing in close analogy to exchange bias systems with antiferromagnetic pinning. Here we study CoPt(35nm)/NiFe(450nm)/Ta(d)/NiFe(450nm) heterostructures with 0.7 <d<5nm. We use alternating gradient force magnetometry to measure the overall magnetization reversal and minor loop behavior. Magnetoresistance (MR) is measured by four-point methodology and modeled using magnetization data thus confirming the assumptions of uniform rotation of the top layer and exchange spring behavior of the pinned NiFe layer. In addition, Polarized Neutron Reflectometry (PNR) provides an independent data set for magnetization depth profiles. We compare and contrast results from our magnetometry and MR technique with PNR results. The objective of this comparison is to show that single-component magnetometry in concert with MR and modeling reveals the full vector and depth profile information of the distinct magnetization reversal mechanisms. Financial support by NSF through Career, MRSEC, DOE-OBES

9:24AM V16.00008 Growth and magnetism of highly (001)-oriented $[Fe/Pt]_n/Pt$ films[1] , T.A. GEORGE, X.Z. LI, L. YUE, DAVID J. SELLMYER, University of Nebraska — Highly (001) textured non-epitaxial $L1_0$ FePt films have been fabricated on SiO_2 substrates by post-deposition annealing 11 nm magnetron sputtered multilayers of Fe and Pt with an additional overlayer of 1 nm Pt. An identical series of films was made without the thick Pt terminating layer for comparison. All films were post-deposition annealed at 600 $^\circ$C for 300 s in a rapid thermal processor and show a high degree of chemical order. The ordered films without a Pt overlayer include a mixture of (001) and randomly oriented grains. In the samples with a Pt overlayer only the $(00l)$ peaks are visible, demonstrating an enormous enhancement in the degree of (001) texture. Structural analysis reveals a decrease in surface roughness from over 2 nm to less than 1 nm, elimination of voided regions, and an increase in average grain size from 50 to 150 nm with the inclusion of a Pt overlayer. Magnetic hysteresis loops show a high squareness ratio for Pt-overlayer samples with coercivities much smaller than their no-overlayer counterparts. The effects of Fe:Pt stoichiometry and bilayer thickness are investigated along with the involved grain-growth process.

[1]This research is supported by NSF-MRSEC, DOE, and NCMN.

9:36AM V16.00009 Exchange bias and magnetic anisotropy in ultrathin iron films grown on (001) GaAs[1] , KRITSANU TIVAKORNSASITHORN, XINYU LIU, MALGORZATA DOBROWOLSKA, JACEK FURDYNA, Department of Physics, University of Notre Dame, Notre Dame, IN 46556 — Ultrathin iron films grown by MBE on GaAs substrates were studied by SQUID and by ferromagnetic resonance (FMR). Exchange bias (EB) was observed in this system at temperatures below 20 K, but disappeared at higher temperatures. The angular dependence of asymmetric hysteresis loops of the sample were understood as resulting from the coexistence of the cubic and uniaxial magnetic anisotropy fields of the Fe film and the EB field arising from a yet unidentified inter-layer between Fe and GaAs (possibly Fe2As). Magnetic anisotropy of the Fe films was investigated by FMR in a manner similar to that described by Aktas et al. [1]. By fitting the angular dependence of the FMR field we have obtained magnetic parameters of the sample, which are similar to those reported in Ref. [1]. However, the g- factor obtained from the fitting shows an unexpected anomalous increase in the low temperature range. Since this behavior occurs exactly in the range where EB appears, it is tempting to speculate that these two effects are causally related.

[1] B. Aktas et al., J. Appl. Phys. 102, 013912 (2007).

[1]Supported by NSF Grant DMR1005851.

9:48AM V16.00010 Measuring Exchange Bias in Patterned Films using Ferromagnetic Resonance , ROHAN ADUR, INHEE LEE, YURI OBUKHOV[1], The Ohio State University, CHRISTINE HAMANN, JEFFREY MCCORD[2], IFW Dresden, DENIS V. PELEKHOV, P. CHRIS HAMMEL, The Ohio State University — Exchange bias exploits the exchange interaction at the interface between a ferromagnet and an adjacent antiferromagnet to create a preferred orientation for the ferromagnet. He-ion bombardment has been used to create stripe-patterned films displaying anti-parallel exchange bias in adjacent stripes. As the width of these stripes approaches micron-size, magnetization reversal within individual stripes can be hindered by dipolar fields from magnetic charges at boundaries, making magnetometry measurements difficult to interpret. Here we report Ferromagnetic Resonance measurements of the magnitudes of the two opposing exchange bias fields perpendicular to the stripe axis, the dipolar fields experienced by neighboring stripes, and we quantify the effect of ion irradiation on the saturation magnetization of the $Ni_{81}Fe_{19}$ films.

[1]Currently at Howard University
[2]Currently at FZD Dresden

10:00AM V16.00011 Scanning Probe Ferromagnetic Resonance Imaging of Stripe Patterned Exchange Bias IrMn-NiFe Film Using Nanoscale Confined Modes , INHEE LEE, ROHAN ADUR, The Ohio State University, CHRISTINE HAMANN, IFW Dresden, YURI OBUKHOV, The Ohio State University, JEFFREY MCCORD, Forschungszentrum Dresden-Rossendorf, DENIS PELEKHOV, The Ohio State University, BERND BUCHNER, IFW Dresden, CHRIS HAMMEL, The Ohio State University — We report scanned probe Ferromagnetic Resonance (FMR) imaging of the spatially modulated internal exchange-bias field in the exchange coupled ferromagnet (FM)/antiferromagnet (AF) $Ni_{81}Fe_{19}$ /$Ir_{23}Mn_{77}$ bilayer material using Magnetic Resonance Force Microscopy (MRFM). The exchange bias is spatially modulated by ion beam irradiation into a periodic stripe pattern having 2 or 20 micron periods. Adjacent stripes have oppositely aligned exchange bias fields. Our new method of FMR imaging employs the locally confined FMR modes created by a strong, non-uniform probe tip field on the out-of-plane saturated $Ni_{81}Fe_{19}$ film. We image the spatial variation of the inhomogeneous internal field with spectroscopic precision clearly resolving two exchange bias regions. Analysis of the local magnetic properties and their transition at the boundary of two exchange bias regions will be presented. This work was supported by the U.S. Department of Energy through Grant No. DE-FG02-03ER46054.

10:12AM V16.00012 Large exchange bias after zero-field cooling from an unmagnetized state[1] , LAN WANG, Nanyang Technological University, BAOMIN WANG, Nanyang Technological Univeristy, YONG LIU, Nanyang Techological University, PENG REN, Nanyang Technological University, BIN XIA, Nanang Technological University, KAIBIN RUAN, Nanyang Technological University, JIABAO YI, National Univeristy of Singapore, JUN DING, National University of Singaore, XIAOGUANG LI, University of Science and Technology of China — Exchange bias (EB) is usually observed in systems with interface between different magnetic phases after *field cooling*. Here, we report an unexpected finding that a *large* EB can be realized in Ni-Mn-In bulk alloys after *zero-field cooling from an unmagnetized state*. We propose that the size of superparamagnetic domains in the alloys can grow up under external magnetic fields, which induces a transition from a superspin glass to a superferromagnetic (SFM) state. The SFM unidirectional anisotropy, which is the origin of EB effect, can be created at the *newly* formed SFM-antiferromgantic interface during the initial magnetizing process.

[1]Singapore National Research Foundation (RCA-08/018) and MOE Tier 2 (T207B1217).

10:24AM V16.00013 High energy product of Sm_2Co_7/FeCo nanocomposites prepared by severe plastic deformation , NARAYAN POUDYAL, CHUANBING RONG, J. PING LIU, Department of Physics, University of Texas at Arlington, Arlington, TX 76019, USA, YING ZHANG, M.J. KRAMER, Division of Materials Science and Engineering, Ames Laboratory, Iowa State University, Ames, IA 50011, USA — Nanocomposite magnets, consisting of exchange coupled hard magnetic and soft magnetic phases exhibit enhanced remanent magnetization and therefore high energy product *(BH)*$_{max}$. In addition to the high performance, nanocomposites magnets are of commercial interest because the alloys require less expensive rare-earth elements. Here, we report Sm_2Co_7+ x wt % FeCo (x = 0 to 50) nanocomposites prepared by high energy ball-milling and subsequent heat treatments. The evolution of structure and magnetic properties with soft phase fraction was systematically studied. Effect of the soft phase composition Fe_{100-X} Co_X (x = 20, 35 and 50) was also investigated. Microstructural studies by energy filter transmission electron microscopy revealed a homogeneous distribution of -Fe phase in the matrix of hard magnetic Sm-Co phase with grain size less than 20 nm after severe plastic deformation. Enhanced remanence and *(BH)* $_{max}$ (up to 17 MGOe) in the nanocomposites with 40 % of the soft phase are obtained.

10:36AM V16.00014 Microstructure refinement in $Nd_2Fe_{14}B$/(Fe,Co) nanocomposite ribbons produced by melt-spinning in a magnetic field , VUONG VAN NGUYEN, CHUANBING RONG, J. PING LIU, Department of Physics, University of Texas at Arlington, Arlington, TX 76019, USA — $Nd_2Fe_{14}B$/(Fe,Co) ribbons were prepared by melt-spinning in a magnetic field perpendicular or parallel to the wheel surface. The starting alloy $Nd_{15}Fe_{77}B_8$ was mixed with soft magnetic Fe, or Co, or $Fe_{65}Co_{35}$. The amount of the soft phases was varied from10 to 40 wt.% of the hard phase. The wheel was reconstructed to provide the surface magnetic fields in the range of 1 to 4 KG perpendicular or parallel to the wheel surface. The obtained results show that grain size in the ribbons was significantly reduced while the texture was enhanced. The mechanism remains to be fully understood, though it may be related to a change of the C-shaped diagram. The observed results suggest that a magnetic field can be used to control and optimize microstructures of nanocomposite ribbons. The effect of field strength and configuration is also discussed in details.

10:48AM V16.00015 Structure and magnetism of epitaxial NiMn single layers and Co/NiMn bilayers on $Cu_3Au(100)$[1] , WALDEMAR MACEDO, (1), WOLFGANG KUCH, (2), PEDRO GASTELOIS, (1), JORGE MIGUEL[2], (2), MAXIMILIANO MARTINS, (1), YAQOOB KHAN, (2), 1- NANOTECNOLOGIA, CENTRO DESENV. TECNOL. NUCLEAR, BELO HORIZONTE, MG, BRAZIL TEAM, 2- EXPERIMENTALPHYSIK, FREIE UNIV. BERLIN, GERMANY TEAM — The structure of single-crystalline NixMn100-x (NiMn) ultrathin films on Cu3Au(100) and also the magnetic properties of Co films on the NiMn/Cu3Au(100) films have been investigated by multiple techniques. For $10 \leq x \leq 77$, our results revealed good epitaxial, layer-by-layer growth at a substrate temperature of 300 K for all NiMn films with near equiatomic composition. The results indicate a face-centered tetragonal (fct) structure for NiMn, as expected for the L1o phase, and with the c-axis along the film normal. For the Co/NiMn bilayers, MOKE hysteresis loops show a thickness independent coercivity, suggesting no magnetic coupling at the Co/NiMn interface. Although the structural results indicate the formation of ftc NiMn in the equiatomic concentration range, we have no indication of antiferromagnetism for NiMn on Cu3Au(100) at room temperature. This is contrary to the observations for Co/NiMn on Cu(100).

[1]Support: CNPq and FAPEMIG (Brazil), DFG (Germany).
[2]Present address: Diamond Light Source, UK

Thursday, March 24, 2011 8:00AM - 10:48AM –
Session V17 DMP GMAG: Focus Session: Bulk Properties of Complex Oxides - 5d Oxides D174

8:00AM V17.00001 Spin-Orbit Interaction Rediscovered in Transition Metal Oxides[1] , GANG CAO, University of Kentucky — The 5d-transition metal oxides are a class of novel materials that exhibit nearly every collective state known for solids. It is commonly expected that iridium oxides should be more metallic and less magnetic than their 3$d$and 4f counterparts due to the extended nature of the 5$d$orbitals. In marked contrast, many iridates are magnetic insulators that exhibit a large array of phenomena seldom or never seen in other materials. We review the anomalous physical properties of several iridates and address potential underlying mechanisms, which include strong orbital magnetism, the $J_{eff} = 1/2$ insulating state, and spin-orbit coupling; the latter strongly competes with other interactions to create an unusual balance between relevant degrees of freedom in this class of materials.

[1]This work was supported by NSF through grants DMR-0856234 and EPS-0814194.

8:36AM V17.00002 Resonant inelastic x-ray scattering study of charge ordering in CuIr2S4 , HLYNUR GRETARSSON, University of Toronto, Canada, JUNG-HO KIM, DIEGO CASA, THOMAS GOG, Argonne National Laboratory, USA, SANG-WOOK CHEONG, Rutgers University, USA, YOUNG-JUNE KIM, University of Toronto, Canada — We present Ir L_3-edge resonant inelastic x-ray scattering (RIXS) spectra and resonant x-ray emission spectra (RXES) on the thiospinel, $CuIr_2S_4$, which has been attracting much interest due to intriguing metal-insulator transitions. At room temperature $CuIr_2S_4$ is metallic, but goes through a metal insulator transition at $T_{MI} \sim 226$ K due to the formation of charge order (CO) of Ir^{3+} and Ir^{4+} together with spin dimerization between Ir^{4+} ions. By exposing the sample to x-ray below T = 50 K, the crystal symmetry goes from triclinic to tetragonal, accompanied by reduced resistivity. The RIXS signal was dominated by a broad and strong feature around 3 eV, arising from t_{2g} to e_g transition, but we were able to observe a clear signature of opening of the insulating gap across the metal-insulator transition. In addition, we also found that this gap is partially filled in the irradiation-induced phase. The emission spectra reveals the existence of an excited Ir-5d t_{2g} state, which is hidden in the Ir L_3-edge XAS of $CuIr_2S_4$. The result indicates that the electronic reconstruction that takes place in the irradiation-induced phase comes from the Ir^{3+} while the Ir^{4+} dimers are unchanged.

8:48AM V17.00003 Electron-doped $Sr_2IrO_{4-\delta}$ $(0 \leq \delta \leq 0.04)$: Evolution of a disordered $J_{eff} = 1/2$ Mott insulator into an exotic metallic state[1] , O.B. KORNETA, T.F. QI, S. CHIKARA, L.E. DE LONG, G. CAO, Department of Physics and Astronomy, University of Kentucky, S. PARKIN, Department of Chemistry, University of Kentucky, P. SCHLOTTMANN, Department of Physics, Florida State University — Stoichiometric Sr_2IrO_4 is a ferromagnetic $J_{eff} = 1/2$ Mott insulator driven by strong spin-orbit coupling. Introduction of very dilute oxygen vacancies into single-crystal $Sr_2IrO_{4-\delta}$ ($\delta < 0.04$) leads to significant changes in lattice parameters and drives a number of intriguing phenomena such as insulator-to-metal transition at $T_{MI} \approx 105K$, anomalous non-Ohmic behavior and an abrupt current-induced transition in the resistivity. Highly-anisotropic resistivity of the samples continues to decrease by several orders of magnitude below T_{MI} without saturation to a residual limit at the lowest temperature studied $T = 1.8K$. The low-temperature metallic state exhibits two distinct regimes (separated at $T \approx 52K$) of switching in the non-linear $I - V$ characteristics. The novel behavior illustrates an exotic ground state and constitutes a new paradigm for device structures.

[1]This work was supported by NSF through grants DMR-0552267, DMR-0856234 (GC) and EPS-0814194 (GC, LED), and by DoE through grants DE-FG02-97ER45653 (LED) and DE-FG02-98ER45707 (PS).

9:00AM V17.00004 Magnetic ordering in Sr_2IrO_4 from first principles , SABINA RUIZ-CHAVARRIA, GREGORIO RUIZ-CHAVARRIA, PABLO DE LA MORA, Facultad de Ciencias, UNAM, CARLOS COSIO-CASTANEDA, GUSTAVO TAVIZON, Facultad de Quimica, UNAM — Sr_2IrO_4 is a layered compound with IrO_2 planes, separated by two SrO planes. Experimentally Sr_2IrO_4 shows weak ferromagnetism. This behavior can be assigned either as band magnetism or canted antiferromagnetic ordering. The latter has been confirmed by Arpes. With DFT calculations (using the WIEN2k package and Quantum Expresso) we show that the antiferromagnetic ordering is more stable than the ferromagnetic one, and due to the Dzyaloshinskii-Moriya rules there is a possibility of canted magnetic ordering.

9:12AM V17.00005 Effect of spin-orbit coupling on the band structure, magnetic ground states and low energy excitations of double perovskites[1] , ONUR ERTEN, ANAMITRA MUKHERJEE, MOHIT RANDERIA, NANDINI TRIVEDI, PATRICK WOODWARD, The Ohio State University — We investigate a model for double perovskites $A_2BB'O_6$ that describes the coupling of local moments on the B site to itinerant electrons contributed by the B′ sites. To model materials like Sr_2CrOsO_6 we examine the role of spin-orbit coupling on the the B′ site, which cannot be ignored because of the large Z of Os. First, we present $T = 0$ results for the net moment in the ferrimagnetic state. We show that direct B′-B′ hopping plays just as important role as the spin orbit coupling in determining the ordered moment. We use our model Hamiltonian approach to discuss the question of metallic versus insulating ground states, by including the effects of Coulomb U on the spin-orbit split electronic structure. Finally, we investigate the low energy excitations of this model to understand the origin of the experimentally observed nonmonotonic behavior of magnetization as a function of temperature.

[1]Supported by the NSF-MRSEC grant DMR-0820414.

9:24AM V17.00006 Magnetic and structural properties of Sr2CrReO6 epitaxial films fabricated by ultra-high vacuum sputtering[1] , A.J. HAUSER, B. PETERS, J. SOLIZ, R.E. WILLIAMS, M. DIXIT, H.L. FRASER, P.M. WOODWARD, F.Y. YANG, The Ohio State University — Sr2CrReO6, a double-perovskite half-metallic ferromagnet, has attracted much attention due to its high Tc of 620 K. However, balancing the stoichiometry and ordering of a quaternary oxide is no trivial matter. We have deposited pure-phase Sr2CrReO6 epitaxial films on SrTiO3 substrates by ultrahigh vacuum off-axis magnetron sputtering with precise control of the oxygen partial pressure and in-situ monitoring by high-pressure residual gas analyzer. The films exhibit saturation magnetization at T = 5K approaching 0.9 Bohr magnetons per formula unit and Tc close to 600 K. X-ray diffractometry spectra demonstrate epitaxy and phase purity with a rocking curve FWHM of 0.012 degrees. Laue oscillations give evidence of exceptionally smooth surface and interface as well as precise film thickness determination. Finally, direct observation of the films by HAADF STEM show nearly defect free films with double-perovskite ordering. We will discuss the effects of stoichiometry, growth pressure and oxygen content on sample properties.

[1]Funding for this research was provided by the Center for Emergent Materials at The Ohio State University, an NSF MRSEC (Award Number DMR-0820414).

9:36AM V17.00007 Electron doped CrO_2: An unsual example of a charge ordered ferromagnet , PRIYA MAHADEVAN, ABHINAV KUMAR, S.N.Bose National Centre for Basic Sciences, DEBRAJ CHOUDHURY, D.D. SARMA, Solid State and Structural Chemistry Unit, Indian Institute of Science — Usually metallicity accompanies ferromagnetism. $K_2Cr_8O_{16}$ is one of the less common examples of magnetic materials, exhibiting ferromagnetism in the insulating state [1]. Analyzing the electronic and magnetic properties within first principle electronic structure calculations, we find [2] that K acts like a donor. The doped electrons associated with the introduction of K in the lattice, induces a charge ordered and insulating ground state and interestingly also introduces a ferromagnetic coupling between the Cr ions. The primary considerations driving the charge ordering are found to be electrostatic ones with the charge being localized on two Cr atoms that minimize the electrostatic energy. The structural distortion that accompanies the ordering, generates a pathway for the electron localized on one site to hop on to the neighboring sites, a process more favorable in the ferromagnetic case, thus, giving rise to a rare example of a charge-order driven ferromagnetic insulator.

[1] Kunihiro Hasegawa *et al.*, Phys. Rev. Lett. **103**, 146403(2009).
[2] Priya Mahadevan, Abhinav Kumar, Debraj Choudhury and D.D. Sarma, Phys. Rev. Lett **104**, 256401 (2010).

9:48AM V17.00008 Ab initio study of the anti-ferromagnetic, non-collinear CuB_2O_4 Crystal[1] , YIING-REI CHEN, Department of Physics, National Taiwan Normal University, Taipei, Taiwan 116, P.-R. LEE, J.-Y. LIN, Institute of Physics, National Chiao Tung University, Hsinchu, Taiwan 300, J.-M. CHEN, National Synchrotron Radiation Research Center, Hsinchu, Taiwan 300, A.N. VASILIEV, Department of Low Temperature Physics, Moscow State University, Moscow 119992, Russia — The spiky features in the crystal absorption spectrum, and the distinct differences in the directional oxygen K-edge absorption spectroscopy of the non-collinear anti-ferromagnetic, incommensurate CuB_2O_4, had led us to this LDA+U study of the crystal, although in the commensurate phase, due to the instrumental limitation. The calculated band structure matches the spiky features in the absorption spectrum, while the orbital analyzed DOS data explain the differences in the directional oxygen K-edge absorption spectroscopy. The two groups of dispersion-less bands, immediately above the gap, come from different groups of plaquettes, of Cu(A) and Cu(B), and are responsible for the spiky features observed experimentally.

[1]This work is supported by NSC grant No.99-2112-M-003 -012-MY2.

10:00AM V17.00009 Doping Rules in A_2BO_4 Spinel Oxides , ALEX ZUNGER, T. PAUDEL, V. STEVANOVIC, S. LANY, Natl. Renewable Energy Lab., CO — Many of the physical phenomena surrounding Complex Oxide involve the creation and annihilation of charge carriers by cross –substitution of atoms or by the formation of vacancies and interstitials. We have used the machinery of First-Principles defect calculation, developed and tested over the years on semiconductors (where experimental data needed to test DFT corrections is rather clear), applying it to a large number of oxides, initially from the Spinel family. We calculate defect formation energies as a function of temperature and oxygen partial pressure, as well as the concentration of donors and acceptors and the ensuing free carriers. A number of regularities emerge. (i) Oxygen vacancies are not a viable source of electrons and cation vacancies are (usually) not a viable source of holes. (ii) Instead, cation-anti-sites (A-on-B donor and B-on-A acceptors) tend to form in significant numbers and release carriers. (iii) For the group of A3+ and B2+ spinels we find four "doping classes" (a) both donor and acceptor are in the gap (Al_2MgO_4) (b) Only acceptor is in the gap (Co_2ZnO_4) (c) only donor in the gap and (d) none in the gap. Simple regularities can be used as first-order rules to guess electrical behavior from composition. This work was supported through the Center for Inverse Design, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

10:12AM V17.00010 Magnetoelectricity and magnetostriction due to the rare-earth moment in $TmAl_3(BO_3)_4$, RAJIT CHAUDHURY, Department of Physics and TcSUH, University of Houston, Houston,TX 77204-5002, B. LORENZ, Y.Y. SUN, C.W. CHU, Department of Physics and TcSUH, University of Houston, Houston,TX 77204-5002, L. N. BEZMATERNYKH, V.L. TEMEROV, Institute of Physics, Siberian Division, Russian Academy of Sciences, Krasnoyarsk 660036, Russia — We investigated the magnetic, magnetostriction and magnetoelectric properties of d-electron free rare-earth aluminum borate $TmAl_3(BO_3)_4$ between room temperature and 2 K. The magnetoelectric polarization along the 'a' and 'c' directions reaches up to 300 μ C/m^2 at 70 kOe with the field is applied along the 'a' axis. 'c' axis magnetic field does not show any significant effect, which correlates with the fact that χ_a changed very rapidly compared to χ_c. We find that the polarization is proportional to the magnetostriction. The result of this investigation prove the existence of a significant coupling between the rare-earth magnetic moment and the lattice in $RAl_3(BO_3)_4$ compounds (R=rare earth). This compound shows that the rare-earth moment is sufficient enough to generate a large magnetoelectric effect. This is comparatively a simpler system to study and understand the origin of magnetoelectric effect.

10:24AM V17.00011 On the Pairing Instability in Rutile MO_2 , L. ANDREA SALGUERO, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — The metal-dioxide family of compounds such as TiO_2, SnO_2, VO_2, NbO_2, and WO_2 have been of much recent interest for reasons as diverse as understanding novel correlated electron physics to designing new photo/electro-catalysis. All can be thought of as forming in a prototypical tetragonal "rutile" structure, yet members with unpaired d^1 and d^2 electrons undergo a structural phase transition to a monoclinic, "distorted rutile," structure. In some cases this metal pairing transition accompanies a metal to insulator transition, the precise role, however, is still not clear. Here we present a comparative first-principles study of the lattice instabilities in d^1 and d^2 MO_2 rutile, paying particular attention to the d^2 system WO_2, which remains metallic even in the distorted phase. We calculate the phonon dispersion in the tetragonal prototypical structure. Using unstable high symmetry modes as a guide, we calculate the energy surface around the high-symmetry structure and perform full structural relaxations in the distorted ground states. We elucidate the interplay between the electronic structure and the pairing transition and discuss the possibility of controlling it with strain.

10:36AM V17.00012 Relativistic effect determines the oxidation states: a study of Rh and Ir oxides by first principles methods , MAOSHENG MIAO, Materials Research Lab, University of California Santa Barbara, RAM SESHADRI, Materials Department & Department of Chemistry and Biochemistry, University of California Santa Barbara — The relativistic effect becomes significant on determining the structure and properties of $4d$ and $5d$ transition-metal compounds. It is found in some iridates that the relativistic effect, mainly contributed as spin-orbit interactions, can enhance the otherwise weak correlation of $5d$ electrons and cause an unusual Mott transition. Utilizing such effects in creating new phase such as topological insulator has grown into a hot spot in the frontier of functional oxide research. However, the relativistic effects on orbital energies, although important on determining the structure, has not been systematically studied. The general trend of the oxidation states of transition metals in the same group is to decrease with increasing atomic number. However, in contrast to this trend, Ir tends to form IrO_2 (4+) whereas Rh forms both Rh_2O_3 (3+) and RhO_2. Using relativistic and non-relativistic first principles calculations, we demonstrate that the unusually high oxidation state of Ir and the high stability of IrO_2 is caused by relativistic effect. Because relativity contracts the s and p orbitals, it repels Ir $5d$ electrons outwards and increases their energies. As a consequence, Ir tends to be oxidized to 4+ state and forms IrO_2.

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V18 GMAG DMP: Focus Session: Low D/Frustrated Magnetism - Spin Ice, et al. D172

8:00AM V18.00001 ABSTRACT WITHDRAWN –

8:12AM V18.00002 Magneto-optical Kerr Effect Studies of Artificial Frustrated Magnets , K.K. KOHLI, A.L. BALK, J. LI, S. ZHANG, P. LAMMERT, V.H. CRESPI, P. SCHIFFER, N. SAMARTH, Pennsylvania State University — We use the magneto-optical Kerr effect (MOKE) to study the collective magnetic behavior of geometrically frustrated arrays of single-domain ferromagnetic islands. By varying the island spacing, lattice geometry and the orientation relative to the magnetic field, we probe the properties of the arrays via MOKE measurements of the net moment of the arrays. We study the influence of local geometry and frustration on the collective magnetization reversal process, using the switching field as a measure. Further, angle-resolved MOKE measurements probe the influence of individual island shape anisotropy on the collective anisotropy of interacting arrays. Finally, we present preliminary measurements in an oscillating magnetic field. The results are compared to the results of micromagnetic simulation. We thank M. Ericson and C. Leighton for sample preparation. This research was supported by the US Dept. of Energy.

8:24AM V18.00003 Measuring Disorder in Artificial Kagome Ice , STEPHEN DAUNHEIMER, JOHN CUMINGS, Dept. of Materials Science & Engineering, University of Maryland — Artificial spin ice is proving to be a valuable tool in understanding magnetic interactions on the nanoscale. It can directly show the interactions responsible for geometric frustration, and different geometries have been used to model real pyrochlore spin ice compounds and other lattices. The strength in the approach lies in the ability of a synthetic material, fabricated from macroscopic artificial "atoms," to mimic real materials, where atoms are essentially identical with low disorder from lattice site to lattice site. However, in artificial spin ice materials there can be substantial variation among the artificial atoms in relevant quantities such as coercive field, with some systems showing standard deviations as high as 20%. By carefully studying the reversal process of artificial kagome ice along specific crystallographic directions, we can directly measure the distribution of coercivities of the individual nanoscale magnets. By using a lattice of connected magnets fabricated from Ni80Fe20, we find that the coercivity distribution can have a deviation of less than 5%. These narrow deviations should allow the observation of behavior that mimics more closely what would be expected in real spin ice materials.

8:36AM V18.00004 Dynamics of magnetization in artificial spin ice on kagome[1] , OLGA PETROVA, YICHEN SHEN, Johns Hopkins University, PAULA MELLADO, Harvard University, OLEG TCHERNYSHYOV, Johns Hopkins University — We model magnetization dynamics in artificial spin ice on kagome under an applied magnetic field. Magnetization reversal is mediated by domain walls carrying two units of magnetic charge emitted from and absorbed by lattice junctions and propagating along the wires. The Coulomb interaction between magnetic charges induces avalanches in magnetization reversal. Distributions of avalanche lengths for various angles between the initial magnetization and the applied magnetic field were considered. We used a Gaussian distribution in the magnitude of the links' critical fields to mimic disorder in a real system [1]. An asymmetric distribution of topological defects at a wire junction gives rise to an offset angle α in the reversal field $H(\theta) = H_c/\cos(\theta + \alpha)$ where θ is the angle between the link and the applied magnetic field [2]. The model reproduces the salient features of magnetization reversal curves observed experimentally.

[1] Y. Qi, T. Brintlinger, and J. Cumings, Phys. Rev. B **77,** 094418 (2008).
[2] P. Mellado, O. Petrova, Y. Shen, and O. Tchernyshyov, Phys. Rev. Lett. **105,** 187206 (2010).

[1]This work was supported in part by the NSF Grant DMR-0520491.

8:48AM V18.00005 Disorder and field-induced dynamics in artificial spin ice , ZOE BUDRIKIS, The University of Western Australia, Perth, Australia, PAOLO POLITI, Instituto dei Sistemi Complessi CNR, Sesto Fiorentino, Italy, ROBERT STAMPS, The University of Western Australia, Perth, Australia — Artificial spin ices are athermal systems for which dynamics are induced by a time varying applied field. The field induced dynamics have received a lot of attention, both experimental and theoretical (see, e.g., [1,2]), but these studies have not dealt explicitly with the effects of disorder. We show, through numerical simulations and studies of the phase space of the system, that disorder in fact has a strong and fundamental effect on the field-induced dynamics. This highlights the fact that an understanding of the dynamics of artificial spin ice must take into account both the sequence of applied fields and the spin ice lattice.

[1] X. Ke, J. Li, C. Nisoli, P. E. Lammert, W. McConville, R. F. Wang, V. H. Crespi, and P. Schiffer, Phys. Rev. Lett. 101, 037205 (2008).
[2] Z. Budrikis, P. Politi, and R. L. Stamps, Phys. Rev. Lett. 105, 017201 (2010).

9:00AM V18.00006 Control of Ground State Order in Artificial Square Ice , JASON MORGAN, University of Leeds, AARON STEIN, CFN, BNL, SEAN LANGRIDGE, ISIS, RAL, CHRIS MARROWS, University of Leeds — Anisotropy in nanomagnet arrays can be tailored to enforce geometrical frustration, so that analogs of spin-ice materials can be fabricated [1-2]. We have studied artificial square ice, which consists of interlinked vertices of four Ising moments. Previously, energy minimisation via ac demagnetization has received significant attention, however, the long-range ordered ground state (GS) is inaccessible via this method. Furthermore, equilibriation is disallowed in the athermal limit so far explored. We show it is possible to realise GS order in as-prepared arrays, fabricated via electron beam lithography and evaporation, due to early-growth thermalization [3]. Monopole and string-like excitations from the GS are seen to be Boltzmann factor-weighted. Monopole propagation and interactions can be inferred within an energy band structure. Lattice spacing and buffer material allow control of ordering.

[1] Wang et al., Nature (2006), **439**, 303-306
[2] Harris et al., PRL (1997), **79**, 2554-2557
[3] Morgan et al., Nature Phys. (at press)

9:12AM V18.00007 Monopole Dynamics in Spin Ice , CLAUDIO CASTELNOVO, Royal Holloway University of London — The last couple of years have witnessed intense interest in spin ice materials due to the unique nature of its low energy excitations, which take the form of emergent magnetic monopoles. Through combined theoretical and experimental work, it has become increasingly apparent that an effective description of these excitations in terms of free, Coulomb interacting point-like quasiparticles is essential to develop an understanding of the thermodynamic properties of these materials beyond numerical simulations. On the other hand, we are only just beginning to unravel the repercussions of such exotic excitations on the dynamics of spin ice, in relation for instance to how the system relaxes when driven out of equilibrium, or in relation to thermal transport experiments. In this talk we review some of the latest theoretical and experimental results on the out of equilibrium properties of spin ice materials, ranging from thermal and field quenches [Castelnovo, Moessner, & Sondhi, PRL 104, 107201 (2010) and ongoing work] to thermal runaways in response to a varying magnetic field [Slobinsky *et al.*, arXiv:1010.4143v1]. In particular, we discuss how these phenomena can be understood as consequences of the specific nature of the low energy excitations.

9:48AM V18.00008 Magnetic Monopoles in Matter: An Analytic Theory , BERNARD KAAS, University of Twente — Transport theory is presented which, starting from the microscopic field equations, incorporates the magnetic monopole physics occurring in materials such as spin ice. Hall effect, Landau levels, and thermopower are calculated for magnetic charges. Magnetic charge currents in elementary lattices are shown to exist even in the absence of geometrical frustration.

10:00AM V18.00009 Theoretical and computational models of emergent magnetic monopoles and Dirac strings in kagome spin-ice , REMO V. HUGLI, HANS-BENJAMIN BRAUN, GERARD DUFF, University College Dublin, CONDENSED MATTER THEORY, UCD TEAM, MAGNETIC NANOSTRUCTURES, PAUL SCHERRER INSTIUTE, SWITZERLAND TEAM — Magnetic monopoles and their associated Dirac strings have recently been experimentally observed as emergent quasiparticles in frustrated magnetic spin-ice systems. Detection of reciprocal signatures of monopoles were reported for 3D pyrochlore systems, and subsequently, direct real-space observations of monopoles and their associated Dirac strings were made in 2D artificial kagome lattices. In contrast to conventional domain growth, the magnetization process in these spin ice systems proceeds through nucleation and avalanche-type propagation of overturned dipoles - physical versions of a Dirac string. The 1D nature of these avalanches in a 2D system provides an example of dimensional reduction through frustration. We establish a theoretical model and perform Monte Carlo simulations which faithfully reproduce the observed hysteresis, string-avalanche statistics and monopole densities.

10:12AM V18.00010 Hunting a [111] magnetization plateau to test the quantum spin ice model in Tb2Ti2O7 , PETER BAKER, ISIS Facility, STFC Rutherford Appleton Laboratory, Didcot OX11 0QX, United Kingdom, MARIA MATTHEWS, Department of Physics and Materials Research Institute, Pennsylvania State University, University Park, Pennsylvania 16802, USA, SEAN GIBLIN, ISIS Facility, STFC Rutherford Appleton Laboratory, Didcot OX11 0QX, United Kingdom, PETER SCHIFFER, Department of Physics and Materials Research Institute, Pennsylvania State University, University Park, Pennsylvania 16802, USA, CHRISTOPHER BAINES, Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institute, Villigen CH-5232, Switzerland, DHARMALINGHAM PRABHAKARAN, Oxford University Department of Physics, Clarendon Laboratory, Parks Road, Oxford OX1 3PU, United Kingdom — The pyrochlore magnet Tb2Ti2O7 may be described by a quantum spin ice model. This model predicts a magnetization plateau will occur for weak fields applied along the [111] axis at low-temperature. We have carried out muon-spin relaxation measurements to test this hypothesis. Features are observed at 15 and 65mT, agreeing with the predicted boundaries of the magnetization plateau. In the intermediate region the field dependence of the muon relaxation rate suggests a constant distribution of local magnetic fields of 10mT, and a constant fluctuation time of 20ns. ac susceptibility measurements are being carried out to investigate the bulk response on a longer timescale.

10:24AM V18.00011 Creation and Measurement of Magnetic Charge Currents in Spin Ice , SEAN GIBLIN, Rutherford Appleton Lab, UK, STEVEN BRAMWELL, Uuniveristy College London, UK, PETER HOLDSWORTH, University of Lyon, France, PRABHAKARAN DHARMALINGAM, University of Oxford, UK, IAN TERRY, University of Durham, UK — The recent discovery of magnetic charge in spin ice raises the question of whether long-lived currents of magnetic "monopoles" can be created and manipulated by applying magnetic fields. Here we show that they can; by applying a magnetic field pulse to a $Dy_2Ti_2O_7$ spin ice crystal at 0.36 Kelvin, we create a relaxing magnetic current that lasts for several minutes. We measure the current by means of the electromotive force it induces in a solenoid coupled to a susceptometer and quantitatively describe it using a chemical kinetic model of point-like charges obeying the Onsager-Wien mechanism of carrier dissociation and recombination.

10:36AM V18.00012 d-wave Metal phase of itinerant electrons with ring exchange on a 2-leg ladder , M.S. BLOCK, Dept. of Physics, UCSB, H.-C. JIANG, Microsoft Research, Station Q, UCSB, R.V. MISHMASH, Dept. of Physics, UCSB, D.N. SHENG, Dept. of Physics and Astronomy, CSU, Northridge, O.I. MOTRUNICH, Dept. of Physics, Caltech, M.P.A. FISHER, Dept. of Physics, UCSB — I will present recent results in the search for theoretical insights into non-Fermi liquid phases in two dimensions. In particular, we propose a novel conducting phase for itinerant electrons on the square lattice with strong d-wave correlations (i.e. a "d-wave metal"; see [1] for the bosonic analog of this phase) and a candidate Hamiltonian (hopping plus four-site electron ring exchange), which we examined in search of this phase (at $T = 0$) over some portion of the phase diagram. For numerical tractability, we specialize to the 2-leg ladder and study this model using variational Monte Carlo (VMC) and the density matrix renormalization group (DMRG). For the VMC, we construct trial wavefunctions corresponding to a particular slave particle decomposition of the electrons and consistent with the properties of the proposed d-wave metal as well as for the "normal" Fermi liquid phase to map out a VMC phase diagram for the candidate Hamiltonian. Meanwhile, DMRG is employed as a quasi-exact probe of this Hamiltonian and the successes and failures of the trial wavefunctions, relative to the unbiased DMRG results, will be presented. [1] O. I. Motrunich and M. P. A. Fisher, Phys. Rev. B, **75**, 235116 (2007).

10:48AM V18.00013 Entanglement Hamiltonians for quantum spin chains[1] , RONNY THOMALE, Princeton University, STEPHAN RACHEL, Yale University, DANIEL AROVAS, UC San Diego, B. ANDREI BERNEVIG, Princeton University — We report on our analysis of entanglement phenomena in gapped and gapless quantum spin chains. In particular we discuss criteria of correspondence between entanglement spectra and Hamiltonian spectra with respect to symmetries, spectral gaps, and eigenstate properties. We find that the structure of the entanglement Hamiltonian associated with the ground state is helpful to discover various spectral properties of the full system.

[1]RT acknowledges support from a Feodor Lynen Fellowship of the Humboldt Foundation.

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V19 GMAG: Focus Session: Spin Transport & Magnetization Dynamics in Metals VIII

D170

8:00AM V19.00001 ABSTRACT WITHDRAWN –

8:36AM V19.00002 Ferromagnetic resonance studies of CoFeB-MgO[1] , ERIK SHIPTON, UC San Diego, KEN LEE, Qualcomm Corporation, JONATHON SAPAN, JIMMY KAN, KEITH CHAN, UC San Diego, ERIC FULLERTON — There has been much interest in ferromagnetic magnetic tunnel junctions (MTJs) as a potential candidate for spin transfer torque memories. Many parameters are important in order to optimize the spin transfer torque effect to minimize the critical switching current density (J_c) without compromising an energy barrier (E_B) between stable states. CoFeB/MgO systems have many desirable properties including high spin polarization and, thereby high tunnel magnetoresistance. Recently, Ikeda et al. reported that Fe-rich CoFeB/MgO MTJs can induce perpendicular anisotropy that is strong enough to overcome the in-plane shape anisotropy, demonstrating CoFeB-based perpendicular MTJs [1]. In this work, we have performed FMR studies as a function of alloy composition, layer thickness, pre and post annealing of CoFeB/MgO systems. Coplanar waveguide method VNA FMR experiments were performed [2]. From the FMR resonance frequency and linewidth we were able to extract the Gilbert damping as well as the effective magnetization. Experimental details as well as results will be presented.

[1] S. Ikeda et al, *Nature Materials* **9**, 721 - 724 (2010)
[2] J.M. Beaujour et al, Eur. Phys. J. B **59**, 475–483 (2007)

[1]This research was partially supported by NSF award # DMR-1008654 and DOE-BES Award # DE-SC0003678.

8:48AM V19.00003 Energy distributions of defects causing barrier-resistance noise in CoFeB/MgO/CoFeB tunnel junctions[1] , RYAN STEARRETT, XIAOMING KOU, JOHN XIAO, ED NOWAK, University of Delaware — Magnetic tunnel junction devices, such as field sensors, are well known to exhibit low frequency resistance noise having a $1/f$ spectrum. This noise has its origins in a combination of electrical and magnetic mechanisms. Previously, we have shown that the resistance noise can be reduced significantly through thermal annealing. Here, we report on the energy distribution of the defects causing tunnel-barrier-resistance noise. The distributions are determined from a Dutta-Horn model for thermally activated charge trapping and detrapping kinetics. We also discuss how the distribution changes as a function of annealing time and its relation to the current-voltage characteristics and the voltage bias dependence of the $1/f$noise.

[1]Supported by DOE under Award No. DE-FG02-07ER46374.

9:00AM V19.00004 Ultrafast Switching in Magnetic Tunnel Junction based Orthogonal Spin Transfer Devices , HUANLONG LIU, DANIEL BEDAU, DIRK BACKES, JORDAN KATINE, JÜRGEN LANGER, ANDREW KENT, NEW YORK UNIVERSITY, NEW YORK, NY 10003 USA TEAM, HITACHI-GST, SAN JOSE, CALIFORNIA 95135 USA TEAM, SINGULUS, 63796 KAHL AM MAIN, GERMANY TEAM — Orthogonal spin-transfer magnetic random access memory (OST-MRAM) uses a spin-polarizing layer magnetized perpendicularly to the free layer to achieve large spin-transfer torques and ultrafast energy efficient switching. We have fabricated and studied OST-MRAM devices that incorporate a perpendicularly magnetized polarizer and a magnetic tunnel junction, which consists of an in-plane magnetized free layer and synthetic antiferromagnetic reference layer. A switching probability of 100% is observed for 500 ps pulses, requiring an energy of 250 fJ. The fast switching process indicates there is no incubation delay of several nanoseconds as observed in conventional collinear magnetized devices. Due to the perpendicular polarizer switching is possible for both pulse polarities. There is also evidence for precessional switching in the non-monotonic dependence of the switching probability versus pulse amplitude. This work was supported by Spin Transfer Technologies.

9:12AM V19.00005 The effect of annealing on the spin-transfer torques of MgO MTJ nanopillars , YUN LI, HSIN-WEI TSENG, PINSHANE HUANG, JOHN READ, DAN RALPH, ROBERT BUHRMAN, Cornell University, Ithaca NY 14853 — Thermal annealing is essential for enhancing the tunneling magnetoresistane (TMR) of magnetic tunnel junctions, and many studies have focused on the effect of annealing on MTJ chemical, structural, and electrical transport properties. Here, we report the magnetic, electronic properties and the in-plane and field-like spin-transfer torques (STT) in both as-grown and post-annealed FeCoB/MgO/FeCoB MTJs nanopillars. We find that the 350 $^\circ$C vacuum annealing breaks the symmetry of the bias dependence of the TMR, conductivity, and switching phase diagram (SPD). Moreover STT-FMR measurements indicate that annealing substantially increases the in-plane torque asymmetry with bias voltage direction, as well as affecting the field-like torque magnitude, with the latter indicating a very significant enhancement of interlayer exchange coupling across the barrier. This STT change is consistent with the change in chemical composition and structural coherency of the MTJ interfaces and electrodes, indicated by XRD and analytical STEM analyzes.

9:24AM V19.00006 Bias voltage dependence of the total magnetic field in CoFeB magnetic tunnel junctions[1] , M.D. RIEMER, NYU/IBM Research, J.Z. SUN, IBM Research, A.D. KENT, NYU — We report experimental thermal-noise spectrum-based ferromagnetic resonance (T-FMR) measurements on CoFeB magnetic tunnel junctions in magnetic fields perpendicular to the film plane. The junctions tested have lateral sizes of 45×80 nm^2. In a simple model a dc junction bias voltage should affect both the slope and the intercept of the T-FMR frequency's dependence on applied magnetic field. The intercept would vary linearly with changes in bias voltage due to an electric field-induced change in uniaxial anisotropy [1]. The slope would have a quadratic dependence on changes in bias voltage based on the existence of a perpendicular spin-torque as discussed by Sankey *et al.* [2]. In this experiment we attempt to de-construct the contribution from these two mechanisms. This is done by a careful analysis of the magnetic field dependence of the T-FMR spectra [3].

[1] Suzuki et al, Appl. Phys. Lett. **96**, 022506 (2010).
[2] Sankey et al, Nature Physics **4**, 67 (2008).
[3] Mascaro et al, Intermag/MMM paper FB-11.

[1]Supported by NSF-DMR-1006575.

9:36AM V19.00007 Confirm existence of 90°-type coupling in Fe/MgO/Fe junction by investigating magnetic components perpendicular to the plane of incidence[1] , XIAOJING TAN[2], Department of Physics & Astronomy, University of California, Riverside — We study 90°-type interlayer exchange coupling (IEC) in a Fe/MgO/Fe junction by linear magneto-optical Kerr effect (MOKE) in $p_{in} - p_{out}$ configuration, in which only in-plane magnetization perpendicular to the external field $H$is detected. By investigating the switching processes of the ferromagnetic vectors from parallel with- to perpendicular to H, we find there is a switching correlation between them: the ferromagnetic vector in the bottom layer always follows the switching direction of that in the top layer. Further analysis shows this kind of switching sequence is the direct consequence of 90°-type coupling between the two magnetic vectors, i.e., 90°-type coupling is indeed exists in Fe/MgO/Fe junction.

[1]NSF 0706681
[2]other authors: Y-F. Chiang, J.J. Wong, R.K. Kawakami, H.W.K. Tom

9:48AM V19.00008 Influence of Interface on Conductance in AlO_x Based Magnetic Tunnel Junctions[1] , FENG GUO, E. DAN DAHLBERG, School of Physics and Astronomy, University of Minnesota — A surprising minimum in the differential conductance at nonzero bias is observed in some magnetic tunnel junctions consisting of CoFe/AlO_x/CoFe; this pronounced conductance feature occurred for electrons tunneling from the bottom to top electrode. The presence of this conductance feature depends upon the oxidation time for creating the barrier from a thin Al layer; for short and moderate oxidation times the feature was present while for long oxidation times the conductance was found to be both symmetric about zero bias and monotonic with increasing bias voltage. To determine the origin of this feature samples were prepared where the oxidation states of the CoFe on each side of the barrier were studied by X-ray photoelectron spectroscopy: the conductance feature is observed only when the top CoFe layer is partially oxidized and it disappears when the CoFe on both sides of the junction has some oxidation present. More interestingly, the bias voltage of the conductance feature decreases with oxidation time. We attribute the differential conductance feature to the electronic structure and the chemical bonding at the bottom CoFe/AlO_x interface.

[1]This work was supported by the MRSEC Program of the National Science Foundation under Award No. DMR-0819885

10:00AM V19.00009 Spin transfer torque in magnetic tunnel junctions with a perpendicularly magnetized polarizer , TAKAHIRO MORIYAMA, THEODORE GUDMUNDSEN, LUQIAO LIU, R.A. BUHRMAN, D.C. RALPH, Cornell University — Spin-torque devices containing magnetic layers with perpendicular magnetic anisotropy are of interest for strategies to reduce the switching currents in memory applications. We report spin-torque-driven ferromagnetic resonance (ST-FMR) measurements of the bias-dependent torque in magnetic tunnel junctions containing $[Co/Ni]_x$ multilayers possessing perpendicular anisotropy, acting as the polarizer layer providing spin-polarized current. We observe unusual dependence of the bias-dependent torque as a function of the magnetic orientation of the $[Co/Ni]_x$ multilayer. We speculate that this sensitivity to the magnetic orientation may originate from changes in the occupation of spin-polarized states at the Co/Ni interfaces associated with the perpendicular magnetic anisotropy.

10:12AM V19.00010 Spin transfer induced domain wall motion by perpendicular current injection in MgO-based magnetic tunnel junctions[1] , A. CHANTHBOUALA, R. MATSUMOTO, J. GROLLIER, V. CROS, A. ANANE, A. FERT, A. V. KHVALKOVSKIY, Unite Mixte de Physique CNRS/Thales, France, K.A. ZVEZDIN, Istituto P.M., Italy, A. FUKUSHIMA, S. YUASA, National Institute of Advanced Industrial Science and Technology, Japan — The spin transfer effect allows to manipulate magnetic domain walls in ferromagnetic wires by current injection. Most experiments use the lateral configuration in which the current is injected directly through the wire where the domain wall (DW) propagates. In this geometry the critical current densities are of the order of 10^8 A.cm^{-2}. Here we show that by using the current-perpendicular to plane geometry, the current densities can be decreased by two orders of magnitude. Depending of the current sign, the DW propagates in the free layer of a magnetic tunnel junction in both directions, inducing large resistance variations. By investigating the physical origin of DW motion, we find that the field-like torque has a large contribution to the effect, as recently predicted by Khvalkovskiy *et al.* (Phys. Rev. Lett. 2009). This result paves the way towards a new type of domain wall based magnetic memories.

[1]Financial support by the ERC 2010 Stg 259068 is acknowledged

10:24AM V19.00011 High Voltage Pulse Measurements of Microwave Emission and Spin-Torque Effects in Magnetic Tunnel Junction , H.W. TSENG, Y. LI, Cornell Univ., J.A. KATINE, HGST, San Jose, CA, P.G. GOWTHAM, D.C. RALPH, R.A. BUHRMAN, Cornell Univ. — The character and strength of the in-plane and field-like spin transfer torque (STT) components in magnetic tunnel junctions at high bias voltages are crucial to the successful utilization of MTJs in STT MRAM. If the field-like torque (FLT), which is generally found to be symmetric with respect to bias direction for moderate voltages, $<$ $\pm$ 0.5 V, is too large it could result in unreliable switching (back-hopping) for negative bias voltage pulses (anti-parallel to parallel switching). Here we discuss pulse measurements of MgO MTJs at high bias that yield important information about the FLT component in the $\pm$ 0.5 to 1.0 V regime through analysis of both the thermally-excited FMR behavior and spin torque driven oscillations. In the structures studied we find a strong and highly asymmetric voltage-dependent FLT at high bias that under some field and voltage conditions can result in large amplitude, incoherent microwave dynamics that could have a strong effect in enhancing back-hopping. We will analyze possible mechanisms, including junction asymmetries and inelastic tunneling.

10:36AM V19.00012 Microwave phase detection with a magnetic tunnel junction[1] , XIN FAN, Department of Physics and Astronomy, University of Delaware, SANGCHEOL KIM, Department of Electrical Engineering and Computer Science, University of Delaware, XIAOMING KOU, Department of Physics and Astronomy, University of Delaware, JAMES KOLODZEY, Department of Electrical Engineering and Computer Science, University of Delaware, HUAIWU ZHANG, State Key Laboratory of Electronic Films and Integrated Devices, University of Electronic Science and Technology of China, JOHN XIAO, Department of Physics and Astronomy, University of Delaware — A magnetic tunnel junction (MTJ) can detect microwave magnetic field due to the interplay between the ferromagnetic resonance and tunneling magneto resistance. Based on the fact that the tunneling resistance change is quadratically proportional to the rf magnetic field, we have designed a mixing circuit in which two microwaves interfere, giving rising to a dc voltage containing the phase difference between the two microwaves. With ability to detect microwave intensity and phase, the MTJ-based device may be used for on-chip microwave network analyzer and spectrum analyzer.

[1]This work has been supported by NSF DMR0827249 and NSF IIP- 1013468. Work at UCD was supported by NSF DMR-1008791 and NSF ECCS-0925626.

10:48AM V19.00013 Time-resolved detection of spin-transfer-driven ferromagnetic resonance and spin torque measurement in magnetic tunnel junctions[1] , CHEN WANG, Y.-T. CUI, R.A. BUHRMAN, D.C. RALPH, Cornell University — Several experimental techniques have been introduced in recent years in attempts to measure spin transfer torque in magnetic tunnel junctions (MTJs). The dependence of spin torque on bias is important for understanding fundamental spin physics in magnetic devices and for applications. However, previous techniques have provided only indirect measures of the torque and their results to date for the bias dependence are qualitatively and quantitatively inconsistent. Here we demonstrate that spin torque in MTJs can be measured directly by using time-domain techniques to detect resonant magnetic precession in response to an oscillating spin torque. The technique is accurate in the high-bias regime relevant for applications, and because it detects directly small-angle linear-response magnetic dynamics caused by spin torque it is relatively immune to artifacts affecting competing techniques. At high bias we find that the spin torque vector differs markedly from the simple lowest-order Taylor series approximations commonly assumed.

[1]We acknowledge J.A. Katine and D. Mauri for fabrication of the devices used in our experiment.

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V20 FIAP/DMP GERA/DCOMP: Focus Session: Physics of Energy Storage Materials V – Thermal Storage and Conventional Hydrides D168

8:00AM V20.00001 Origin of the Diverse Melting Behaviors of Aluminum Nanoclusters with Around 55 Atoms[1] , JOONGOO KANG, SU-HUAI WEI, National Renewable Energy Laboratory, YONG-HYUN KIM, Korea Advanced Institute of Science and Technology — Microscopic understanding of thermal behaviors of metal nanoparticles is important for nanoscale catalysis and thermal energy storage applications. Using first-principles molecular dynamics simulations, we reveal the microscopic origin of the diverse melting behaviors of Al_N clusters with N around 55 [1,2]. The conceptual link between the degree of symmetry (e.g., T_d, D_{2d} and C_s) and solidity of atomic clusters is quantitatively demonstrated through the analysis of the configuration entropy. The size-dependent, diverse melting behaviors of Al clusters originate from the reduced symmetry ($T_d \rightarrow D_{2d} \rightarrow Cs$) with increasing the cluster size. In particular, the sudden drop of the melting temperature and appearance of the dip at N = 56 are due to the T_d-to-D_{2d} symmetry change, triggered by the surface saturation of the tetrahedral Al_{55} with the T_d symmetry.

[1] G. A. Breaux, C. M. Neal, B. Cao, and M. F. Jarrold, Phys. Rev. Lett. **94**, 173401 (2005).
[2] J. Kang, S.-H. Wei, and Y.-H. Kim, J. Am. Chem. Soc. (in press).

[1]This work was funded by the U.S. DOE EERE CSP and NREL LDRD programs.

8:12AM V20.00002 Azonbenzene-functionalized carbon nantubes as a high energy density solar thermal fuel , ALEXIE KOLPAK, ENGIN DURGAN, JEFF GROSSMAN, Massachusetts Institute of Technology — Solar thermal fuels, which store energy from the sun in the chemical bonds of molecules, are a fascinating energy storage prospect: in principle they are 100% renewable, produce no emissions or by-products, are easily transportable in the form of liquids or powders, and can be recharged by the sun without any special equipment. However, adaptation of solar fuels as a viable, low-cost, large-scale means of energy storage will require the discovery of new materials other than the one known case based on Ruthenieum that can perform the process over many cycles with no degradation. Here we discuss a novel approach to the design of solar fuels based on photoswitchable molecules covalently bonded to carbon nanotubes (CNTs). Using density functional theory, we examine the potential for maximizing the energy density via a combination of steric and intermolecular interactions between metastable azobenzene photoisomers and a CNT substrate. In addition, we investigate how a tuning parameter unique to the nanoparticle/molecule geometry — the packing density of the molecules on the nanotube — can be varied to produce significant, controlled changes in the transition pathway and barriers via ordered molecule-molecule interactions, potentially leading to new classes of nanoparticle-based solar fuels.

8:24AM V20.00003 A high volume, high throughput volumetric sorption analyzer[1] , Y.C. SOO, M. BECKNER, J. ROMANOS, C. WEXLER, P. PFEIFER, U of Missouri, P. BUCKLEY, J. CLEMENT, MRI — In this talk we will present an overview of our new Hydrogen Test Fixture (HTF) constructed by the Midwest Research Institute[2] for The Alliance for Collaborative Research in Alternative Fuel Technology[3] to test activated carbon monoliths for hydrogen gas storage. The HTF is an automated, computer-controlled volumetric instrument for rapid screening and manipulation of monoliths under an inert atmosphere (to exclude degradation of carbon from exposure to oxygen). The HTF allows us to measure large quantity (up to 500 g) of sample in a 0.5 l test tank, making our results less sensitive to sample inhomogeneity. The HTF can measure isotherms at pressures ranging from 1 to 300 bar at room temperature. For comparison, other volumetric instruments such as Hiden Isochema's HTP-1 Volumetric Analyser can only measure carbon samples up to 150 mg at pressures up to 200 bar.

[1]Work supported by the US DOD Contract # N00164-08-C-GS37.
[2]http://www.mriresearch.org
[3]http://all-craft.missouri.edu

8:36AM V20.00004 Synthesis of Li_2MgIr and $LiMgIrH_6$: Guidance from DFT , JAN HERBST, JAMES SALVADOR, MARTIN MEYER, GM R&D Center — Formation of Li_2MgIr was suggested by theoretical modeling of Li_2MgX systems and their hydrides with density functional theory (DFT). Verifying our DFT results, we have synthesized Li_2MgIr and determined its crystal structure and hydrogen sorption behavior. The phase crystallizes in the cubic $P\bar{4}3m$ space group and is isostructural to the known ternary Li_2MgSi. Its reaction with hydrogen proceeds according to $Li_2MgIr + \frac{7}{2}H_2 \rightarrow LiMgIrH_6 + LiH$. The hydride $LiMgIrH_6$ also features $P\bar{4}3m$ symmetry; its detailed crystal structure is established via a combination of x-ray diffraction and DFT analyses. A metal $\rightarrow$ insulator transition accompanies formation of the hydride.

8:48AM V20.00005 Thermodynamics of MgH_2 hydrogen storage materials: nanoparticle size and topological structure effects[1] , JASON REICH, Chemisry, University of Illinois, Urbana-Champaign, IL 61801, LINLIN WANG, DUANE JOHNSON, Ames Laboratory/US DoE, Iowa State University, Ames, IA 50011-3020 — Via plane-wave-based Density Functional Theory calculations, we investigate H-desorption from (110) rutile MgH_2, a surface step, and surfaces of nanoscale $Mg_{30}XH_{62}$ clusters having catalytic dopants (X=Mg, Ti, or Fe). All calculated desorption enthalpies are endothermic, in contrast to results in the literature,[2] and no particle size effect is found for desorption of H singly, doubly, or triply-bonded to metal atoms, indicating only local bond energy is relevant. In contrast to recent results, we show that exothermic results are not obtained when initial cluster structures are carefully relaxed globally via simulated annealing, in which amorphous structures are found to be favored. A topological feature is identified that offers potential utility for using nanostructured MgH_2 as a hydrogen-storage solution.

[1]Work supported in part by the DoE, BES Catalysis (DEFG02-03ER15476), Energy (DEFC36-05GO15064) with Sandia MHCoE, BES Materials (DEFG02-03ER46026), and Ames Laboratory (DE-AC02-07CH11358) operated by Iowa State University.
[2]Larsson, P.; Araujo, C. M.; Larsson, J. A.; Jena, P.; Ahuja, R. *P Natl Acad Sci USA* 2008, 105, 8227

9:00AM V20.00006 Hydrogen desorption from $MgH_2(110)$ surface with transition-metal catalyst: a DFT study of energetics and barriers[1] , LIN-LIN WANG, DUANE D. JOHNSON, Division of Materials Science and Engineering, Ames Laboratory/US DoE, Iowa State University, Ames, IA 50011-3020 — Transition-metal (TM) catalysts are widely used in hydrogen-storage materials to increase hydrogen absorption and desorption kinetics. Using density functional theory calculations, we elucidate the catalytic effect of Ti on H-desorption from $MgH_2(110)$ surface. Kinetic energy barriers of different reaction pathways of hydrogen desorption are calculated via nudged-elastic-band method. We find that Ti dopant is effective in reducing kinetic barriers, in agreement with experimental observations. We also find that magnetic degrees of freedom must be carefully included to describe the change of magnetic states during catalytic-enhanced desorption. As vacancy migration barriers are lower than desorption barrier, bulk diffusion of H inherently feeds into the favorable surface desorption mechanism.

[1]Supported by the DOE/BES under DE-FG02-03ER15476 (Catalysis), DEFC36-05GO15064 (Sandia Metal-Hydride Center of Excellence), DE-FG02-03ER46026 (Materials), and DE-AC02-07CH11358 at the Ames Laboratory operated by Iowa State University

9:12AM V20.00007 Tuning the Hydrogen Storage in Magnesium Alloys , SULEYMAN ER, University of Twente, GILLES A. DE WIJS, GEERT BROCKS — We investigate the hydrogen storage properties of promising magnesium alloys. MgH_2 (7.6 wt % H) would be a very useful storage material if the (de)hydrogenation kinetics can be improved and the desorption temperature is markedly lowered. Using first principles calculations, we show that hydrides of Mg-transition metal (TM) alloys adopt a structure that promotes faster (de)hydrogenation kinetics, as is also observed in experiment [1]. Within the lightweight TMs, the most promising alloying element is titanium. Alloying Mg with Ti alone, however, is not sufficient to decrease the stability of the hydride phases, which is necessary to reduce the hydrogen desorption temperature [2]. We find that adding aluminium or silicon markedly destabilizes Mg-Ti hydrides and stabilizes Mg-Ti alloys. Finally, we show that controlling the structure of Mg-Ti-Al(Si) system by growing it as multilayers, has a beneficial influence on the thermodynamic properties and makes it a stronger candidate for hydrogen storage [3].

Ref: [1] S. Er *et al.*, Phys. Rev. B, **79**, 024105 (2009). [2] S. Er *et al.*, J. Phys.: Condens. Matter, **22**, 074208 (2010). [3] S. Er *et al.*, J. Phys. Chem. Lett., **1**, 1982 (2010).

9:24AM V20.00008 Neutron, Thermodynamic, and Modeling Studies of Hydrogen Interaction with MgO(100) , JOHN LARESE, University of Tennessee, L.L. DAEMEN, Los Alamos National Lab, J. OLLIVIER, T. SEYDEL, Institut Laue-Langevin, E. CRUZ SILVIA, B. SUMPTER, Oak Ridge National Lab — We report our investigations of thermodynamic, neutron diffraction, inelastic and quasielastic neutron scattering (INS and QENS) studies of hydrogen adsorbed onto MgO(100). Guided by our volumetric adsorption measurements, we used INS and QENS to probe the dynamics of the adsorbed H2 molecules. Our structural studies indicate that near monolayer completion the intermolecular distance of the H2 molecules on MgO are $\sim$20% more compressed than the closest packed bulk solid plane. The melting of this compressed solid takes place at temperatures above the bulk triple point, whereas most other 2D films melt at about 70% of the triple point. Using INS, the motion of the adsorbed hydrogen is examined as a function of film thickness. For rotational motions, we use the ortho-to-para transition as a guide and find that the rotational barrier for H2 adsorbed on MgO is shifted to lower energy at low surface coverage. These results are compared with modeling for additional insight into the microscopic processes that underpin the observed behavior. This work partially supported by the U.S. DOE, BES under contract DE-AC05-00OR22725 with ORNL managed and operated by UT-Battelle, LLC, the NSF under grant DMR-0412231 and a grant from the University of TN, JINS.

9:36AM V20.00009 Enhanced Hydrogen Storage Properties of Magnesium Nanotrees by Glancing Angle Deposition , MEHMET CANSIZOGLU, TANSEL KARABACAK, Department of Applied Science, University of Arkansas at Little Rock, Little Rock, AR, 72204 — Magnesium has a high hydrogen storage capacity of 7.6 wt %. In addition it is one of the most abundant low cost materials in nature. However, absorption/desorption of hydrogen in Mg mainly suffer from slow kinetics. In this study, we investigate the hydrogen storage properties of Mg "nanotrees with nanoleaves" fabricated by glancing angle deposition (GLAD) method and compare to those of conventional thin films of Mg. A recently developed quartz crystal microbalance (QCM) gas absorption/desorption technique was used for hydrogen storage measurements on our thin film and nanostructured coatings. Storage experiments were performed at temperatures between 100-300 $^{\circ}$C, and at 30 bars of H_2 pressure. Our results reveal that Mg nanotrees have significantly faster kinetics and lower absorption temperatures for hydrogen storage compared to Mg thin films. The enhancement in absorption properties is believed to be due to decreased diffusion lengths, favorable crystal orientations for diffusion of hydrogen, and resistance to surface oxidation of Mg nanotrees.

9:48AM V20.00010 Neutron spectroscopy of gamma-MgH2 , ALEXANDER KOLESNIKOV, Oak Ridge National Laboratory, VLADIMIR ANTONOV, VADIM EFIMCHENKO, Inst. Solid State Phys. RAS, Chernogolovka, Russia, GARRETT GRANROTH, Oak Ridge National Laboratory, S.N. KLYAMKIN, Moscow State Un., Russia, A.V. LEVCHENKO, MICHAEL SAKHAROV, Inst. Solid State Phys. RAS, Chernogolovka, Russia, YANG REN, Argonne National Laboratory, TIMMY RAMIREZ-CUESTA, ISIS, Rutherford Appleton Laboratory, UK — Under ambient conditions, magnesium dihydride exists in two forms, alpha-MgH2 (the most stable modification) and gamma-MgH2 (a less stable modification). The alpha-phase partly transforms to gamma-MgH2 in the course of ball-milling and under high pressure and temperature. Due to the high hydrogen content of 7.6 wt.%, MgH2 has been intensively studied as a prospective material for hydrogen storage. By exposing of alpha-MgH2 to a pressure of 5 GPa and temperature 840 K, we prepared a sample, in which about 60% of the alpha-MgH2 was transformed to gamma-MgH2. We have measured inelastic neutron scattering (INS) spectra of both the high pressure treated MgH2 and starting alpha-MgH2, and extracted the spectrum for gamma-MgH2. The differences between the INS spectra and their agreement with the first-principles calculations for these compounds will be discussed.

10:00AM V20.00011 The chemical potential of hydrogen in Mg-films and metal-doped carbon nanostructures[1] , MINA YOON, Oak Ridge National Laboratory and Fritz-Haber-Institut der Max-Planck-Gesellschaft, HANNO WEITERING, ZHENYU ZHANG, Oak Ridge National Laboratory — We use first-principles density functional theory to study the binding mechanism of hydrogen to nanoscale systems. We investigate the performance of the exchange-correlation functional in describing the interaction between hydrogen and metal systems and the importance of the vibrational contribution in the formation enthalpy. In ultrathin Mg films the stability of hydrides is much lower than in the corresponding bulk systems and it can be modified by metal alloying. We calculate the chemical potential of hydrogen in Mg films for different dopant species and film thicknesses while including all vibrational degrees of freedom. By comparing the chemical potential with that of free hydrogen gas at finite temperature and pressure, we construct a hydrogenation phase diagram and identify the conditions for hydrogen absorption/desorption. The vibrational contribution to the chemical potential of hydrogen becomes more prominent for dihydrogen adsorption to metals, where its significance dramatically changes depending on the binding characteristics. This feature is illustrated by the example of metal-doped nanocarbon systems.

[1]Supported by the US DOE, Office of Basic Energy Sciences, Materials Sciences and Engineering Division and the Max Planck Society

10:12AM V20.00012 Computational search for hydrogen storage materials: accuracy and alloys[1] , LUCAS WAGNER, Massachusetts Institute of Technology, ERIC MAJZOUB, University of Missouri-Saint Louis, MARK ALLENDORF, Sandia National Labs, JEFFREY GROSSMAN, Massachusetts Institute of Technology — Metal hydride materials are among the strongest contenders for hydrogen storage, offering good weight and volume density. The main reason that these materials are not used now is that it is very challenging to find a material that is both light enough and has the proper binding to allow for easy absorption/desorption near room temperature. We will evaluate two routes to controlling the binding energy: particle size and alloy composition using the highly accurate quantum Monte Carlo method. We find that traditional methods of calculating the binding energy such as the Wulff construction and density functional theory should be applied with caution, as they can lead to misleading results. We will also report on the prospects for finding a sweet spot of size and alloy composition that has the correct binding energy for hydrogen storage applications.

[1]Supported by the Department of Energy.

10:24AM V20.00013 Ultra-low diffusion barriers for the AlH_3-related vacancies in γ-$NaAlH_4$, FENG ZHANG, YAN WANG, MEI-YIN CHOU, School of Physics, Georgia Institute of Technology — It has been suggested that the diffusion of AlH_3-related vacancies plays an essential role in the decomposition of $NaAlH_4$, a prototypical material for hydrogen storage[1,2]. We find from first-principles calculations that the diffusion barrier for both the neutral AlH_3 vacancy and the charged AlH_4^- vacancy in the newly proposed γ-phase of $NaAlH_4$ [3] is only about 0.1 eV, much lower than the barrier for the diffusion of corresponding vacancies in the conventional α-phase 0.5 eV, calculated with the same method. Possible schemes to facilitate the $\alpha \rightarrow \gamma$ phase transformation in order to improve the kinetics of the decomposition reaction of $NaAlH_4$ will also be discussed.

[1] H. Gunaydin, K. N. Houk, and V. Ozoliņš, Proc Natl Acad Sci USA **105**, 3673 (2008).
[2] G. B. Wilson-Short, A. Janotti, K. Hoang, A. Peles, and C. G. Van de Walle, Phys. Rev. B **80**, 224102 (2009).
[3] B. Wood and N. Marzari, Phys. Rev. Lett. **103**, 185901; **104**, 019901.

10:36AM V20.00014 Defect-mediated Alane formation on Ti-doped Al(111) surfaces: a DFT study , ADITI HERWADKAR, LIN-LIN WANG, DUANE D. JOHNSON, Ames Laboratory/US Department of Energy, Iowa State University — Understanding of Alane (AlH_3) formation on Al surface remains elusive, including interpreting STM results under various conditions. Using density functional theory calculations, we study Alane formation on close-packed (111) and stepped surfaces with {111} and {100} microfacets of Al, with and without Ti as a catalyst. We find that Ti dopants act as catalyst in the formation of Alane on Al(111) via a vacancy-mediated mechanism. Additionally, we find the Alane formation energy at steps is 40% less than that from the flat surface. We assess the energetics of various surface-defect configurations to understand the concerted roles that Ti dopants, surface vacancies, and step defects play in Alane formation. Work was supported in part by Department of Energy, Office of Basic Energy Science under contract DEFC36-05GO15064 (Sandia Metal-Hydride Center of Excellence), DE-FG02-03ER15476, DE-FG02-03ER46026, and DE-AC02-07CH11358 at the Ames Laboratory operated by Iowa State University.

10:48AM V20.00015 Molecular hydrogen interaction with Ti doped Al(111) surfaces , IRINDER CHOPRA, University of Texas at Dallas, SANTANU CHAUDHURI, Washington state University, JEAN-FRANCOIS VEYAN, YVES CHABAL, University of Texas at Dallas — Alanates are promising hydrogen storage materials, but have poor re-hydrogenation kinetics. Decomposition[1] of $NaAlH_4$ can be made reversible at reasonable temperatures and pressures by adding titanium. There is however little understanding of the role of Ti as a catalyst,[2] and no experimental evidence for H_2 dissociation on Ti-doped Al surfaces. Using CO as a probe molecule in conjunction with in-situ infrared absorption spectroscopy, we present unambiguous evidence for molecular hydrogen dissociation, chemisorptions and spill over on with Ti doped Al(111) surfaces. The optimum catalytic activity of the Ti-doped Al surface occurs for a Ti coverage of 0.1 monolayer. At high hydrogen coverage, no CO physisorption is observed, indicating that the dissociated hydrogen spill over from the catalytic active Ti site. CO molecules can be chemisorbed at the catalytic sites but do not spill over. These findings provide important information on the nature of the catalyst during the hydrogenation reactions.

[1] *J. Alloys Compd.* 1997, 253, 1.
[2] *J Am Chem Soc* 2006, 128, (35), 11404-11415.

Thursday, March 24, 2011 8:00AM - 10:36AM –

Session V21 DCOMP FEd: Focus Session: Teaching Computational Physics to Classroom and Research Students D161

8:00AM V21.00001 Computational (Physics Education) vs. (Computational Physics) Education: Many Body for Anybody , ROBERT PANOFF, Shodor Education Foundation — The substantial role of computational approaches to physics research is not currently reflected proportionately in how we prepare future physicists. We can do better in using computation to teach the concepts of physics –Computational (Physics Education) – and to prepare students to be computational physicists – (Computational Physics) Education. We have the opportunity to demonstrate that effective use of computing in physics really matters. A computational approach in physics education is essential because quantitative reasoning, computational thinking, and multiscale modeling are the intellectual "heart and soul" of 21st Century physics and therefore are the essential skills of the 21st Century physicist. Computing matters because we can apply the power of interactive computing to reach a deeper understanding of physics and the mathematics underlying the theory and their role in understanding the world. We will explore a transformation in physics education, supported by interactive computing resources, promoting a dynamic encounter with the world through guided discovery. We will explore a variety of free and low-cost sources for modeling tools from Shodor and its Computational Science Education Reference Desk, a pathway project of the National Science Digital Library.

8:36AM V21.00002 ABSTRACT WITHDRAWN –

8:48AM V21.00003 Computing Band Structures in Undergraduate Solid State , JAVIER HASBUN, University of West Georgia — Understanding band structures is quite challenging for undergraduate solid state physics students. Calculating the band structures is even more difficult. However, using the techniques developed earlier [1], and which were applied to the simple cubic structures, it is possible to extend them to semiconducting systems in a simple way. The idea is to employ the 8-band model concept of Harrison's Hamiltonian approach [2] to model and parametrize the bands. The method also uses the system's band structure's Green's function and employs the k-space Brillouin-zone ray approach [3] combined with a complex integration method [4] to obtain the density of states. The number of occupied electron states up to a certain energy is obtained using Romberg's method and example results will be shown. [1] Javier Hasbun (J42.00013) http://meetings.aps.org/Meeting/MAR10/Event/119248 [2] S. Froyen, and W. A. Harrison, Phys. Rev. B Vol. 20, 2420 (1979). [3] An-Ban Chen, Phys. Rev. B, Vol. 16, 3291 (1977). [4] Javier Hasbun http://meetings.aps.org/link/BAPS.2009.MAR.L29.12

9:00AM V21.00004 Introducing Computational Physics in Introductory Physics using Intentionally Incorrect Simulations[1] , ANNE COX, Eckerd College — Students in physics courses routinely use and trust computer simulations. Finding errors in intentionally incorrect simulations can help students learn physics, be more skeptical of simulations, and provide an initial introduction to computational physics. This talk will provide examples of electrostatics simulations that students can correct using Easy Java Simulations and are housed in the Open Source Physics Collection on ComPADRE (http://www.compadre.org/osp).

[1]Partial support through the Open Source Physics Project, NSF DUE-0442581.

9:12AM V21.00005 Computational ... Physics Education: Letting physics learning drive the computational learning[1] , NORMAN CHONACKY, Yale University — For several years I have been part of a team researching and rethinking why physicists are more willing to admit the value of computational modeling than to include it in what they teach. We have concluded that undergraduate faculty face characteristic barriers that discourage them from starting to integrate computation into their courses. Computational tools and resources are already developed and freely available for them to use. But there loom ill-defined "costs" to their course learning objectives and to them personally as instructors in undertaking this. In an attempt to understand these issues more deeply, I placed myself in the mindset of a relative novice to computational applications. My approach: focus on a physics problem first and then on the computation needed to address it. I asked: could I deepen my understanding of physics while simultaneously mastering new computational skills? My results may aid appreciation of the plight of both a novice professor contemplating the introduction of computation into a course and the students taking it. These may also provide insight into practical ways that computational physics might be integrated into an entire undergraduate curriculum.

[1]Research support from: Shodor Education Foundation; IEEE-Computer Society; and Teragrid Project. Research collaboration from Partnership for Integration of Computation into Undergraduate Physics.

9:48AM V21.00006 Teaching computational physics: An embarrassment of riches for teaching computational physics , AMY BUG, Swarthmore College, LARRY ENGELHARDT, Francis Marion University — The first decade of the 21st century has provided a wealth of exceptional resources for teaching computational physics, including numerous textbooks, libraries of computer codes (visual as well as numerical), and high-level interfaces for accessing these libraries. We are now faced with the very real challenge of choosing which of these resources to incorporate into the finite number of courses available in a given curriculum. This choice depends on several factors: How much time can be allocated to teaching computational methods and at what stage in the curriculum? What are the goals? (Learning physics better? Being prepared to work in research labs studying large-scale problems?) Are commercial packages an appropriate option for your student population? In recent years one of us (L.E.) has taught three undergraduate computational physics courses per year. The other (A.B.) has taught at various points in the undergraduate spectrum (a seminar for seniors, a computational methods lab for sophomores, a summer research experience for freshmen from underrepresented groups). Thus, while there are no right or wrong answers to these questions, we will present some of the decisions we have made, and will discuss the consequences.

10:00AM V21.00007 A course in Computational Physics , GEORGE RAWITSCHER, University of Connecticut — This course, taught at UConn, has several objectives: 1) To make the students comfortable in using MATLAB; 2) To reveal the existence of unavoidable inaccuracies due to numerical roundoff errors and algorithm inaccuracies; 3) to introduce modern spectral expansion methods [1], and compare them with conventional finite difference methods. Some of the projects assigned in the course will be described, such as the motion of a falling parachute, and the vibrations of an inhomogeneous vibrating string [2].

[1] Lloyd N. Trefethen, "Spectral Methods in MATLAB (SIAM, Philadelphia, PA, 2000)"; John P. Boyd, "Chebyshev and Fourier Spectral Methods," (Dover Publications, Inc. Mineola, New York, Second revised edition, 2001).
[2] G. Rawitscher and J. Liss, "The vibrating inhomogeneous string," Am. J. of Phys., to be published; and arXiv:1006,1913v1 [physics.comp-ph]

10:12AM V21.00008 Using Python as a first programming environment for computational physics in developing countries , GODFREY AKPOJOTOR, Physics Department, Delta State University, Abraka, Nigeria, LOUIS EHWERHEMUEPHA, Physics Department, University of Lagos, Lagos, Nigeria, MYRON ECHENIM, Physics Department, Delta State University, Abraka, Nigeria, FAMOUS AKPOJOTOR, Physics Department, University of Benin, Benin City, Nigeria — Python unique features such its interpretative, multiplatform and object oriented nature as well as being a free and open source software creates the possibility that any user connected to the internet can download the entire package into any platform, install it and immediately begin to use it. Thus Python is gaining reputation as a preferred environment for introducing students and new beginners to programming. Therefore in Africa, the Python African Tour project has been launched and we are coordinating its use in computational science. We examine here the challenges and prospects of using Python for computational physics (CP) education in developing countries (DC). Then we present our project on using Python to simulate and aid the learning of laboratory experiments illustrated here by modeling of the simple pendulum and also to visualize phenomena in physics illustrated here by demonstrating the wave motion of a particle in a varying potential. This project which is to train both the teachers and our students on CP using Python can easily be adopted in other DC.

10:24AM V21.00009 Undergraduate research in numerical relativity: How to put a black hole on a graphics card , JASON D. GRIGSBY, Friedrich-Schiller-University of Jena — Andreas Weyhausen, a diploma student at the Friedrich-Schiller University, ported a standard code for the full 3D stable simulation of black holes to run on a graphics processing unit (GPU), a first in the field. A presentation will be made describing the task he accomplished with key results, including a speed-up comparison to the serial code. This will be placed in context of the course work that prepared him for the project and advising provided by the FSU gravity group prior, during and after the execution leading to his thesis on Numerical Algorithms of General Relativity for Heterogeneous Computing Environments.

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V22 DCMP: Magnetic Phase Transitions I D163

8:00AM V22.00001 Pressure-induced antiferromagnetism in pure CeFe2 , JIYANG WANG, THOMAS ROSENBAUM, U. of Chicago, YEJUN FENG, Argonne National laboratory, RAFAEL JARAMILLO, Harvard University, SARA HARAVIFARD, Argonne National laboratory — CeFe2 is a ferromagnet that exhibits antiferromagnetic fluctuations in its ground state at low temperature. We use x-ray diffraction to measure directly the emergence of antiferromagnetic order in pure CeFe2 at high pressure. We present an analysis of both the magnetic and lattice symmetries in the newly discovered high pressure phase, and compare our results to those from doped CeFe2 systems. This comparison provides insights into the roles of pressure and chemical doping in driving the magnetic quantum phase transition.

8:12AM V22.00002 Transition-metal dihalide MX_2 as magnetoelectric multiferroics , SHINICHIRO SEKI, TAKASHI KURUMAJI, SHINTARO ISHIWATA, HIROYUKI MATSUI, YOSHINORI TOKURA, University of Tokyo, HIROSHI MURAKAWA, YUSUKE TOKUNAGA, YOSHIO KANEKO, ERATO-JST, TATSUO HASEGAWA, AIST — Magnetoelectric properties were investigated for transition-metal dihalide MX_2, which turns out to be the first example of non-chalcogen based spiral-spin induced multiferroics. We discovered the emergence of ferroelectric polarization (P) in helimagnetic state for several compounds such as $CuCl_2$ with edge-shared $S = 1/2$ chain and MnI_2 with stacked triangular lattice. In the latter material, in-plane magnetic field (H) was found to induce the rearrangement of six possible multiferroic domains. With every $60°$-rotation of H around the c-axis, discontinuous $120°$-flop of P-vector is observed as a result of the flop of magnetic modulation vector (q). In-plane H also alters the stable direction of q-vector from original $q \parallel \langle 1\bar{1}0 \rangle$ to $q \parallel \langle 110 \rangle$ above 3 T, which leads to significant change of P-flop patterns under rotating H. At the critical field region ($\sim$ 3T), due to the enhanced q-flexibility, P-vector smoothly rotates clockwisely twice while H rotates counter-clockwisely only once.

8:24AM V22.00003 Infrared spectroscopy of phonons and electromagnons in multiferroic $TbMnO_3$, R.P.S.M. LOBO, R. SCHLECK, LPEM, ESPCI-ParisTech, CNRS, Paris, France, R.L. MOREIRA, Depto. Fisica, UFMG, Brazil, H. SAKATA, Dept. Physics, Tokyo Univ. Science, Japan — We measured the temperature dependent infrared reflectivity spectra of $TbMnO_3$ with the electric field of light polarized along each of the three crystallographic axes. We analyzed the effect, on the phonon spectra, of the different phase transitions occurring in this material. We show that the antiferromagnetic transition at T_N renormalizes the phonon parameters along the three directions. Our data indicate that the electromagnon, observed along the a direction, has an important contribution in building the dielectric constant. We show that this electromagnon spectral weight comes only from a few phonons which can be clearly identified. We also determined that only one phonon, observed along the c-axis, has anomalies at the ferroelectric transition. This phonon is built mostly from Mn vibrations, suggesting that Mn displacements are closely related to the formation of the ferroelectric order.

8:36AM V22.00004 Ultrafast pump-probe spectroscopy of multiferroic $TbMnO_3$, JINGBO QI, LI YAN, STUART TRUGMAN, JIANXIN ZHU, ALEXANDER BALATSKY, QUANXI JIA, ANTOINETTE TAYLOR, ROHIT PRASANKUMAR, Los Alamos National Laboratory, CENTER FOR INTEGRATED NANOTECHNOLOGIES TEAM — $TbMnO_3$, exhibiting simultaneously both magnetic and ferroelectric phases, is an excellent multiferroic candidate for demonstrating the strong coupling between different degrees of freedom, i.e. spin, orbital and charge order. Previously, ultrafast optical pump-probe spectroscopy has proven to be an ideal technique for unraveling the interplay between different orders in the time domain. In this work, we used this technique to study ultrafast dynamics in multiferroic $TbMnO_3$. At low temperatures, we initially observed an extraordinarily slow rising process, with a timescale of tens of picoseconds, followed by another decay process with a relaxation time of hundreds of picoseconds. An analysis of these two processes as a function of temperature reveals the influence of the magnetic and ferroelectric phase transitions on carrier dynamics in $TbMnO_3$, which agrees well with other experimental results.

8:48AM V22.00005 Photoinduced Femtosecond Formation of Ferromagnetism in a Strongly Correlated Antiferromagentic Manganite , TIANQI LI, AARON PATZ, Dept. of Physics and Astronomy, Iowa State University; Ames Lab - USDOE, JIAQIANG YAN, THOMAS LOGRASSO, Ames Lab - USDOE, JIGANG WANG, Dept. of Physics and Astronomy, Iowa State University; Ames Lab - USDOE — There has been strong current interest to manipulate collective spins and even induce magnetic phase transitions in their highly *non-equilibrium, non-thermal* states at *femtosecond* time scales. Such processes offer opportunities to exceed the upper limit of the magnetic switching speed (0.1-10 GHz) in modern magneto-optical recording industry and magnetic storage/logic devices. One prominent system to explore such femtosecond magnetism is strongly correlated manganites, which are truly "responsive" near the phase boundary, exhibiting extreme sensitivity to external stimuli, such as light, electric and magnetic fields. Using ultrafast two-color magnetic circular dichroism spectroscopy, we have observed a substantial photoinduced magnetization enhancement in $Pr_{0.7}Ca_{0.3}MnO_3$ within 180 fs above a threshold pump fluence and at low temperature. Such a photoinduced critical behavior vanishes at elevated temperature. These results clearly show a photoinduced ultrafast antiferromagnetic to ferromagnetic phase transition, demonstrating particularly, that one can reveal a hidden, thermally inaccessible ground state at fs time scales.

9:00AM V22.00006 Polaron Glass in $La_{0.35}Pr_{0.275}Ca_{0.375}MnO_3$[1] , MARK BURKHARDT, Stanford University and SLAC National Accelerator Laboratory, M.A. HOSSAIN, S. SARKAR, J. STÖHR, SLAC National Accelerator Laboratory, Y.-D. CHUANG, A.G. CRUZ GONZALEZ, A. DORAN, A. SCHOLL, A.T. YOUNG, Advanced Light Source, Lawrence Berkeley National Laboratory, Y.J. CHOI, S.-W. CHEONG, Rutgers Center for Emergent Materials and Department of Physics & Astronomy — Manganite compounds in the $La_{1-x-y}Pr_yCa_xMnO_3$ series are known for exhibiting phase separation over a large temperature range. We combined the x-ray photoemission electron microscopy (PEEM) and resonant elastic soft x-ray scattering (REXS) techniques to study the interplay between the ferromagnetic and charge-ordered/antiferromagnetic phases, respectively, in $La_{0.35}Pr_{0.275}Ca_{0.375}MnO_3$. We found a polaronic glassy state at intermediate temperatures, when the material is dominated by charge- and orbital-order domains. When the sample is cooled below T_C, the magnetization increases, accompanied by a relaxation of the lattice deformations that accompany the polaron glass.

[1]This Work and the Advanced Light Source are funded by the DOE Office of Basic Energy Science.

9:12AM V22.00007 The role of oxygen in the colossal magnetoresistance in manganites[1] , M.A. HOSSAIN, M.H. BURKHARDT, SIMES, Stanford, S. SARKAR, H. OHLDAG, S. DE JONG, SLAC, A. SCHOLL, A.T. YOUNG, A. DORAN, Y.-D. CHUANG, Berkeley Lab, D. DESSAU, U. Colorado, J. MITCHELL, Argonne Lab, H.A. DÜRR, J. STÖHR, SLAC — We have used Low temperature Photo-Emission Electron Microscopy (PEEM) measurements on the bi-layered manganite compound $La_{1.8}Sr_{1.2}Mn_2O_7$ to explore the origin of the colossal magnetoresistance (CMR) effect. It is generally agreed that CMR cannot be explained by double exchange only, and that other interactions mediated by oxygen atoms such as polarons must be important. We have imaged the magnetic domain structure by x-ray magnetic circular dichroism PEEM spectro-microscopy at both the O and Mn sites. By probing the ferromagnetic domain formation below T_c, we find that the insulator-to-metal transition is mediated by magnetic interactions involving a strong magnetic moment on oxygen. The spatially resolved oxygen K-edge XMCD signal reveals the role of the in-plane and out-of- plane e_g orbitals in the magnetic transitions and thereby sheds light on the very origin of CMR.

[1]DOE, NSERC

9:24AM V22.00008 Momentum-Space Dichotomy in the Metal-Insulator Transition in doped EuO , DANIEL SHAI, ALEXANDER MELVILLE, JOHN HARTER, ERIC MONKMAN, DAWEI SHEN, DARRELL SCHLOM, KYLE SHEN, Cornell University — EuO possesses a wide variety of remarkable properties, most which can be accessed only upon carrier doping. In addition to its large ferromagnetic moment (S = 7/2), doped EuO exhibits a metal-insulator transition with a change in resistivity of over 10^{13} and highly spin polarized carriers. Furthermore, the ferromagnetic Curie temperature can be enhanced from 69 K in undoped EuO to over 200 K in carrier doped EuO. We present angle-resolved photoemission studies of $Eu_{1-x}Gd_xO$ thin films which elucidate the electronic structure and mechanism of the metal-insulator transition. Our ARPES studies verify that the exchange coupling between the Eu 4f moments and the delocalized Eu 5d states pushes the bottom of the majority-spin conduction band through E_F below T_C. We also reveal a surprising dichotomy between the delocalized carriers at the Brillouin zone boundary below T_C, and localized carriers around the zone center above T_C which are responsible for the respective low-temperature ferromagnetic metallic and high-temperature paramagnetic semiconducting behaviors observed in transport measurements.

9:36AM V22.00009 Anharmonic Lattice Effect in the Giant Negative Thermal Expansion Antiperovskite $Cu_{1-x}Sn_xNMn_3$, PENG TONG, DESPINA LOUCA, Department of Physics, University of Virginia, GRAHAM KING, ANNA LLOBET, Los Alamos National Laboratory, BOSEN WANG, YUPING SUN, Institute of Solid State Physics, Chinese Academy of Sciences — The antiperovskite $ANMn_3$ (A: transitional metals and semiconducting elements) often shows a large, discontinuous volume contraction at the magnetic transition associated with a large negative thermal expansion (NTE). The NTE property was initially observed in $Cu_{1-x}Ge_xNMn_3$ where Ge-doping broadens the discontinuous volume contraction. It was recently reported that although the average symmetry is cubic in the solid solutions, locally, the symmetry is tetragonal with the I4/mcm symmetry of the end member $GeNMn_3$. We investigated the local structure of a "Ge"-free NTE system, the $Cu_{1-x}Sn_xNMn_3$ with x= 0.1 and 0.5. On average, both compounds are cubic at all temperatures. At base temperature, the local structure is cubic as well. As the temperature rises however, local lattice distortions evidenced by the splitting of the Mn-Cu and Mn-Sn bonds are observed. This local distortion can be described by the I4/mcm symmetry but this symmetry is different from the P4/mmm symmetry of $SnNMn_3$. The splitting of the Mn-Cu and Mn-Sn bond gives rise to a local lattice anharmonicity that may in turn be significant in the NTE behavior in this class of compounds.

9:48AM V22.00010 Magneto-elastic coupling in molecule-based materials: $[Ru_2(O_2CMe)_4]_3[Cr(CN)_6]$ and $Mn[N(CN)_2]_2$[1] , T.V. BRINZARI, Q.-C. SUN, J.L. MUSFELDT, University of Tennessee, L.-C. TUNG, Y.J. WANG, National High Magnetic Field Laboratory, J. LIU, M.-H. WHANGBO, North Carolina State University, J.S. MILLER, University of Utah, J.L. MANSON, Eastern Washington University, J.A. SCHLUETER, Argonne National Laboratory — We measured the infrared vibrational response of two prototypical molecule-based magnets, $[Ru_2(O_2CMe)_4]_3[Cr(CN)_6]$ and $Mn[N(CN)_2]_2$. We find that both temperature and magnetic field driven transitions impact spin-lattice interactions in these materials. For instance, through the Néel transition, Cr–CN stretching and bending modes as well as Ru-O stretching mode in $[Ru_2(O_2CMe)_4]_3[Cr(CN)_6]$ display sudden frequency shifts and a strong hysteresis that reveal local structure changes around Cr and Ru centers in response to magnetic ordering. On the other hand, the dicyanamide ligands in $Mn[N(CN)_2]_2$ display pronounced sensitivity to the 30 T magnetic quantum critical transition, in line with our calculations that point toward the importance of N–C–N and C–N–C angles for the mediation of Mn$\cdots$Mn spin exchange interactions.

[1]This work is supported by the U.S. Department of Energy.

10:00AM V22.00011 Neutron diffraction study of the magnetic order in magnetic coordination polymer $CuF_2(H_2O)_2(pyz)$ (pyz=pyrazine) , CUIHUAN WANG, MARK D. LUMSDEN, ANDREW D. CHRISTIANSON, Oak Ridge National Laboratory, JOHN A. SCHLUETER, Material Science Division, Argonne National Laboratory — The new linear chain coordination polymer $CuF_2(H_2O)_2(pyz)$(pyz=pyrazine) provides an interesting example for the study of low dimensional physics. $CuF_2(H_2O)_2(pyz)$ has a monoclinic structure where the Cu^{2+} ions form a 2 dimensional (2D) square lattice in the bc-plane. Short range magnetic order appears below 10 K followed by a transition to long range antiferromagnetic order with $T_N \sim 2.6$ K. To further understand the magnetic behavior of $CuF_2(H_2O)(pyz)$, we have performed neutron diffraction experiments on deuterated single crystals $CuF_2(D_2O)_2(d_4\text{-pyz})$. Below 2.6 K we observe magnetic Bragg peaks which are consistent with the propagation vector (1/2 1 0). Refinement of the data shows that the magnetic moment lies in the ac-plane. Fitting the temperature dependence of the magnetic order parameter to a power-law form in the reduced temperature range of 1-T/T_N = 0.01-0.4 yields a critical exponent, β, of 0.25±0.01. This result is consistent with the expectation for a 2D XY model where β=0.23 [1].

[1] S. T. Bramwell and P. C. W. Holdsworth, J. Phys.: Condens. Matter. **5** L53-L59 (1993).

10:12AM V22.00012 Valence instability of Eu in $EuPd_3B_x$ $(0 < x < 0.53)$, ANDREAS LEITHE-JASPER, ROMAN GUMENIUK, MIRIAM SCHMITT, WILDER CARILLO-CABRERA, WALTER SCHNELLE, CHRISTOPH GEIBEL, HELGE ROSNER, MPI CPfS Dresden — In a joint theoretical and experimental study large series of intermetallic compounds $EuPd_3B_x$ and $GdPd_3B_x$ are characterized by X-ray diffraction, metallography, EPMA and chemical anlysis assessing the range of formation up to $x < 0.53$ and $x < 0.42$, respectively. Density functional based electronic structure calculations predict a valence change in $EuPd_3B_x$ above $x = 0.19(0.02)$ from a non-magnetic Eu^{3+} state into a magnetic Eu^{2+} state which is reflected in a discontinuity of the lattice parameter. Consistent with the calculations X-ray diffraction data show a kink in the lattice parameter at $x = 0.22(0.02)$. X-ray absorption spectroscopy measurements assign this kink to a transition into a heterogeneous mixed valence state of Eu. The influence of external pressure on the valence instability will be discussed.

10:24AM V22.00013 Efficient First-principles Wang-Landau Calculations , G. BROWN, Florida State University, A. RUSANU, KH. ODBADRAKH, M. EISENBACH, D.M. NICHOLSON, Oak Ridge National Laboratory — The Wang-Landau (WL) method of finding the density of states g(E) contributing to the partition function Z(kT) is useful for determining thermodynamic properties from first-principles energy calculations for magnetic systems. Since DFT calculations require significant computer resources, it is important to make the convergence of the WL method to a self-consistent g(E) as efficient as possible. We present approaches for making accurate initial estimates of g(E) based on similar Hamiltonians or estimates of g(E) for a different number of atoms. These approaches can include workstation-based calculations using classical Heisenberg Hamiltonians based on exchange parameters calculated from initial data from DFT WL calculations. In addition, we annunciate serveral insights we have gained into the convergence of the WL method. For instance, the minimum curvature of the calculated g(E) is limited by the update parameter and the maximum energy step of the Markov chain. This material is based upon work supported as part of the Center for Defect Physics, an Energy Frontier Research Center funded by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences. This research used resources of the Oak Ridge Leadership Computing Facility at Oak Ridge National Laboratory, which is supported by the Office of Science of the Department of Energy.

10:36AM V22.00014 First principles calculations of magnetic properties of Fe and Fe_3C at finite temperature , MARKUS EISENBACH, GREGORY BROWN, AURELIAN RUSANU, DON M. NICHOLSON, Oak Ridge National Laboratory — We demonstrate a method to investigate finite temperature magnetism from first principles that harnesses massively parallel computers to obtain the free energy, specific heat, magnetization, susceptibility, and other quantities as function of temperature by combining classical Wang-Landau Monte-Carlo calculations with a first principles electronic structure code that allows the energy calculation of constrained magnetic states. Here we will present our calculations of finite temperature properties such as specific heat, magnetization and susceptibility of Fe and Fe_3C using this approach where we find the Curie temperatures to be in good agreement with experiment at 980K and 425K respectively. This work was conducted at Oak Ridge National Laboratory (ORNL), which is managed by UT-Battelle for the U.S. Department of Energy (US DOE) under contract DE-AC05-00OR22725 and sponsored in parts by the Center for Nanophase Material Sciences, Scientific User Facilities Division, the Center for Defect Physics, an Energy Frontier Research Center funded by the US DOE Office of Basic Energy Sciences and by the US DOE Office of Energy Efficiency and Renewable Energy, Industrial Technologies Program. This research used resources of the Oak Ridge Leadership Computing Facility at ORNL, which is supported by the US DOE, Office of Science.

10:48AM V22.00015 Fist Principles Approach to the Magneto Caloric Effect: Application to Ni_2MnGa , KHORGOLKHUU ODBADRAKH, DON NICHOLSON, AURELIAN RUSANU, MARKUS EISENBACH, GREGORY BROWN, BOYD EVANS III, ORNL — The magneto-caloric effect (MCE) has potential application in heating and cooling technologies. In this work, we present calculated magnetic structure of a candidate MCE material, Ni_2MnGa. The magnetic configurations of a 144 atom supercell is first explored using first-principle, the results are then used to fit exchange parameters of a Heisenberg Hamiltonian. The Wang-Landau method is used to calculate the magnetic density of states of the Heisenberg Hamiltonian. Based on this classical estimate, the magnetic density of states is calculated using the Wang Landau method with energies obtained from the first principles method. The Currie temperature and other thermodynamic properties are calculated using the density of states. The relationships between the density of magnetic states and the field induced adiabatic temperature change and isothermal entropy change are discussed. This work was sponsored by the Laboratory Directed Research and Development Program (ORNL), by the Mathematical, Information, and Computational Sciences Division; Office of Advanced Scientific Computing Research (US DOE), and by the Materials Sciences and Engineering Division; Office of Basic Energy Sciences (US DOE).

Thursday, March 24, 2011 8:00AM - 10:36AM –
Session V23 DCMP: Superconductivity: Josephson Effects II D165

8:00AM V23.00001 Lorentzian crater in superconducting microwave resonators with inserted nanowires , ALEXEY BEZRYADIN, MATTHEW W. BRENNER, SARANG GOPALAKRISHNAN, JASEUNG KU, University of Illinois at Urbana-Champaign, NAYANA SHAH, University of Cincinnati, PAUL M. GOLDBART, University of Illinois at Urbana-Champaign — We report on observations of nonequilibrium pulsing states in microwave (i.e., GHz) coplanar waveguide(CPW) resonators consisting of superconducting MoGe strips interrupted by a trench and connected by one or more suspended superconducting nanowires. The Lorentzian resonance peak shows a "crater" when driven past the critical current of the nanowire, leading to a "pulsing" state. In the pulsing state, the supercurrent grows until it reaches the critical current, at which point all stored energy quickly dissipates through Joule heating. We develop a phenomenological model of resonator-nanowire systems, which explains the experimental data quantitatively. For the case of resonators comprising two parallel nanowires and subject to an external magnetic field, we find field-driven oscillations of the onset power for crater formation, as well as the occurrence of a new state, in which the periodic pulsing effect is such that only the weaker wire participates in the dissipation process.

8:12AM V23.00002 Characterizing Chiral Domains in Sr2RuO4 via Nanoscale Josephson Junctions[1] , D. BAHR, University of Illinois, J.D. STRAND, Syracuse University, D.J. VAN HARLINGEN, University of Illinois, Y. MAENO, Kyoto University — There is substantial evidence that the ruthenate superconductor Sr_2RuO_4 has a chiral order parameter of the form $p_x \pm ip_y$ and forms chiral domains. In order to verify this picture and determine the size of the domains, we have fabricated Josephson junctions on the order of and smaller than the domain width of $\sim 1\mu$m implied by Josephson interferometer experiments. Using Focused Ion Beam milling, we have patterned Sr_2RuO_4-Cu-PbIn junctions ranging in size from 0.5μm x 0.5μm to 4μm x 4μm on the edge face of a Sr_2RuO_4 crystal. By measuring the magnetic field modulation of the Josephson critical current, we can probe the phase anisotropy across the junction and determine the size and dynamics of chiral domains. Our data is consistent with the predicted domain width but also exhibits signatures that suggest the formation of chiral domain structure along the c-axis. The theoretical model of domain wall movement proposed by Bouhon and Sigrist is supported by our data.

[1]Work supported by the Department of Energy Basic Energy Sciences grant DE-FG02-07ER46453.

8:24AM V23.00003 Josephson effect and Andreev scattering in a three-terminal quantum dot in the Kondo regime , AKIRA OGURI, Osaka City University, YOICHI TANAKA, RIKEN — We study low-temperature transport through a single quantum dot (QD) connected to three terminals, consisting of two superconducting (SC) leads and one additional normal lead. This system shows interesting behavior caused by an interplay between Josephson, Andreev and Kondo physics. The low-energy excitations of this system can be described by a local Fermi liquid theory for the renormalized Bogoliubov particles. We calculate the renormalized parameters using the Wilson numerical renormalization group approach. The Kondo temperature and the residual interaction between the renormalized Bogoliubov particles depend sensitively on the Josephson phase ϕ at the crossover region between the local Cooper paring and the Kondo singlet. This crossover reflects the quantum phase transition between non-magnetic singlet and magnetic doublet states, which takes place in the case where the addition normal lead is disconnected. We will also discuss the results for the Josephson current and the DC conductance due to the Andreev reflection.

8:36AM V23.00004 Dissipation of mobile vortices in self-dual Josephson junction arrays , SAID SAKHI, American University of Sharjah — Mutual U(1) $\times$ U(1) Chern-Simons Landau-Ginzburg theory appears as an effective field theory in self-dual Josephson junction arrays. In this theory two complex fields associated with disordering electric and magnetic charges are minimally coupled to two gauge fields related to the currents of Cooper pairs and vortices. The condensation of disorder fields is employed to explore the various phases (superconducting, insulating, and metallic) of the model. In this work we investigate the interplay between the dissipation of mobile vortices and the condensation of magnetic and charge excitations. We evaluate the electromagnetic response functions of the system, and we analyze the longitudinal and the Hall conductivities as a function of the strength of dissipation.

8:48AM V23.00005 Measurement of a weak-link Josephson junction in a p-wave superconducting ring , JOONHO JANG, RAFFI BUDAKIAN, DAVID FERGUSON, University of Illinois at Urbana-Champaign, VICTOR VAKARYUK, Argonne National Laboratory, PAUL GOLDBART, University of Illinois at Urbana-Champaign, YOSHITERU MAENO, Kyoto University, Japan — We report the fabrication of a weak-link Josephson junction in a micron-size Sr_2RuO_4 ring by focused ion beam milling, and the measurement of the current-phase relation (CPR) using cantilever torque magnetometry. In the presence of a magnetic field applied perpendicular to the crystal $c-$axis, a second harmonic term in the CPR appears which may be related to the underlying spin texture of the spin-triplet condensate. The observed CPR is similar to that previously reported for weak-link junctions in ^{3}He-B. By including the contribution from both the charge and the spin current into the Gibbs-free energy, we can accurately model the observed CPR of the Sr_2RuO_4 weak-link junction.

9:00AM V23.00006 Periodic critical current pattern in the superconductor-graphene-superconductor junction induced by the current in one of the leads , ULAS COSKUN, UT Dallas, IVAN BORZENETS, GLEB FINKELSTEIN, Duke University — We have formed superconducting metal contacts to graphene, resulting in supercurrent through graphene visible up to several degrees Kelvin. In our geometry, graphene bridges a gap between two closely spaced superconducting wires. We have found that passing a current along the length of one of the wires periodically modulates the magnitude of the supercurrent through graphene. We discuss the origins of the observed interference patterns

9:12AM V23.00007 Intrinsic Josephson Junctions with Intermediate Damping[1] , PAUL A. WARBURTON, SAJID SALEEM, JON C. FENTON, University College London, SUSIE SPELLER, CHRIS R.M. GROVENOR, University of Oxford — In cuprate superconductors, adjacent cuprate double-planes are intrinsically Josephson-coupled. For bias currents perpendicular to the planes, the current-voltage characteristics correspond to those of an array of underdamped Josephson junctions. We will discuss our experiments on sub-micron Tl-2212 intrinsic Josephson junctions (IJJs). The dynamics of the IJJs at the plasma frequency are moderately damped (Q $\approx$ 8). This results in a number of counter-intuitive observations, including both a suppression of the effect of thermal fluctuations and a shift of the skewness of the switching current distributions from negative to positive as the temperature is increased. Simulations confirm that these phenomena result from repeated phase slips as the IJJ switches from the zero-voltage to the running state. We further show that increased dissipation counter-intuitively increases the maximum supercurrent in the intermediate damping regime (PRL vol. 103, art. no. 217002). We discuss the role of environmental dissipation on the dynamics and describe experiments with on-chip lumped-element passive components in order control the environment seen by the IJJs.

[1]Work supported by EPSRC.

9:24AM V23.00008 Intrinsic Josephson effect in $Bi_2Sr_2CaCu_2O_{8+\delta}$ after doping by current injection , S. PROBST, X.Y. JIN, Y. SIMSEK, C. STEINER, C. BERGMANN, Y. KOVAL, P. MÜLLER, Department of Physics and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg — By current injection we can change the properties of $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystals electronically in a wide range. In this work the properties of the same sample were changed multiple times in very small steps in order to investigate the doping process by current injection in greater detail. By measuring the IV characteristic of the intrinsic Josephson junctions as well as doping current and doping voltage simultaneously, the change of superconducting properties is monitored. Macroscopic quantum tunneling experiments in intrinsic Josephson junctions were performed. An exponential increase of the critical current density with hole concentration was observed. Simultaneously, the capacitance of the intrinsic Josephson junctions increases with the doping level by a factor of 5. We will discuss possible reasons for these results.

9:36AM V23.00009 Statistics of voltage fluctuations in resistively shunted Josephson junctions , MICHAEL MARTHALER, Institut fuer Theoretische Festkoerperphysik and DFG Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, 76128 Karlsruhe, DMITRY GOLUBEV, Karlsruhe Institute of Technology, Institut fuer Nanotechnologie, 76021 Karlsruhe, Germany, YASUHIRO UTSUMI, Department of Physics Engineering, Faculty of Engineering, Mie University 1577, Kurimamachiya-cho, Tsu, Mi-e, 514-8507, Japan, GERD SCHÖN, Institut fuer Theoretische Festkoerperphysik and DFG Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, 76128 Karlsruhe — The intrinsic nonlinearity of Josephson junctions converts Gaussian current noise in the input into non-Gaussian voltage noise in the output. For a resistively shunted Josephson junction with white input noise we determine numerically exactly the properties of the few lowest cumulants of the voltage fluctuations, and we derive analytical expressions for these cumulants in several important limits. The statistics of the voltage fluctuations is found to be Gaussian at bias currents well above the Josephson critical current, but Poissonian at currents below the critical value. In the transition region close to the critical current the higher-order cumulants oscillate and the voltage noise is strongly non-Gaussian. For coloured input noise we determine the third cumulant of the voltage.

9:48AM V23.00010 Josephson effect in S/F/S junctions: spin bandwidth asymmetry vs. Stoner exchange , HENRIK ENOKSEN, Norwegian University of Science and Technology, GAETANO ANNUNZIATA, Universita di Salerno, JACOB LINDER, Norwegian University of Science and Technology, MARIO CUOCO, CANIO NOCE, Universita di Salerno, ASLE SUDBO, Norwegian University of Science and Technology — We analyze the dc Josephson effect in a ballistic S/F/S junction in the quasiclassical Andreev approximation. We consider the possibility of ferromagnetism originating from a mass renormalization of carriers of opposite spin, i.e. a spin bandwidth asymmetry (SBAF). We provide a general formula for Andreev levels which is valid for arbitrary interface transparency, exchange interaction, and bandwidth asymmetry. We analyze the current-phase relation, the critical current, and the free energy in the short junction regime, showing that a larger number of $0-\pi$ transitions is expected when the ferromagnetism is driven by SBAF compared to Stoner magnetism. We compare the phase diagrams of two identical junctions differing only in the mechanism by which the mid layer becomes magnetic, pointing out that the phase difference across the junction in the ground state need not be the same, even for equal polarizations.

10:00AM V23.00011 Fluxon dynamics in two-band superconductor-based long Josephson junctions , BAL-RAM GHIMIRE, HAO-YU TSAI, JU KIM, Department of Physics and Astrophysics, UNIVERSITY OF NORTH DAKOTA TEAM — We investigate the phase dynamics of a long Josephson junction (LJJ) with two-band superconductors such as MgB_2 and iron pnictides. Due to two condensates in each superconductor layer, the phase dynamics of a two-band LJJ, described by the perturbed sine-Grodon equation, becomes more complex than that for the usual LJJ with one-band superconductors. This complexity arises from the presence of inter-band Josephson current that yields soliton-like excitation. This excitation represents a large stable variation of the phase difference of the two condensates. Accounting for the soliton- like excitation, we find that the fluxon dynamics in the LJJ with two-band superconductors is influenced by the modulation of Josephson current. The Josephson current modulation yields radiation emission by the moving fluxon. Also, we discuss the effects of this current modulation on the current- voltage characteristics of the LJJ.

10:12AM V23.00012 Enhancement of macroscopic quantum tunneling in Josephson junctions with multigap superconductors through zero-point fluctuations of Josephson-Leggett mode[1] , YUKIHIRO OTA, MASAHIKO MACHIDA, Japan Atomic Energy Agency, TOMIO KOYAMA, Tohoku Univ. — We theoretically study macroscopic quantum tunneling (MQT) in a hetero Josephson junction formed by a conventional single-gap superconductor and a multigap one such as MgB_2 and iron-based superconductors. In such a Josephson junction, multiple phase differences are defined and MQT dynamics are extended on a space expanded by the multiple phases. We clarify the quantum dynamics of the multiple phase differences and construct a theory for the MQT in Josephson junctions with multiple gaps. The dynamics of the phase differences are strongly affected by Josephson-Leggett mode, i.e., the fluctuation mode between the multiple phase differences and the escape rate characterizing MQT dynamics is calculated based on the effective action renormalized by the Josephson-Leggett mode. We show that the escape rate is drastically enhanced when the frequency of the Josephson-Leggett mode is less than the Josephson-plasma frequency.

[1]CREST(JST), JST-TRIP

10:24AM V23.00013 Parametric Amplification in Discrete Josephson Transmission Line , HAMID REZA MOHEBBI, A. MAJEDI MAJEDI, University of Waterloo, Institute for Quantum Computing — A Series-connected discrete Josephson transmission line (DJTL) which is periodically loaded by open stubs is studied to investigate various aspects of traveling-wave parametric amplification. The dispersion analysis is made to ensure the existence of three non-degenerate time-harmonic waves interacting with each other through the phase matching condition which is imposed by the cubic nonlinearity associated with each junction. Having weak nonlinearity and slow varying assumptions, we exploit the perturbation theory with the multiple scale technique to derive the three coupled nonlinear partial differential equations to describe their spatial and temporal amplitude variations in this parametric interaction. Cases of perfect phase-matching and slight mismatching are addressed in this work. The numerical analysis based on the spectral method in space and finite difference in time domain are used to monitor the unilateral gain, stability and bandwidth of the proposed structure. This structure can be used as a mesoscopic platform to study the creation of squeezed states of the microwave radiation. These properties make this structure desirable for applications ranging from superconducting optoelectronics to dispersive readout of superconducting qubits where high sensitivity, fast speed and low-noise operation is required.

Thursday, March 24, 2011 8:00AM - 10:00AM –
Session V24 FHP FIP: History of Physics and International Programs D167

8:00AM V24.00001 Castles in the Air: The Einstein-De Sitter Debate, 1916-1918 , CHARLES MIDWINTER, MICHEL JANSSEN, University of Minnesota — The Einstein De Sitter debate marked the birth of modern cosmology and the infamous cosmological constant. For Einstein, the controversy was essentially a philosophical one. Einstein's insistence on a static Universe and Mach's Principle guided him in the construction of his own cosmological model, and compelled him to criticize De Sitter's. For De Sitter, the debate began as idle conjecture. Before long, however, he began to wonder if the "spacious castles" he and Einstein had constructed might actually represent physical reality. We plan to write a volume that reproduces the documents relevant to the debate. Our commentary will retrace and explain the arguments of the historical players, complete with calculations. For the first time readers will be able to follow the arguments of Einstein and De Sitter in a detailed exploration of the first two relativistic cosmological models. Readers will see how Einstein's flawed criticisms of De Sitter were supported by Herman Weyl, and finally how Felix Klein settled the whole matter with a coordinate transformation.

8:12AM V24.00002 Ettore Majorana, Ugo Fano and Autoionization , ENNIO ARIMONDO, University of Pisa, CHARLES W. CLARK, Joint Quantum Institute, National Institute of Standards and Technology and University of Maryland, WILLIAM C. MARTIN, National Institute of Standards and Technology — In his brief career, Ettore Majorana posed some questions that remain of compelling interest today, such as the nature of the neutrino. Less remembered now is his virtuosity as an atomic theorist. His first published paper (1928) dealt successfully with complex atomic structures like those of Gd and U, using Fermi's statistical model which was only a few months old at the time. In the early 1930s he solved two outstanding problems of atomic spectroscopy, correctly interpreting them as involving multiply-excited discrete states of atoms that were embedded in single-electron continuua, and thus first identifying the phenomenon of autoionization in atomic spectra.[1] His unpublished notebooks[2] show that he grasped this phenomenon at a level of detail comparable to that of modern theory, which derives from the independent work of Ugo Fano.[3] We review Majorana's work on this subject and show how it still guides present understanding. [1]E. Arimondo, C. W. Clark and W. C. Martin, *Rev. Mod. Phys.* **82**, 1947 (2010) [2]E. Di Grezia and S. Esposito, *Found. Phys.* **38**, 228 (2008) [3]U. Fano, Nuovo Cimento **12**, 154 (1935); *Phys. Rev.* **124**, 1866 (1961); *J. Res. Natl. Inst. Stand. Technol.* **110**, 583 (2005)

8:24AM V24.00003 The Golden Age of Radio: Solid State's Debt to the Rad Lab[1] , JOSEPH D. MARTIN, University of Minnesota — While MIT's Radiation Laboratory is rightly celebrated for its contributions to World War II radar research, its legacy extended beyond the war. The Rad Lab provided a model for interdisciplinary collaboration that continued to influence research at MIT in the post-war decades. The Rad Lab's institutional legacy–MIT's interdepartmental laboratories–drove the Institute's postwar research agenda. This talk examines how solid state physics research at MIT was shaped by a laboratory structure that encouraged cross-disciplinary collaboration. As the sub-discipline of solid state physics emerged through the late-1940s and 1950s, MIT was unique among universities in its laboratory structure, made possible by a large degree of government and military funding. Nonetheless, the manner in which MIT research groups from physics, chemistry, engineering, and metallurgy interfaced through the medium of solid state physics exemplified how the discipline of solid state physics came to be structured in the rest of the country. Through examining the Rad Lab's institutional legacy, I argue that World War II radar research, by establishing precedent for a particular mode of interdisciplinary collaboration, shaped the future structure of solid state research in the United States.

[1]Research supported by a grant-in-aid from the Friends of the Center for the History of Physics, American Institute of Physics.

8:36AM V24.00004 Willie Hobbs Moore (1934-1994): The First Female African American Physicist , RONALD MICKENS, Clark Atlanta University — We discuss the life and career of Willie Hobbs Moore, the first African American woman to receive a doctorate degree in physics. This achievement occurred in June 1972 at the University of Michigan, Ann Arbor, MI. Her dissertation, directed by the renowned spectroscopist Samuel Krimm, was on the subject of "A Vibrational Analysis of Secondary Chlorides," and focused on a theoretical analysis of the secondary chlorides for polyvinal-chlorine polymers. From 1972–1977, she, Krimm, and collaborators published more than thirty papers on this and related research issues. In addition to an overview of her family background, her careers as a research physicist and scientist working in various industrial laboratories, we discuss the obstacles and successes she encountered at various stages of her life.

8:48AM V24.00005 Encounters with John Van Vleck: Elevating the Self-Esteem of an Experimentalist , JAMES WYNNE, IBM TJ Watson Research Center — As a Harvard freshman in 1960, John H. Van Vleck was assigned to guide me through physics course selections. As a Harvard first year graduate student in 1964, I took his course on Group Theory. He was an esteemed theoretician, and I was an experimentalist. Nevertheless, I liked him, and he both educated me and gave me good advice. Later, I learned that Van Vleck was responsible for bringing Nicolaas Bloembergen, my Ph. D. advisor, back to Harvard from Holland, with a faculty appointment in the Division of Engineering and Applied Physics. (Bloembergen had done his Ph.D. thesis with Ed Purcell, making NMR into a science, and Purcell was one of the best teachers I encountered in 9 years at Harvard.) Stepping forward in time to May, 1969, just after defending my doctoral thesis, I ran into Van Vleck in the hallway. I told him I had earned my Ph.D., and he asked me what I had done for my thesis. Feeling defensive while talking to a great theoretician, I started out cautiously to say that I had built a carbon dioxide laser. He immediately started praising me as the best of the breed, someone who could build things and actually make them work. The praise continued, he told some stories (which I will share), and I left the building on "Cloud 9." It was a really good day.

9:12AM V24.00006 US-Finland Planning Visit: Cooperative Research and Education Activities in Integrated Access Networks[1] , ARLENE MACLIN, Morgan State University, UNIVERSITY OF ARIZONA-CIAN COLLABORATION, AALTO UNIVERSITY IN FINLAND COLLABORATION — This planning grant visit sponsored by the NSF Office of International Science and Engineering occurred from October 3-10, 2010. The Dean of the School of Computer, Mathematical and Natural Sciences from Morgan State University (MSU), the PI and a faculty member from engineering at MSU along with a faculty member from the University of Arizona and two advanced level graduate students from the NSF-funded Center for Integrated Access Networks participated in this visit. The topic of novel low dimensional nano-materials was determined to be one possible area for future collaboration. As a result of this visit, a Materials World Network proposal has been submitted to the NSF involving MSU and CIAN in the US and Aalto University in Finland. A companion proposal on novel low dimensional nano- materials has also been submitted to the Academy of Finland. Another anticipated outcome of this collaboration of MSU with Aalto University and CIAN expands the outreach and diversity component to MSU, an institution serving largely an underrepresented minority student.

[1]Sponsor for this work was NSF # 1042309.

9:24AM V24.00007 ABSTRACT WITHDRAWN –

9:36AM V24.00008 ABSTRACTWITHDRAWN –

9:48AM V24.00009 ABSTRACT WITHDRAWN –

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V25 DCMP: Superconductivity: HTSC Theory, Mostly Nematics and Inhomogeneous Systems D166

8:00AM V25.00001 The role of nematic fluctuations in the thermal melting of pair-density-wave phases in superconductors[1] , DANIEL BARCI, Department of Physics, Universidade Estadual do Rio de Janeiro, Brazil, EDUARDO FRADKIN, Department of Physics, University of Illinois — We study properties of phase transitions of the superconductor liquid crystal phases, and analyze the competition between the recently proposed Pair Density Wave (PDW) and nematic $4e$ superconductor (4eSC). Nematic fluctuations enhance the 4eSC and suppress the PDW phase. For a system decoupled from a lattice, the PDW state exists only at $T = 0$ and the low temperature phase is a nematic $4e$SC with short ranged PDW order.

[1]This work was partially supported by CNPq and FAPERJ, by NSF grant DMR 0758462, and by DOE, under Contract DE-FG02-91ER45439

8:12AM V25.00002 Nematicity in 3-band Hubbard model of cuprate superconductors , KYUNGMIN LEE, JUNPING SHAO, Cornell University, RICHARD SCALETTAR, University of California - Davis, MICHAEL LAWLER, SUNY Binghamton, EUN-AH KIM, Cornell University — The recent discovery of intra-unit-cell nematicity in STM studies of cuprate superconductors [1] underscores the importance of the role played by oxygen orbitals in CuO2 plane. Motivated by this observation we study 3-band Hubbard model using exact diagonalization. In particular, we investigate the effects various interaction parameters (Ud, Up, Vpd, Vpp) have on nematicity. Interestingly, we find that Ud, the on-site repulsion at copper sites, enhances nematicity in the strongly coupled regime.

[1] Lawler, M. J. *et al.* Intra-unit-cell electronic nematicity of the high-Tc copper-oxide pseudogap states. *Nature* **466**, 347 (2010).

8:24AM V25.00003 Mean-Field Nematic Phase Diagram for the Three-Band Hubbard Model , MARK H. FISCHER, LASSP, Department of Physics, Cornell University, MICHAEL J. LAWLER, Department of Physics, Applied Physics and Astronomy, Binghamton University, EUN-AH KIM, LASSP, Department of Physics, Cornell University — We map out the phase diagram of the three-band Hubbard model of a CuO_2 plane for nematic order in the parameter space of various on-site and nearest-neighbor interactions. For this, we define an intra-unit cell nematic order parameter in terms of a charge imbalance between the two oxygen sites in the unit cell and employ a self-consistent mean-field analysis. This study is motivated by recent STM experiments on high-T_c cuprate superconductors pointing towards intra-unit cell nematicity.

8:36AM V25.00004 Dynamical electronic nematicity from Mott physics , SATOSHI OKAMOTO, Materials Science and Technology Division, Oak Ridge National Laboratory, DAVID SENECHAL, Department de Physique and RQMP, Universite de Sherbrooke, MARCELLO CIVELLI, Laboratoire de Physique des Solides, Univ. Paris-Sud, ANDRE-MARIE TREMBLAY, Department de Physique and RQMP, Universite de Sherbrooke, and Canadian Institute for Advanced Research — We study the two-dimensional Hubbard model with small band anisotropy using dynamical-mean-field theory for clusters. We found that very large transport anisotropies can be induced by very small band anisotropy as in many strongly correlated materials. This happens when the interaction is large enough to yield a Mott transition. The maximum effect on conductivity anisotropy occurs in the underdoped regime as observed in high temperature superconductors. The anisotropy decreases at large frequency and is not associated with static stripe order. Thus we call the phenomenon "dynamical electronic nematicity". This work was supported by the Materials Sciences and Engineering Division, Office of Basic Energy Sciences, U.S. DOE (S.O.), NSERC (Canada) and the Tier I Canada Research Chair Program (A.- M.T.), with part of the computational resources by RQCHP and Compute Canada.

8:48AM V25.00005 Quantum Nematic Physics in the Hubbard Model of Cuprate Superconductors , SHI-QUAN SU, GONZALO ALVAREZ, MICHAEL SUMMERS, THOMAS MAIER, Oak Ridge National Lab — Recent experiments have provided strong evidence that quantum electronic nematic order plays an important role in characterizing the pseudogap region of the cuprate superconductors. Starting from the generic Hubbard model of the cuprates, we introduce a small anisotropy in the hopping integral to model a small orthorhombic distortion. We perform a dynamic cluster quantum Monte Carlo approximation of this model, in order to study the effects of this anisotropy on various properties. In particular, we investigate the effects on superconductivity and pseudogap behavior, as well as the competition between different effects.

9:00AM V25.00006 On the origin of quantum criticality found at finite doping in 2D Hubbard model[1] , SHUXIANG YANG, HERBERT FOTSO, JUANA MORENO, MARK JARRELL, Louisiana State University — To better understand the excitations responsible for quantum criticality (QC) found at finite doping in the 2D Hubbard model, we analyze the vertices for different scattering channels obtained from the Dynamical Cluster Continuous-Time Quantum Monte Carlo simulation. By decomposing these vertices using the parquet equations we find that both superconductivity and the charge instabilities responsible for the QC come from the crossed spin channel contribution, and thus are driven by the spin-fluctuations. On contrast, the spin instability comes from the fully irreducible spin vertex contribution.

[1]We acknowledge the support from NSF OISE-0730290 and DOE SciDAC DE-FC02-06ER25792

9:12AM V25.00007 Superconductivity from purely repulsive interactions in the 2D electron gas , SRINIVAS RAGHU, Rice University, STEVEN KIVELSON, Stanford University — We present a well-controlled perturbative renormalization group (RG) treatment of superconductivity from short-ranged repulsive interactions in a variety of model two dimensional electronic systems. Our analysis applies in the limit where the repulsive interactions between the electrons are small compared to their kinetic energy.

9:24AM V25.00008 Effect of competing orders on superconductivity in the Hubbard model , WEEJEE CHO, Stanford University, SRINIVAS RAGHU, Rice University, STEVEN KIVELSON, Stanford University — We study the superconducting transition in the repulsive Hubbard model incorporating different competing orders at the mean field level. To the model on the square lattice with nearest and next-nearest neighbor hopping amplitudes, we add appropriate modulations of the hopping terms or onsite energies, such that they produce the desired broken symmetry. We then study the superconducting instability in the (theoretically tractable) limit in which the onsite repulsion U is small compared to the bandwidth. We obtain the pairing symmetry and strength as a function of the magnitude of the order parameter. Specific cases of broken symmetry states we study include antiferromagnetism, ferromagnetism, nematic order, d-density wave, and orbital loop order.

9:36AM V25.00009 d-wave Cooper pairing in multiband models for the high-T_c cuprates , CARSTEN HONERKAMP, STEFAN UEBELACKER, RWTH Aachen — We investigate possible reasons for the significant differences of T_cs in high-T_c cuprate compounds, based on renormalization group treatments of downfolded models for the electronic structure. Generally, cuprates with a square like Fermi surface exhibit lower critical temperatures than materials with a more rounded Fermi surface, which contradicts with many theoretical studies of the one band Hubbard model. To resolve this contradiction we study multiband models which in addition to the d_{x2-y2} orbital contain $4s$ and d_{z2} orbitals using different approximation levels of the functional renormalization group technique. Our results suggest that the observed material trend can be explained in parts by the influence of orbital mixing, which can dominate over the effect of the Fermi surface shape.

9:48AM V25.00010 Inhomogeneity and d-wave superconductivity in the Hubbard model[1] , S. CHAKRABORTY, D. SÉNÉCHAL, A.-M.S TREMBLAY, Dept. de physique, RQMP, Sherbrooke — Whether or not inhomogeneity plays a significant role in determining the superconducting properties of the cuprate high-Tc superconductors remains an open issue, in spite of extensive theoretical and experimental focus. To this end, we study d-wave superconductivity in the checkerboard Hubbard model on a square lattice. We employ the Cellular Dynamical Mean Field theory method with an exact diagonalization solver at zero temperature. The d-wave order parameter is computed for various inhomogeneity levels over the entire doping range of interest. We find a monotonic decrease in the maximum amplitude of the superconducting order parameter with inhomogeneity. However, the order parameter increases with inhomogeneity in a small doping interval lying in the extreme overdoped regime. For any doping, an inhomogeneity-induced change in the height of the lowest energy peak in the antiferromagnetic spin susceptibility correlates with the change in amplitude of the order parameter.

[1]Supported by NSERC (Canada), CRC (A.-M.T.), RQCHP and Compute Canada.

10:00AM V25.00011 Disorder effects on pair binding in the checkerboard Hubbard model , PETER SMITH, MALCOLM KENNETT, Simon Fraser University — The checkerboard Hubbard model is an inhomogeneous fermionic Hubbard model in which hopping on plaquettes takes a different value to hopping between plaquettes. The pair binding energy in the clean checkerboard Hubbard model, interpreted as a tendency towards superconducting order, is positive over a wide part of the zero temperature phase diagram. We perform exact diagonalization studies of the checkerboard Hubbard model with on-site disorder. For systems up to twelve sites, we study the distribution of pair binding energies that results from the introduction of potential disorder and find that weak disorder enhances the region of the phase diagram over which there is a non-zero probability of pair binding, without greatly changing the average pair binding energy. We also study how stronger disorder destroys pair binding.

10:12AM V25.00012 Theoretical investigation of superconductivity and antiferromagnetism in trilayer cuprate superconductors , YAN CHEN, Fudan University, China — Recent ARPES experiment on the optimally doped trilayer cuprate superconductors Bi2223 has revealed a layer variation of both doping density and d-wave gap. In particular, the two outer layers are overdoped with a gap which is larger than the gap for optimally doped single layer cuprates while the inner layer is underdoped with an even larger gap. Here we propose a minimal model composed of three layer t-J model, single particle interlayer tunneling as well as Cooper pair tunneling terms. By using renormalized mean field method, both the superconducting (SC) and antiferromagnetic (AFM) properties are theoretically investigated. Both tunneling effects may influence the phase configurations of both d-wave SC and AFM order parameters on each layer which plays a crucial role in determining the electronic structures of trilayer cuprates. In particular, the inphase state for both SC and AFM phases is found to be relevant to the Bi2223 trilayer system. In such a state, the superconducting order parameter of inner plane will be further enhanced due to the constructive proximity effect from the two outer planes and the hole density of inner plane will be much suppressed. Furthermore we predict that the appearance of interlayer ferromagnetic correlations for such system which could be tested by future NMR experiments. **This work is in collaboration with Chun Chen and A. Fujimori.

10:24AM V25.00013 Confinement-deconfinement interplay in quantum phases of doped Mott insulators , PENG YE, Institute for Advanced Study, Tsinghua University, Beijing, 100084, P. R. China, CHU-SHUN TIAN, Institute of Theoretical Physics, Cologne University, D-50937 Cologne, Germany, XIAO-LIANG QI, Department of Physics, Stanford University, Stanford, CA 94305, USA, ZHENG-YU WENG, Institute for Advanced Study, Tsinghua University, Beijing, 100084, P. R. China — It is generally accepted that doped Mott insulators can be well described by the t-J model. In the latter, the electron fractionalization is dictated by the phase string effect. We found that in underdoped regime, the antiferromagnetic and superconducting phases are dual: in the former, holons are confined while spinons are deconfined, and vice versa in the latter. These two phases are separated by a novel phase, the so- called Bose-insulating phase, where both holons and spinons are deconfined. A pair of Wilson loops was found to constitute a complete set of order parameters determining this zero- temperature phase diagram. The quantum transitions between these phases are suggested to be of non-Landau-Ginzburg-Wilson type.

10:36AM V25.00014 FLEX calculation of the pairing state symmetry and quasiparticle excitations for $SrRu_2O_4$, JOHN DEISZ, Department of Physics, University of Northern Iowa — We calculate the superconducting phase diagram for a two-dimensional, three-band tight-binding model of $SrRu_2O_4$ using the fluctuation exchange approximation (FLEX). Electron interactions are modeled by an atomically-local interaction with intra-band, inter-band and exchange terms and an atomically-local spin-orbit interaction is included as well. Preliminary results suggest that FLEX produces a singlet-pairing state with $d_{x^2-y^2}$ orbital symmetry, a result that is not in agreement with many experimental results. However, we do find that the values for the interaction strengths that are required to generate $T_c \simeq 1.5\,K$ lead to normal state quasiparticle line widths that are in reasonable agreement with experimental results.

10:48AM V25.00015 Diagrammatic Quantum Monte Carlo Solution of Two dimensional Cooperon-Fermion model , KAIYU YANG, ETHZ & Boston College — We investigate the two-dimensional Cooperon-fermion model in the strong coupling limit with continuous-time diagrammatic determinant quantum monte carlo (DDQMC). We obtained the same Kosterlitz-Thouless transition temperature T_c for the fermion's off-diagonal long range order χ_{OD} ($\boldsymbol{k}$=0,$\omega = 0$) and cooperon's Greens function $G^b(\boldsymbol{k}$=0,$\omega = 0)$ as expected. The renormalized cooperon's band (band gap and mass) is examined carefully. The delocalization of the cooperons enhances the diamagnetism. When applied to study the diamagnetism of pseudogap state in high-T_c cuprate, the results we obtained is in good agreement with recent torque magnetization measurements.

Thursday, March 24, 2011 8:00AM - 10:48AM –

Session V26 DMP DCOMP: Focus Session: Iron Based Superconductors – Doping Studies D162/164

8:00AM V26.00001 Isotope substitution induced lattice expansion in the iron based superconductors , MATS GRANATH, University of Gothenburg, OLEG KIM, ITAI PANAS, Chalmers University of Tech. — In the iron based superconductors there are indications of a wide range of exponents for the iron isotope effect on Tc in different families of these materials. In this work we explore to what extent this spread of exponents may be a result of different isotope induced lattice expansions in combination with an extreme sensitivity of Tc to the interatomic distances. We estimate the magnitude of anharmonicity in the dominant Fe-As(Se) bond based on a model fit of the temperature dependence of Raman phonon frequencies. Using a variational approach to treat the effect of the anharmonic potential we calculate the magnitude and sign of the expansion of lattice parameters and interatomic distances due to Fe isotope substitution in several different iron-based superconductors.

8:12AM V26.00002 Doping evolution of the electronic structure in $Ba(Fe_{1-x}Co_x)_2As_2$ as revealed by polarization dependent ARPES and soft X-ray absorption , PAOLO VILMERCATI, CHRISTINE CHENEY, University of Tennessee Knoxville, SUNG-KWAN MO, Lawrence Berkely National Laboratory, FEDERICA BONDINO, ELENA MAGNANO, Consiglio Nazionale delle Ricerche, MARCO MALVESTUTO, Sictrotrone Trieste, ATHENA SEFAT, MICHAEL MCGUIRE, BRIAN SALES, DAVID SINGH, DAVID MANDRUS, Oak Ridge National Laboratory, NORMAN MANNELLA, University of Tennessee Knoxville — Here we present a study based on ARPES and X-ray absorption spectroscopies in order to unveil the electronic structure evolution upon Co-doped in BaFe2As2 high Tc superconductors, for the doping levels x=(0,6,8,12,22)%. This study focuses on two points: i) the effective role of Co at different doping levels; ii) the shift upon doping of the band structure. X-ray absorption experiments carried out at the Co L23 edge highlight the chemical state of cobalt at the various doping levels, thus unveiling its role as charge donor. The orbital selectivity of polarization dependent ARPES is used to show the filling evolution of each band. The spectra have been collected in different geometries along the ΓX and ΓM high symmetry crystallographic directions and at two different photon energies. The experimental results show a general rearrangement of the charge within the various orbitals upon doping, with a non rigid band shift.

8:24AM V26.00003 Doping dependence of the optical spectra in $Fe_{1.02}Te_{1-x}Se_x$ [1] , CATALIN MARTIN, X. XI, K. MILLER, D. KOUKIS, University of Florida, J. HU, Z.Q. MAO, Tulane University, G.L. CARR, Brookhaven National Laboratory, D.B. TANNER, University of Florida — We measured the optical reflectivity and extracted the optical conductivity over a broad spectral range of the Fe-chalcogenide $Fe_{1.02}Te_{1-x}Se_x$, at various doping levels, from x=0.12 to x=0.45. Except for the highest concentration of Se (x=0.45), optical properties show unusual frequency and temperature dependence. The zero frequency Drude peak is absent in optical conductivity, a plasma edge cannot be unambiguously defined and both reflectivity and optical conductivity have non-monothonic temperature dependence. For the superconducting samples, we found a weak enhancement of the reflectivity in the far-infrared region upon cooling below Tc and its possible association with the superconducting gap will be discussed.

[1]Supported by the US DOE through contracts DE-FG02-02ER45984 and DE-AC02-98CH10886.

8:36AM V26.00004 Doping-Induced Evolution of Superconducting Order Parameter in Ba(Fe1-xNix)2As2 Single Crystals[1] , CONG REN, Laboratory for Superconductivity, Institute of Physics, China, ZHAOSHENG WANG, HUIQIAN LUO, HUAN YANG, LEI SHAN, HAIHU WEN, Laboratory for Superconductivity, IOP — We report a systematic investigation on the c-axis point-contact Andreev reflection (PCAR) in $BaFe_{2-x}Ni_xAs_2$ superconducting single crystals with the Ni concentrations from underdoped to overdoped regions ($0.075 \leq x \leq 0.15$). At low temperatures, an in-gap peak at low-bias voltage is observed in PCAR for overdoped samples, in contrast to the case of underdoped junctions, in which an in-gap plateau is observed. The spectra are fitted using a generalized Blonder- Tinkham-Klapwijk (BTK) formalism with two gaps: one isotropic and another angle dependent. The second gap, resulted from the fitting, shows a clear crossover from a nodeless in the underdoped side to a nodal feature in the overdoped region. This intriguing observation provides strong evidence of the doping induced evolution of the superconducting order parameter when the inter-pocket and intra-pocket scattering are tuned through doping, as expected in the $s_{\pm}$ scenario.

[1]This work is supported by the Natural Science Foundation of China, the Ministry od Science and Technology of China.

8:48AM V26.00005 First-principles study of light-element doping effects on iron-based superconductors , HIROKI NAKAMURA, MASAHIKO MACHIDA, Japan Atomic Energy Agency — Since the discovery of the iron-based superconductor, $LaFeAsO_{1-x}F_x$ whose Tc reached 26K, various types of iron-based superconductors have been fabricated to attain higher T_c. Recently, it is reported that Tc of an iron-based superconductor $LaFeAsO_{1-y}$ is enhanced to 35K by doping hydrogen. This result implies that atoms of light elements penetrate into the crystal of iron-based superconductors and transform their structures into more useful ones for superconductivity. In this talk, we investigate how the light elements are doped in the iron-based superconductors by using the first-principles density functional theory. Furthermore, we evaluate the effects of doping on the crystal structures and electronic states and explore the origin of the T_c enhancements.

9:00AM V26.00006 Electron spin resonance in iron pnictides , H.-A. KRUG VON NIDDA, J. DEISENHOFER, N. PASCHER, S. SCHAILE, E. DENGLER, A. LOIDL, Experimentalphysik V, Center for Electronic Correlations and Magnetism, Institute for Physics, Augsburg University, D-86135 Augsburg, Germany, H.S. JEEVAN, P. GEGENWART, I. Physik. Institut, Georg-August-Universitaet Goettingen, D-37077 Goettingen, Germany — We report on electron spin resonance studies in Eu based 122-superconductors where the Eu^{2+} ions serve as a probe of the normal and superconducting state. In polycrystalline $Eu_{0.5}K_{0.5}Fe_2As_2$ the spin-lattice relaxation rate $1/T_1^{\rm ESR}$ obtained from the ESR linewidth exhibits a Korringa-like linear increase with increasing temperature above T_c evidencing a normal Fermi-liquid behavior. Below T_c the spin lattice relaxation rate $1/T_1^{\rm ESR}$ follows a $T^{1.5}$-behavior without any appearance of a coherence peak. In superconducting $EuFe_2As_{1.8}P_{0.2}$ single crystals we find a similar Korringa slope in the normal state and observe anisotropic spectra for measuring with the external field parallel and perpendicular to the c-axis. In addition, we will discuss the ESR properties of selected systems from the 1111 and 11 families.

9:12AM V26.00007 Effect of Isoelectronic Doping at the As Site in Iron-based Superconducting Systems , GUANG-HAN CAO, Department of Physics, Zhejiang Uinversity — FeAs-based superconductivity can be induced with various doping strategies—either electron doping, hole doping or isoelectronic doping. In this talk, we will focus on the unique isoelectronic doping at the As site. By using different dopants such as P [1,2] or Sb [3], positive or negative chemical pressure can be generated onto the FeAs layers. The positive chemical pressure suppresses/destroys the spin-density-wave (SDW) ordering, and then superconductivity emerges around a quantum critical point. In contrast, the negative pressure tends to recover the suppressed/hidden SDW ordering. The isoelectronic doping also influences the electronic and magnetic state of 4f electrons in the rare-earth atomic layers and 3d electrons of the Fe planes, especially in the case of proximity between 4f and 3d energy levels. This was manifested by the observation of local-moment ferromagnetism of 4f electrons in $EuFe_2(As_{1-x}P_x)_2$, $CeFeAs_{1-x}P_xO$ and $CeFeAs_{1-x}P_xO_{0.95}F_{0.05}$ [4] systems. Our results demonstrate the intriguing interplay/competition of intersite RKKY coupling among 4f-moments, intrasite Kondo interaction between 4f- and 3d- electrons, and **k**-space Cooper pairing of 3d electrons. This work was done in collaboration with Zhu-An Xu and Jian-Hui Dai, and was supported by National Basic Research Program of China (Grant Nos. 2007CB925001 and 2010CB923003).

[1] Zhi Ren et al., *Phys. Rev. Lett.* 102, 137002 (2009).
[2] C. Wang et al., *EPL* 86, 47002 (2009) ; S. Jiang et al., *JOP-CM* 21, 382203 (2009) .
[3] C. Wang et al., *Science China G* 53, 1225 (2010).
[4] Y. K. Luo et al., *Phys. Rev. B* 81, 134422 (2010) ; Y. K. Luo et al., to be published.

9:48AM V26.00008 Suppression of critical temperature in proton irradiated $Ba(Fe_{1-x}Co_x)_2As_2$, YASUYUKI NAKAJIMA, University of Tokyo, JST- TRIP, TOSHIHIRO TAEN, YUJI TSUCHIYA, University of Tokyo, TSUYOSHI TAMEGAI, University of Tokyo, JST- TRIP, HISASHI KITAMURA, TAKESHI MURAKAMI, NIRS — The study on the superconducting gap structure of iorn-pnictide superconductor is one of the most important issues to uncover the pairing mechanism of high temperature superconductivity. To elucidate the superconducting gap structure, a detailed study on the effect of defects is very crucial because the pair-breaking effects due to scattering centers are phase-sensitive. We report the suppression of T_c due to the pair- breaking effect introduced by 3 MeV proton irradiation in $Ba(Fe_{1-x}Co_x)_2As_2$ single crystals at under-, optimal-, and over-doping levels. We find that T_c decreases and residual resistivity increases monotonically with increasing the proton dose. We also find no resistive upturn at low temperatures, which suggests that the proton irradiation provides nonmagnetic scattering centers. The critical scattering rate for all samples estimated by three different ways is much higher than that expected in $s_{\pm}$-pairing scenario based on inter-band scattering due to antiferro-magnetic spin fluctuations.

10:00AM V26.00009 Nanometer Scale Phase Separation and Chemical Inhomogeneity in the Iron Chalcogenide Superconductor $Fe_{1+y}Te_xSe_{1-x}$, HEFEI HU, JIAN-MIN ZUO, University of Illinois at Urbana-Champaign, JINSHENG WEN, ZHIJUN XU, ZHIWEI LIN, QIANG LI, GENDA GU, Brookhaven National Laboratory, WAN KYU PARK, LAURA GREENE, University of Illinois at Urbana-Champaign — We report direct evidences of phase separation and chemical inhomogeneity in $Fe_{1+y}Te_xSe_{1-x}$ single crystals from scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy (EELS). In STEM, images recorded using an annular dark field (ADF) detector show characteristic nanometer scale patterns of phase separation from the Z dependent contrast. The separation was observed in both non-superconducting samples with excess iron as well as superconducting samples. Using the line scan EELS technique, we determined ~20%, or less, fluctuation in Te concentration from the local average compositions by integrating the intensity of the Te-$M_{4,5}$ edge. The energy-loss near-edge structure (ELNES) of the Fe-$L_{2,3}$ edge changes as the composition varies, especially the L_3 and L_2 ratio, which is sensitive to the d-state occupancy of the Fe atom. The results suggest a miscibility gap in the $Fe_{1+y}Te_xSe_{1-x}$ system and changes in the d-electron states at the nanometer scale from the separated phases.

10:12AM V26.00010 Local topography and spectroscopy of the doped chalcogenide $FeTe_xSe_{1-x}$[1] , XIAOBO HE, GUORONG LI, JIANDI ZHANG, RONGYING JIN, Louisiana State University, Baton Rouge, LA 70803, USA, A.S. SEFAT, M.A. MCGUIRE, B.C. SALES, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, D. MANDRUS, University of Tennessee, Knoxville, TN, 37996, E.W. PLUMMER, Louisiana State University, Baton Rouge, LA 70803, USA — The atomically resolved structural and electronic properties of FeTe and $FeTe_{0.55}Se_{0.45}$ have been investigated using scanning tunneling microscopy/spectroscopy. The STM topography of the doped sample clearly distinguishes two types of atoms. Statistically the topography shows the correct concentration of the two species and reveals that they are not randomly distributed but prefer to congregate with tens of identical atoms in nanometer scale. Consequently, in contrast to extremely flat surface of parent compound FeTe, $FeTe_{0.55}Se_{0.45}$ shows structural phase separation globally breaking the pure *p4/nmm* symmetry. Surprisingly the local density of states on tellurium and selenium atoms in $FeTe_{0.55}Se_{0.45}$ are identical, but not the same as that in pure FeTe. This indicates an itinerant (rather than localized) electronic character in this doped system. This behavior is opposite to phase separation in many other doped materials.

[1]Supported by NSF DMR-1002622.

10:24AM V26.00011 Revealing the electronic structure of the iron pnictides with electron energy-loss spectroscopy , J.C. IDROBO, W. ZHOU, Vanderbilt U./ORNL, M.F. CHISHOLM, ORNL, M.P. PRANGE, Vanderbilt U./ORNL, A.S. SEFAT, M.A. MCGUIRE, B.C. SALES, ORNL, S.J. PENNYCOOK, ORNL/Vanderbilt U., S.T. PANTELIDES, Vanderbilt U./ORNL — We report electron energy-loss spectroscopy (EELS) studies of the parent compounds (LnFeAsO, Ln=La, Ce, Pr, Nd, Sm, Gd) using scanning transmission electron microscopy. We find that all the studied LnFeAsO present a Fe L-edge fine structure closer to that of metallic iron than iron oxides. We observe a direct correlation between the Fe valence state (obtained from EELS) and T_C, i.e. the smaller the calculated Fe valence state, the larger is the T_C for that compound. We also find an anomalous crystallographic orientation-dependence of the Ln M_{45} edge fine structure. In particular, we find difference in the apparent crystal field splitting of Ce and Gd f- bands when the spectra are collected parallel and perpendicular to the c-axis. This research was partially supported by NSF Grant No. DMR-0938330 (JCI, WZ), by ORNL's Shared Research Equipment (SHaRE) User Facility, which is sponsored by the Office of Basic Energy Sciences, U.S. Department of Energy (JCI) and the Office of Basic Energy Sciences, Materials Sciences and Engineering Division, U.S. Department of Energy (MC, ASS, MAM, BCS & SJP), DOE grant DE- F002-09ER46554 (MP, STP), and by the McMinn Endowment (STP) at Vanderbilt University.

10:36AM V26.00012 Doping dependent vortex pinning in single crystal $BaFe_2(As_{1-x}P_x)_2$, LEI FANG, Y. JIA, Argonne National Laboratory, Argonne, IL 60439, USA, C. CHAPARRO, Argonne National Laboratory and Department of Physics, University of Notre Dame, J. SCHLUETER, Argonne National Laboratory, Argonne, IL 60439, USA, Z.L. XIAO, Argonne National Laboratory and Northern Illinois University, H. HELMUT, A.E. KOSHELEV, U. WELP, G.W. CRABTREE, W.K. KWOK, Argonne National Laboratory, Argonne, IL 60439, USA — We report on magnetization measurements on doped single crystals of superconducting $BaFe_2(As_{1-x}P_x)_2$. For optimum doped crystals, we observe a second magnetization peak effect (fish tail). With further doping of phosphur for arsenic, the fish tail effect evolves into a peak effect close to H_{c2}, similar to that found in conventional type II superconductors. In heavily overdoped crystals, the magnetization loop is mostly reversible and no peak effect is observed. The evolution of the peak effect with doping is attributed to the reduction in defects as the crystal's purity is increased, going from optimum doping to over-doping. Possible pinning mechanism for the peak effect will be discussed within the framework of recent heat capacity and resistivity measurements.

Thursday, March 24, 2011 8:00AM - 10:48AM –

Session V27 GQI: Focus Session: Semiconductor Qubits- Dynamic Decoupling, Dephasing, and Relaxation C155

8:00AM V27.00001 Increasing Quantum Dot Electron Spin Coherence with Persistent Spin Narrowing[1] , BO SUN, University of Michigan, COLIN CHOW, Univeristy of Michigan, ALLAN BRACKER, DANIEL GAMMON, Naval Research Laboratory, LU SHAM, University of California San Diego, DUNCAN STEEL, University of Michigan — We demonstrate reproducible initialization of the Overhauser field in a single InAs self-assembled quantum dot using the hole assisted nuclear feedback mechanism. This fixes the mean the Overhauser field to a value determined by two pump lasers and dramatically reduces the statistical broadening of the electron spin resonance arising from averaging over the nuclear spin ensemble, (1/T2*). By initializing for tens of milliseconds, the prepared Overhauser field distribution lasts for well over a second even in the presence of a fluctuating electron spin. Furthermore, we find a mechanism which will initialize the nuclear spins using only a single laser, and that this mechanism involves the evolution of the nuclear spins "in the dark", that is, absent any optical field. This new method is directly compatible with the CW readout technique used in recent time-domain spin manipulation experiments.

[1]The authors would like to acknowledge ARO, NSF, AFOSR, and DAPRA for their support

8:12AM V27.00002 Effects of Multi-pulse Dynamical Decoupling Schemes on Dephasing in a GaAs Spin Qubit[1] , JAMES MEDFORD, CHRISTIAN BARTHEL, CHARLES MARCUS, Harvard University, MICAH HANSON, ARTHUR GOSSARD, Materials Department, University of California, Santa Barbara — Coherence time (T_2) of a singlet-triplet qubit in a GaAs double quantum dot is studied as a function of the number of π-pulses in a Carr-Purcell-Meiborn-Gill (CPMG) dynamical decoupling sequence. In this system, the dominant forms of dephasing are expected to be hyperfine coupling to the nuclei and electrical noise. For n_π ranging from 2 to 32, we find a power law dependence of T_2 with the number of pulses, $T_2 \propto n_\pi^\beta$, where n_π is the number of pulses and $\beta \sim 0.7$ is a fit parameter.

[1]Support from iARPA, Department of Defense

8:24AM V27.00003 The central spin problem: electron spin qubit evolution due to coherently evolving nuclear spins , IZHAR NEDER, MARK RUDNER, HENDRIK BLUHM, BERTRAND HALPERIN, AMIR YACOBY, Harvard University — In recent years, electron spin qubits in solid state quantum dots have emerged as promising candidates for the implementation of quantum information processing. We study the dephasing of two electron spins in a double quantum dot system due to the evolution of the underlying nuclear spins, as was measured in a recent spin echo experiments. We develop a semi-classical model for such a system, by treating the Overhauser field induced by the nuclear spins as a classical time-dependent vector. Comparing the outcome of this model to experimental echo signal of the electron qubit allows us to identify MNR-like signatures from the nuclear spin evolution, such as spin diffusion, coherent nuclear Larmor precession and the spread of the Larmor frequencies by various mechanisms.

8:36AM V27.00004 Generating Entanglement and Squeezed States of Nuclear Spins in Quantum Dots

, MARK RUDNER, Harvard University, LIEVEN VANDERSYPEN, TU Delft, VLADAN VULETIC, LEONID LEVITOV, MIT — Entanglement generation and detection are two of the most sought-after goals in the field of quantum control. Besides offering a means to probe some of the most peculiar and fundamental aspects of quantum mechanics, entanglement in many-body systems can be used as a tool to reduce fluctuations below the standard quantum limit. For spins, or spin-like systems, such a reduction of fluctuations can be realized with so-called squeezed states [1]. Here we present a scheme for achieving coherent spin squeezing of nuclear spin states in single electron quantum dots [2]. This work represents a major shift from earlier studies, which have explored classical "narrowing" of the nuclear polarization distribution through feedback involving stochastic spin flips. In contrast, we use the nuclear-polarization-dependence of the electron spin resonance (ESR) line to provide a non-linearity which generates a non-trivial, area-preserving, "twisting" dynamics which squeezes and stretches the nuclear spin Wigner distribution without the need for nuclear spin flips.

[1] M. Kitagawa, M. Ueda, Phys. Rev. A 47, 5138 (1993).
[2] M. S. Rudner, L. V. M. Vandersypen, V. Vuletic, L. S. Levitov, to be published.

8:48AM V27.00005 Dephasing of two-spin qubits due to their charge and nuclear environments[1]

, GUY RAMON, Santa Clara University — We consider dephasing of qubits encoded in the singlet and unpolarized triplet states of pairs of spins localized in biased double quantum dots. The charge environment is modeled by both two-center charge traps in the insulator (where electrons tunnel between the two centers), and single charge traps located near the gate electrodes and QPCs (where electrons charge and empty the trap). The couplings of these trapped charges to the qubits are calculated by considering their charge distributions within a multipole expansion. It is demonstrated that the summation over these random telegraph processes in mesoscopic devices results in non-Markovian and non-Gaussian noise. For the nuclear environment we consider hyperfine-induced electron-spin dephasing in a nuclear spin bath with narrowed distribution. Nuclear state preparation using dynamical polarization cycles was experimentally achieved recently, and it is also essential to enable X-rotations for two-spin qubits. Our analysis is performed for both free induction and echo signals. The scaling of these dephasing mechanisms with the number of qubits is also discussed.

[1]Supported by Research Corporation

9:00AM V27.00006 Noisy (spin) neighbors of a solid state (spin) qubit[1]

, WAYNE WITZEL, MALCOLM CARROLL, Sandia National Laboratories, NM, LUKASZ CYWINSKI, Institute of Physics, Polish Academy of Sciences, SANKAR DAS SARMA, University of Maryland, College Park — Powerful computational methods have been developed in recent years for understanding decoherence induced by environmental spins. Specifically, the cluster correlation expansion [Phys. Rev. B 78, 085315 (2008)] and adaptations [Phys. Rev. Lett. 105, 187602 (2010)] provide successive approximations that approach the solution to the full quantum mechanical problem for small and large spin baths with good efficiency. We present our findings from these computations. These have implications for solid state spin qubit fabrication and materials choices. In silicon where nuclear spins may be eliminated through isotopic enrichment, we consider other sources of bath spins in the bulk and near interfaces. We also investigate the conditions under which we may abstract out an approximate noise model that is independent of operations applied to the qubit.

[1]Sandia National Laboratories is a multiprogram laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL850

9:12AM V27.00007 Competing effects of hyperfine and spin-orbit interactions in two-electron spin qubits[1]

, ERNESTO COTA, Centro de Nanociencias y Nanotecnología, UNAM, Ensenada, Mexico, SERGIO ULLOA, Ohio University — We analyze the dynamics of a double quantum dot system with two electrons in a uniform magnetic field, taking into account the hyperfine interaction as well as the interdot tunneling-induced Rashba spin-orbit coupling. The former mixes the singlet and triplet (1,1) states while the latter accounts for mixing triplet states and the doubly occupied (0,2) singlet. We focus on the effects on experimental results in GaAs dots [1], involving the generation and control of a nuclear field gradient, necessary for full quantum control of this electron spin qubit. Using a complete description of the quantum states involved in the dynamics and numerical solution of the time-dependent Schrödinger equation, we study different pumping processes used to polarize (and read) the nuclear system, creating a large inhomogeneous nuclear field. We evaluate the fidelity of gate operations involving the two-electron qubit in the presence of competing spin-flip interactions as well as the implementation of these operations in quantum computation with characteristic experimental dot systems.

[1] S. Foletti et al., Nature Physics 5, 903 (2009)

[1]Supported by OU-NQPI/CMSS,NSF-MWN/CIAM and DGAPA-UNAM.

9:24AM V27.00008 Two-eletron spin relaxation in double quantum dots and P donors[1]

, CHIA-WEI HUANG, Department of Physics, Bar-Ilan University, Ramat Gan, 52900, Israel, MASSOUD BORHANI, XUEDONG HU, Department of Physics, University at Buffalo, SUNY, Buffalo, NY 14260-1500, USA — We study singlet-triplet relaxation of two electrons confined in a double quantum dot or bound to P donors in Silicon. Hyperfine interaction of the electrons with the host/phosphorus nuclei, in combination with the electron-phonon interaction, leads to relaxation of the triplet states. We calculate the triplet relaxation rates in the presence of an applied magnetic field. This relaxation mechanism affects, for example, the resonance peaks in current Electron Spin Resonance (ESR) experiments on P-dimers. Moreover, the estimated time scales for the spin decay put an upper bound on the gate pulses needed to perform fault-tolerant two-qubit operations in spin-based quantum computers. We have found the optimal regimes, which mitigate this relaxation mechanism, yet permit sufficiently fast two-qubit operations.

[1]We thank support by NSA/LPS thorugh ARO.

9:36AM V27.00009 Spin-orbit induced two-electron spin relaxation in double quantum dots[1]

, MASSOUD BORHANI, XUEDONG HU, SUNY at Buffalo, NY — We study the spin decay of two electrons confined in a double quantum dots via the spin-orbit interaction and acoustic phonons. We have obtained a generic form for the spin Hamiltonian for two electrons confined in (elliptic) harmonic potentials in doubles dots and in the presence of an arbitrary applied magnetic field. Our focus is on the interdot bias regime where singlet-triplet splitting is small, in contrast to the spin-blockade regime. Our results clarify the spin-orbit mediated two-spin relaxation in lateral/nanowire quantum dots, particularly when the confining potentials are different in each dot.

[1]We thank support by NSA/LPS thorugh ARO.

9:48AM V27.00010 Impurity effects on coupled quantum dot spin qubits in semiconductors , NGA NGUYEN, SANKAR DAS SARMA, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742-4111, USA — Localized electron spins confined in semiconductor quantum dots are being studied by many groups as possible elementary qubits for solid-state quantum computation. We theoretically consider the effects of having unintentional charged impurities in laterally coupled two-dimensional double (GaAs) quantum dot systems, where each dot contains one or two electrons and a single charged impurity in the presence of an external magnetic field. We calculate the effect of the impurity on the 2-electron energy spectrum of each individual dot as well as on the spectrum of the coupled-double-dot 2-electron system. We find that the singlet-triplet exchange splitting between the two lowest energy states, both for the individual dots and the coupled dot system, depends sensitively on the location of the impurity and its coupling strength (i.e. the effective charge). We comment on the impurity effect in spin qubit operations in the double dot system based on our numerical results. This work is supported by LPS-CMTC and CNAM.

10:00AM V27.00011 Theory of anisotropic exchange in laterally coupled quantum dots , FABIO BARUFFA, Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany, PETER STANO, Institute of Physics, Slovak Academy of Sciences, 84511 Bratislava, Slovak Republic, JAROSLAV FABIAN, Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — We consider an interacting pair of quantum dot electron spin qubits (a two electron double quantum dot). In this setup, two-qubit operations are generated by the (isotropic) exchange interaction, which results from the tunable inter-dot coupling. In the presence of spin-orbit interactions, additional effective inter-qubit coupling arises, termed anisotropic exchange. We show that in GaAs, where spin-orbit interactions are weak, the magnitude of the anisotropic exchange is proportional to the external magnetic field and therefore directly controllable, boosting prospects for spin-based quantum computing. We show how the form of anisotropic exchange follows from its spin-orbit origin and that its magnitude can be traced down to dipole moment matrix elements. Based on this findings, we propose an effective spin Hamiltonian suitable for practical modeling of two-electron spin dynamics. We prove the effective Hamiltonian quantitative accuracy confronting it with a microscopic numerical model.

[1] F. Baruffa, P. Stano, J. Fabian, Phys. Rev. Lett. 104, 126401 (2010)
[2] F. Baruffa, P. Stano, J. Fabian, Phys. Rev. B 82, 045311 (2010)

10:12AM V27.00012 Many-body singlets of nuclear spins[1] , WANG YAO, The University of Hong Kong — We show that dynamic spin polarization by collective raising and lowering operators can drive a spin ensemble from arbitrary initial state to many-body singlets, the zero-collective-spin states with large scale entanglement. For an ensemble of N arbitrary spins, both the variance of the collective spin and the number of unentangled spins can be reduced to $O(1)$ (versus the typical value of $O(N)$), and many-body singlets can be occupied with a population of $\sim 20\%$ independent of the ensemble size. We implement this approach in a mesoscopic ensemble of nuclear spins through dynamic nuclear spin polarization by an electron. The result is of two-fold significance for spin quantum technology: (1) a resource of entanglement for nuclear spin based quantum information processing; (2) a cleaner surrounding and less quantum noise for the electron spin as the environmental spin moments are effectively annihilated.

[1]The work was supported by the Research Grant Council of Hong Kong.

10:24AM V27.00013 Atomistic theory of spin relaxation in self-assembled (In, Ga)As/GaAs quantum dots at zero magnetic field , LIXIN HE, Univ. Sci & Tech. of China, HAI WEI, MING GONG, G.-C. GUO — We investigated the spin-flip time (T_1) of electrons and holes mediated by acoustic phonons in self-assembled In(Ga)As/GaAs quantum dots at zero magnetic field, using an atomistic pseudopotential method. At low magnetic field, the first-order process is suppressed, and the second-order process becomes dominant. We find that the spin-phonon-interaction induced spin relaxation time is 40 - 80 s for electrons, and 1 -20 ms for holes at 4.2 K. The calculated hole-spin relaxation times are in good agreement with recent experiments, which suggests that the two-phonon process is the main relaxation mechanism for hole-spin relaxation in the self-assembled quantum dots at zero field. We further clarify the structural and alloy composition effects on the spin relaxation in the quantum dots.

10:36AM V27.00014 Optically controlled electron-nuclear spin dynamics in a quantum dot[1] , EDWIN BARNES, Condensed Matter Theory Center, Dept. of Physics, University of Maryland, SOPHIA ECONOMOU, Naval Research Lab — In recent years, a large number of experiments involving coherent and incoherent control of electron spins in quantum dots have revealed the important role of the nuclear spins of the host material. Experiments with optical controls, both pulsed and continuous wave, have shown that the feedback of the nuclear spins on the electron spin strongly affects the electron spin response. However, a microscopic theory of this mechanism is not available at present. We introduce a formalism that allows us to investigate this system without invoking any phenomenological spin-flip rates for the nuclei. We derive the electron-nuclear dynamics under the influence of external periodic pulsed control to second order in the electron-nuclear hyperfine coupling. Our formalism should have wide applications in both coherently and incoherently driven electron spins interacting with a nuclear spin bath, including self-assembled and gated quantum dots.

[1]Work (EB) supported by LPS-CMTC and CNAM

Thursday, March 24, 2011 8:00AM - 11:00AM –
Session V28 DMP: Focus Session: Carbon Nanotubes and Related Materials: Devices III C156

8:00AM V28.00001 High Frequency Rectification by Carbon Nanotube Schottky Diodes[1] , ENRIQUE D. COBAS, STEVEN M. ANLAGE, MICHAEL S. FUHRER, Center for Nanophysics and Advanced Materials, University of Maryland, College Park, MD 20742-4111, USA — Carbon nanotubes (CNTs) display many properties that make them appealing for RF electronics, including room-temperature mean-free paths approaching 1 μm and a carrier mobility of 10^5 cm^2 / Vs. Further, small junction capacitances on the order of 10 aF promise cut-off frequencies approaching 1 THz, but high impedances make microwave measurements of individual CNTs challenging. We have fabricated single and few-tube CNT Schottky diodes on high-frequency compatible substrates and measured their ac rectification as a function of dc bias, ac power and frequency, up to 40 GHz. The bias dependence of the cut-off frequency is used to extract the effective junction capacitance for diodes of various channel lengths. This capacitance is found to have a weak dependence on applied bias and a strong relation to channel length. Electrostatic simulations corroborate that stray capacitance from the 1D channel to the metal electrode dominates over the effect of carrier depletion near the junction. The results demonstrate that chottky rectification is a viable method of probing transport in high-impedance semiconducting nanostructures.

[1]This work is supported in part by the ONR/Maryland AppEl, Task D10, through grant number N000140911190.

8:12AM V28.00002 Logarithmic time response of carbon nanotube field-effect transistors , ANDREW TUNNELL, University of Maryland, VINCE BALLAROTTO, Laboratory for Physical Sciences, MERIJNTJE BRONSGEEST, JOHN CUMINGS, University of Maryland — When observing the source-drain current of a carbon nanotube field effect transistor (FET) held at constant bias, several different processes can produce a time response of the current, including fluctuations due to current noise, heating of contacts, and releasing of trapped charges in the gate dielectric. This third phenomenon is investigated by pulsing voltages on the gate and observing the source-drain current over time. Instead of a typical exponential decay with one or a few time constants, the current was observed to decrease linearly with the logarithm of time, possibly indicating exponential decay with multiple time constants. This trend was seen to continue for over 20 hours, which spans five orders of magnitude in time with respect to the measurement resolution. This trend of scaling logarithmically with time is also seen with the rate of current change with respect to a gate voltage pulse width. This behavior has been investigated in various FET geometries and different materials, all with comparable results. These measurements may be a new way to investigate and characterize the hysteresis in carbon nanotube FETs and the materials used in their fabrication.

8:24AM V28.00003 Mirage Effect From Thermally-Modulated Transparent Carbon Nanotube Sheet , ALI ALIEV, RAY BAUGHMAN — The single beam mirage effect, also known as photothermal deflection, is studied using a free-standing, highly-aligned carbon nanotube sheet as a heat source whose temperature can be modulated over a wide frequency range. The extremely low thermal capacitance and high heat transfer ability of these transparent forest-drawn carbon nanotube sheets enables high frequency modulation of sheet temperature over an enormous temperature range, thereby providing a sharp, rapidly changing gradient of refractive index in surrounding liquid or gas. The advantages of temperature modulation using carbon nanotube sheets are multiple: in inert gases the temperature can reach $>$2500 K; the obtained frequency range for photothermal modulation is $\sim$100 kHz in gases and over 100 Hz in high refractive index liquids; and the heat source is transparent for optical and acoustical waves. The remarkable light deflection in gases and liquids suggests possible application of carbon nanotube sheets for large laser projectors and cloaking systems.

8:36AM V28.00004 Application of Carbon Nanotube Assemblies for Sound Generation and Heat Dissipation , MIKHAIL KOZLOV, CARTER HAINES, JIYOUNG OH, MARCIO LIMA, SHAOLI FANG, University of Texas at Dallas — Nanotech approaches were explored for the efficient transformation of an electrical signal into sound, heat, cooling action, and mechanical strain. The studies are based on the aligned arrays of multi-walled carbon nanotubes (MWNT forests) that can be grown on various substrates using a conventional CVD technique. They form a three-dimensional conductive network that possesses uncommon electrical, thermal, acoustic and mechanical properties. When heated with an alternating current or a near-IR laser modulated in 0.01–20 kHz range, the nanotube forests produce loud, audible sound. High generated sound pressure and broad frequency response (beyond 20 kHz) show that the forests act as efficient thermo-acoustic (TA) transducers. They can generate intense third and fourth TA harmonics that reveal peculiar interference-like patterns from ac-dc voltage scans. A strong dependence of the patterns on forest height can be used for characterization of carbon nanotube assemblies and for evaluation of properties of thermal interfaces. Because of good coupling with surrounding air, the forests provide excellent dissipation of heat produced by IC chips. Thermoacoustic converters based on forests can be used for thermo- and photo-acoustic sound generation, amplification and noise cancellation.

8:48AM V28.00005 Thermoelectric Transport Through Arrays Of Carbon Nanotube Junctions , IRMA KULJANISHVILI, JIM CHOE, VENKAT CHANDRASEKHAR, SERHII SHAFRANIUK, Northwestern University — The work addresses the voltage-controlled thermal flow and electric current through the carbon nanotube (CNT) junction arrays. The CNT thermoelectric generation (TEG) promises a high efficiency for thermal and electric energy conversion in a variety of applications. [1] The energy generation had been studied using advanced methods of the condensed matter physics and nanotechnology. We will outline our experimental findings based on CNTs - TEG devices. We will report on our results that involve TEG-CNTs devices in array and /or single CNTs junctions geometries. We will describe fabrications protocols for preferential CVD growth of CNTs and nanoscale precision patterning of the catalyst on predefined device architectures. Electronic transport and optical properties of the CNTs-TEG nanostructures will also be discussed. I.K. and S.S. acknowledge support from the U.S. Army CECOM Acquisition Center #W909MY-10-C-0032. I.K. acknowledge collaboration with NanoInk Inc.

9:00AM V28.00006 Carbon nanotube quantum dot in a dissipative environment , HENOK MEBRAHTU, IVAN BORZENETS, YURIY BOMZE, Duke University, ALEX SMIRNOV, North Carolina State University, GLEB FINKELSTEIN, Duke University — We study conductance through a resonant level in a single-walled carbon nanotube quantum dot embedded in a dissipative environment. The dissipation is provided by environmental modes in the nanotube leads and the strength of the dissipation is experimentally controlled in several samples. At base temperature, dissipation suppresses the resonant tunneling peak height while maintaining resonant level width. We also observe a regime where the height and the width of a conductance peak demonstrate qualitatively different energy scaling.

9:12AM V28.00007 Energy Dissipation and Transport in Carbon Nanotube Devices , ERIC POP, University of Illinois Urbana-Champaign — Power consumption is a significant challenge in electronics, often limiting the performance of integrated circuits from mobile devices to massive data centers. Carbon nanotubes have emerged as potentially energy-efficient future devices and interconnects, with both large mobility and thermal conductivity. This talk will focus on understanding and controlling energy dissipation [1-3] and transport [4-6] in carbon nanotubes, with applications to low-energy devices, interconnects, heat sinks, and memory elements [7]. Experiments have been used to gain new insight into the fundamental behavior of such devices, and to better inform practical device models. The results suggest much room for energy optimization in nanoelectronics through the design of geometry, interfaces, and materials.

[1]. E. Pop, "Energy Dissipation and Transport in Nanoscale Devices," Nano Research 3, 147 (2010).
[2]. Z.-Y. Ong and E. Pop, "Molecular Dynamics Simulation of Interfacial Thermal Resistance between Single-Wall Carbon Nanotubes and SiO2," Phys. Rev. B 81, 155408 (2010).
[3]. A. Liao, R. Alizadegan, Z.-Y. Ong, S. Dutta, F. Xiong, K. J. Hsia, E. Pop, "Thermal Dissipation and Variability in Electrical Breakdown of Carbon Nanotube Devices," Phys. Rev. B 82, 205406 (2010).
[4]. A. Liao, Y. Zhao, E. Pop, "Avalanche-Induced Current Enhancement in Semiconducting Single-Walled Carbon Nanotubes," Phys. Rev. Lett. 101, 256804 (2008).
[5]. Y. Zhao, A. Liao, E. Pop, "Multiband Mobility in Semiconducting Carbon Nanotubes," IEEE Elec. Dev. Lett. 30, 1078 (2009).
[6]. D. Estrada, A. Liao, S. Dutta, E. Pop, "Reduction of Hysteresis for Carbon Nanotube Mobility Measurements Using Pulsed Characterization," Nanotechnology 21, 085702 (2010).
[7]. F. Xiong, A. Liao, E. Pop, "Inducing Chalcogenide Phase Change with Ultra-Narrow Carbon Nanotube Heaters," Appl. Phys. Lett. 95, 243103 (2009).

9:48AM V28.00008 Proximal heating by a current-carrying nanotube , KAMAL H. BALOCH, NORVIK VOSKANIAN, MERIJNTJE S. BRONSGEEST, JOHN CUMINGS, University of Maryland — The 1D nature of carbon nanotubes makes them an excellent candidate for thermal management and thermal logic devices. Using an established thermal measurement technique based on the melting of indium islands [1], we have studied the thermal characteristics of Joule-heated MWNTs. Our experimental observations contradict prevailing theoretical models for heat dissipation in CNT. Despite the high thermal contact resistance between the CNT and the substrate we observe that a current-carrying nanotube dissipates power readily into the substrate, suggesting an alternate mode of heat transport based on scattering of hot electrons in the CNT from the substrate phonons. Experimental results, simulations, and a review of the experimental technique will be presented in this talk.

[1] T. Brintlinger, et al., Nano Lett. **8**, 582 (2008).

10:00AM V28.00009 Correlated breakdown of carbon nanotubes in an ultra-high density aligned array , SHASHANK SHEKHAR, MIKHAIL EREMENTCHOUK, MICHAEL LEUENBERGER, SAIFUL KHONDAKER, NanoScience Technology Center and Department of Physics, University of Central Florida, 12424 Research Parkway, Orlando, 32826, USA. — Many proposed applications of single walled carbon nanotubes (SWNTs) require a massively parallel array and selective removal of metallic pathways from the array via electrical breakdown. Since experimental and theoretical studies of individual SWNTs demonstrate that the breakdown is due to Joule heating which occurs at defect sites, a straightforward extrapolation to an array would suggest that the breakdown would occur at random point inside each SWNT. Here we demonstrate that in a densely packed aligned array of SWNTs containing up to 30 SWNT/μm, the breakdown of one of the SWNTs leads to a highly correlated breakdown of neighboring SWNTs, thereby producing a "nano fissure" shaped pattern. We show theoretically that the correlated breakdown is due to the electrostatic field of broken nanotubes that produces locally inhomogeneous current distributions in the neighboring nanotubes triggering their breakdowns in the vicinity of the broken nanotubes. Our results suggest that the densely aligned array works like a correlated solid and have strong implications in the future development of fault-tolerant nano-electronic circuits based on SWNT array.

10:12AM V28.00010 Thermionic Emission Properties of Surface modified conical carbon nano tubes (CCNT) , ANDRIY SHEREHIY, GAMINI SUMANASEKERA, University of Louisville, Department of Physics and Astronomy, SANTOSHRUPA DUMPALA, MAHENDRA SUNKARA, University of Louisville, Department of Chemistry Engineering, ROBERT COHN, University of Louisville, Department of Electrical and Computer Engineering — We have studied field emission and thermionic emission properties of surface modified arrays of CCNTs. The CCNTs with narrow tip radii (about 10 nm) were synthesized using microwave plasma assisted chemical vapor deposition on platinum wire and planar graphite foils. They show enhanced field emission properties with geometrical enhancement factor as high as about 7000 and turn-on electric field as low as approximately 0.7 V/μm. The thermionic emission characteristics show work function of aproximately 4.2 eV which is considerably lower than that of aligned MWNT (4.8 eV). The reduced work function value was further confirmed using ultraviolet photoemission spectroscopy (UPS). The surface modified CCNT arrays were also studied and shown to exhibit poorer emission properties compared to pristine CCNTs. We have further coated CCNTs with diamond nanocrystals and doping of the nanocrystals is underway.

10:24AM V28.00011 Highly Efficient Field Emission from Carbon Nanotube-Nanohorn Hybrids Prepared by Chemical Vapor Deposition , RYOTA YUGE, NEC Corporation, JIN MIYAWAKI, Japan Science and Technology Agency, TOSHINARI ICHIHASHI, SADANORI KUROSHIMA, TSUTOMU YOSHITAKE, NEC Corporation, TETSUYA OHKAWA, YASUSHI AOKI, NEC Lighting, Ltd., SUMIO IIJIMA, Meijo University, MASAKO YUDASAKA, National Institute of Advanced Science and Technology — It is reported that the carbon nanotube (CNT) is one of the best cold cathode emitters for field emission display (FED) and field emission lamp (FEL) due to their large aspect ratio, high mechanical strength, and high electrical conductivity. For the manufacture of highly efficient field emission (FE) devices, we synthesized single-wall carbon nanotube (SWNT) on catalyst-supported single-wall carbon nanohorn (SWNH). We incorporated Fe acetate into SWNHs, heat-treated them, and obtained Fe oxide nano-particles attached to the tips of SWNHs (Fe@NHox). Using Fe@NHox as the catalyst, SWNTs were grown by ethanol-CVD technique (NTNH). In the obtained NTNH, the SWNTs diameters were 1–1.7 nm and the bundle diameters became almost uniform, $i.e.$, less than 10 nm, since the SWNTs were separated by SWNH aggregates. We also confirmed that a large-area FE device with NTNH cathodes made by screen printing was highly and homogeneously bright, suggesting the success of the hybrid strategy.

10:36AM V28.00012 Enhanced electron field emission from simultaneously purified and nitrogen incorporated CNTs via tip opening by Novel *in-situ* nitrogen ECR plasma[1] , SWATHI IYER, PAUL MAGUIRE, NIBEC, University of Ulster — We report a novel single step process by means of *in-situ* nitrogen ECR plasma treatment with very low power and treatment time for the simultaneous metal catalyst (iron) removal via tip opening and nitrogen functionalization/incorporation of the vertically aligned multiwalled carbon nanotubes synthesised using a microwave plasma enhanced chemical vapour deposition. Microscopic (SEM) and spectroscopic (NEXAFS, XPS and Raman) studies reveal negligible remaining Fe content (0%) and limited/no damage structure and alignment of the nanotubes. The incorporation of nitrogen was elucidated by the N-k edge NEXAFS spectra, where the sharp π* peak splits into three distinct peaks at energies 399, 399.5 and 401.1 eV. Increase in the at. % conc. of N 1s from 0.7 to 6.9 % and the disappearance of the peak at 780 eV by XPS and Raman corroborate the inclusion of nitrogen in the CNTs and the complete removal of iron metal catalyst. Metal catalyst removal and nitrogen addition by N-ECR plasma leads to enhanced field emission with very low turn on and threshold fields of 0.52 V/μm and 0.76 V/μm as compared to the recent studies of other nitrogen doped nanomaterials by plasma treatments.

[1]VCRS Scholarship

10:48AM V28.00013 Spin-polarized field emission from nanotubes[1] , JOSEPH DRISCOLL, BRANDON COOK, SERGIY BUBIN, KALMAN VARGA, Vanderbilt University Department of Physics and Astronomy — Time-dependent density functional theory has been used to calculate the spin-polarized field emission from carbon nanotubes with and without Fe adsorbates (atoms and clusters). Using our previously-developed approach [1], the electronic wave function was propagated in real time. Complex absorbing potentials have been employed to avoid artificial reflections from the boundaries and to allow long time simulations. It was observed that various adsorbates cause the separation of density into spin-polarized regions. The calculations predict that carbon nanotubes with various adsorbates can be used as spin-polarized current sources.

[1] J. A. Driscoll and K. Varga, Phys. Rev. B 80, 245431 (2009).

[1]This work is supported by NSF Grants No. ECCS0925422 and CMMI0927345.

Thursday, March 24, 2011 8:00AM - 11:00AM –
Session V29 GQI DAMOP: Quantum Control and Measurement C148

8:00AM V29.00001 Robust high-fidelity universal quantum gates , RAN LI, Kent State University, FRANK GAITAN, Laboratory for Physical Sciences, University of Maryland — We show how a robust high-fidelity universal set of quantum gates can be produced using a single form of non-adiabatic rapid passage whose parameters are optimized to enhance gate fidelity and robustness. All gates in the universal set are found to: (i) operate with fidelities in the range 0.999 — 0.99999, and (ii) use control parameters requiring no more than 14-bit precision. Such precision is within the reach of commercially available arbitrary waveform generators, suggesting the feasibility of an experimental study of this approach to high-fidelity quantum control.

8:12AM V29.00002 Exact, Floquet-based, Single Qubit Control[1] , ANDREW SORNBORGER, University of Georgia, EMILY PRITCHETT, Institute for Quantum Computing — Single-qubit gate design using oscillatory controls is related to the Rabi problem of rotating a spin. In the classical solution one drives the spin with an oscillatory electromagnetic field orthogonal to a background field. Here, we introduce a new, general method for constructing continuous, oscillatory quantum controls based on Floquet's theorem. We then derive a family of exact, analytical solutions to the generalized Rabi problem of completely controlling a single-qubit in a fixed background field.

[1]NSF 1029764, NSF 0939853

8:24AM V29.00003 Protection of quantum systems by nested Uhrig dynamical decoupling[1] , ZHEN-YU WANG, REN-BAO LIU, Department of Physics, The Chinese University of Hong Kong — Based on a theorem we establish on dynamical decoupling of time-dependent systems, we present a scheme of nested Uhrig dynamical decoupling (NUDD) to protect multi-qubit systems in generic quantum baths to arbitrary decoupling orders. This scheme uses only single-qubit operations. Higher order decoupling is achieved at the cost of a polynomial increase in pulse number. For general multi-level systems, this scheme protects a set of unitary Hermitian system operators which mutually either commute or anti-commute, and hence all operators in the Lie algebra generated from this set of operators, generating an effective symmetry group for the system up to a given order of precision. We also show how to implement NUDD with pulses of finite amplitude, up to an error in the second order of the pulse durations.

[1]This work was supported by Hong Kong GRF CUHK402209.

8:36AM V29.00004 Quantum noise of an electromagnetically controlled two level system , CHING-KIT CHAN, L.J. SHAM, Department of Physics, University of California San Diego — A coherent control of a spin is limited by both the decoherence due to coupling with the environment and noise coming from the quantized control. A quantum noise study is particularly important in fault tolerant quantum computation where a very high fidelity is demanded. Here, we present a time evolution study of a two level system interacting with a laser pulse and the electromagnetic vacuum based on the multimode Jaynes- Cummings model. We develop a diagrammatic formalism in which one can easily identify the coherent Rabi oscillation of the TLS and its relaxation from corresponding diagrams. In the small time limit ($t \ll T_1$), where the noise level is small but still an issue to fault tolerant quantum computing, this method gives a quantitative evaluation of the quantum noise of the TLS under an optical control with an arbitrary pulse shape. Furthermore, this approach can be naturally extended from the Markovian to the non-Markovian regime, resulting in dynamics different from that obtained in the optical Bloch analysis. All these calculations are done without any stochastic assumption.

8:48AM V29.00005 Optimal control of an ensemble of atoms in an optical lattice[1] , BOTAN KHANI, SETH MERKEL, JAY GAMBETTA, FELIX MOTZOI, FRANK K. WILHELM, University of Waterloo, QUANTUM DEVICE THEORY GROUP TEAM — Controlling quantum systems in a manner that is robust to experimental errors and inhomogeneities is vital for practical realization of quantum gates. We demonstrate numerically the control of motional degrees of freedom of an ensemble of neutral atoms in an optical lattice of shallow trapping potential. Taking into account the range of quasi-momenta across different Brillouin zones results in an ensemble whose members effectively have inhomogeneous control fields as well as spectrally distinct control Hamiltonians. We present a modified optimal control technique that yields high fidelity control pulses, irrespective of quasi-momentum, with average fidelities above 90%. The resultant controls show a broadband spectrum with gate times in the order of several Rabi oscillations to optimize gates with up to 75% dispersion in the energies from the band structure.

[1]Work supported by NSERC discovery grants, quantumworks, SHARCNET, and IARPA-MQCO. Jay Gambetta was supported by CIFAR, MRI, MITACS, NSERC, and DARPA.

9:00AM V29.00006 High Fidelity State Transfer Over an Unmodulated Linear XY Spin Chain , C. ALLEN BISHOP, Department of Physics, Southern Illinois University Carbondale, YONG-CHENG OU, Department of Physics, Texas Tech University, ZHAO-MING WANG, Department of Physics, Ocean University of China, MARK BYRD, Department of Physics, Southern Illinois University Carbondale — We provide a class of initial encodings that can be sent with a high fidelity over an unmodulated, linear, XY spin chain. As an example, an average fidelity of 96% can be obtained using an 11-spin encoding to transmit a state over a chain containing 10,000 spins. An analysis of the magnetic-field dependence is given, and conditions for field optimization are provided.

9:12AM V29.00007 Geometric Phase Gates via Adiabatic Control Using Electron Spin Resonance , HUA WU, ERIK GAUGER, Department of Materials, Oxford University, Oxford OX1 3PH, UK, RICHARD GEORGE, Clarendon Laboratory, Department of Physics, Oxford University, Oxford OX1 3PU, UK, JOHN MORTON, Department of Materials, Oxford University, Oxford OX1 3PH, UK, MIKKO MÖTTÖNEN, 1)Department of Applied Physics/COMP, Aalto University, FI-00076 AALTO, Finland 2)Low Temperature Laboratory, Aalto University, FI-00076 AALTO Finland — High fidelity operations are essential elements of quantum information processing. In contrast with the dynamic pulses that are routinely used in electron spin resonance for spin qubit manipulation, geometric phase gates achieved via adiabatic control are less sensitive to certain kinds of noise and field inhomogeneities. Here, we employ theoretical and numerical tools to show that these geometric operations can be realized in electron spin systems with greater fidelities than composite dynamic pulses for large inhomogeneities in the microwave field. We further show that the adiabatic geometric phase is robust against fast fluctuations in the static magnetic field. Finally, we investigate adiabatic geometric phase operations experimentally, showing that we are able to apply such robust phase gates to the electron spin on the microseconds timescale.

9:24AM V29.00008 Nanoscale control of individual proximal NV spins via a scanning magnetic field-gradient , MICHAEL GRINOLDS, PATRICK MALETINSKY, SUNGKUN HONG, MIKHAIL LUKIN, RONALD WALSWORTH, AMIR YACOBY, Harvard University — Nanoscale ensembles of nitrogen-vacancy (NV) spins have been proposed for implementing quantum information protocols as well as performing sensitive nanoscale magnetometry. However, it has proven experimentally difficult to control individual NV spins without affecting the state of other, proximal spins, as spins are read-out optically and are often collectively driven by applied radio-frequency fields. We demonstrate that single-spin control in NV-spin ensembles can be achieved via a scanning magnetic field-gradient, which locally splits the electron spin resonances of proximal NVs. With this method, we achieve 9 nm spatial resolutions in imaging, characterization, and simultaneous manipulation of individual NVs, roughly two orders of magnitude better than the optical diffraction limit. We discuss applications of this individual control such as generating entangled spin-states and performing sensitive magnetometry.

9:36AM V29.00009 Nested Uhrig Dynamical Decoupling with Non-uniform Error Suppression , GREGORY QUIROZ, DANIEL LIDAR, University of Southern California — Here the performance of Nested Uhrig Dynamical Decoupling (NUDD) for qubit systems is analyzed when error suppression is non-uniform. The error suppression provided by NUDD is controlled by the sequence order of each nested sequence. The properties of the error suppression are characterized with respect to varying sequence order to verify the expected error suppression scaling of UDD, order $N+1$ error suppression with respect to the total time of evolution for an Nth order sequence. The system operators present in the system-environment evolution are isolated and used to quantify the order of error suppression associated with each system error operator. Using this as a measurement, error suppression is examined with respect to the strength of system-enviroment interaction, as well as the pure bath strength. In the case of single-qubit NUDD, known as Quadratic Dynamical Decoupling (QDD), the results show that the error suppression provided by the inner sequence scales exactly with that of UDD, while the outer sequence dynamics leads to error suppression greater than or equal to that expected from UDD. These results can be extended to multi-qubit systems where the error suppression scaling for the inner sequence applied to each qubit follows that of UDD and the outer sequence applied to each qubit gives an error suppression greater than or equal to $N+1$.

9:48AM V29.00010 Pulsed Quantum Optomechanics , MICHAEL R. VANNER, University of Vienna, IGOR PIKOVSKI, GARRETT D. COLE, MYUNGSHIK KIM, CASLAV BRUKNER, KLEMENS HAMMERER, GERARD J. MILBURN, MARKUS ASPELMEYER — By combining quantum optics with mechanical resonators an avenue is opened to extend investigations of quantum behavior into unprecendented mass regimes. The field resulting from this combination - "cavity quantum optomechanics" – is receiving a surge of interest for its potential to contribute to quantum measurement and control, studies of decoherence and non-classical state preparation of macroscopic objects. However, quantum state preparation and especially quantum state reconstruction of mechanical oscillators is currently a significant challenge. We are pursuing a scheme that employs short optical pulses to realize quantum state tomography, squeezing via measurement and state purifcation of a mechanical resonator. The pulsed scheme has considerable resilience to initial thermal occupation, provides a promising means to explore the quantum nature of massive oscillators and can be applied to other systems such as trapped ions. Our theoretical proposal and experimental results will be discussed.

10:00AM V29.00011 Quantum measurement with Mach-Zehnder Interferometer , YUNJIN CHOI, JUSTIN DRESSEL, ANDREW JORDAN, University of Rochester — We use an electronic Mach-Zehnder Interferometer (MZI) as a measurement device. We perform a measurement on a system by coupling with MZI using a phase shift induced by Clulombic coupling. By reading current and noise cross-correlations, strange conditioned averages can be constructed using the contextual values technique.

10:12AM V29.00012 Continuous phase amplification with a Sagnac interferometer , NATHAN WILLIAMS, DAVID STARLING, BEN DIXON, ANDREW JORDAN, JOHN HOWELL, University of Rochester — We describe a weak value inspired phase amplification technique in a Sagnac interferometer. We monitor the relative phase between two paths of a slightly misaligned interferometer by measuring the average position of a split-Gaussian mode in the dark port. Although we monitor only the dark port, we show that the signal varies linearly with phase and that we can obtain similar sensitivity to balanced homodyne detection. We derive the source of the amplification both with classical wave optics and as an inverse weak value.

10:24AM V29.00013 Conservation of Vacuum in an Interferometer , DOMINIC BERRY, University of Waterloo, ALEXANDER LVOVSKY, University of Calgary — Source efficiency and photon loss are major problems in optical metrology and quantum information. To understand how to address loss for these applications, it is vital to know how the loss behaves under linear optical (LO) processing including conditional measurements. We have developed a theory for the behavior of loss under LO processing, resolving many long-standing questions from previous work [1,2]. In particular, we have shown that, provided the efficiency of the sources is appropriately quantified, the efficiency of the state in any single mode cannot be increased beyond that of the highest-efficiency mode available at the input [1]. It is also not possible to increase efficiency in a catalytic way, using some high-efficiency modes to increase the efficiency of other modes [2]. The results provide a powerful unifying framework for quantifying efficiency by the incoherent vacuum contribution to optical states, even when entangled over multiple modes. The amount of vacuum is invariant under interferometers, and can only be increased by measurement.

[1] D. W. Berry and A. I. Lvovsky, Phys. Rev.Lett.**105**, 203601 (2010).
[2] D. W. Berry and A. I. Lvovsky, e-print:1010.6302 (2010).

10:36AM V29.00014 Dynamics of entanglement in two-dimensional spin system , QING XU, SABRE KAIS, Purdue University, GEHAD SADIEK, King Saud University and Ain Shams University — We consider the time evolution of entanglement in a finite two dimensional transverse Ising model. The model consists of a set of 7 localized spin-$\frac{1}{2}$ particles in a two dimensional triangular lattice coupled through exchange interaction J in presence of an external time dependent magnetic field $h(t)$. The magnetic field is presented in various function forms. We find that the magnetic field with sudden change does not provide a way to control or tuning the entanglement. While for the smoothly changing field, when its the character frequency is small, entanglement tends to follow the change of external magnetic field; when it gets larger, entanglement gradually loses pace with the field. It is also shown that the mixing of even a few excited states by small thermal fluctuation is devastating to the entanglement of the ground state.

10:48AM V29.00015 Probing Majorana edge states with a qubit , CHANG-YU HOU, FABIAN HASSLER, Institute Lorentz, Leiden University, JOHAN NILSSON, Department of Physics, University of Gothenburg, ANTON AKHMEROV, Institute Lorentz, Leiden University — A pair of counter-propagating Majorana edge modes can be described by an Ising conformal field theory. These modes appear in a chiral p-wave superconductor or in some superconducting system belonging to the same universality class. We show how a superconducting flux qubit attached to a such system couples to the two chiral edge modes via the disorder field of the Ising model. Thus, measuring the back-action of the edge states on the qubit allows to probe the properties of Majorana edge modes.

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V30 DCMP: Nanowires and Nanotubes: Thermal and Mechanical Properties C147/154

8:00AM V30.00001 Thermal boundary resistance between carbon nanotubes in nanocomposites with Monte Carlo simulations[1] , KHOA BUI, BRIAN GRADY, DIMITRIOS PAPAVASSILIOU, The University of Oklahoma — Enhancing the thermal conductivity of composites by incorporating carbon nanotubes (CNTs) has been an area of vigorous research recently. Measurements of the effective thermal conductivity (keff) for CNT-polystyrene composites at high CNT %wt found that the ratio (keff/kpolymer) at high concentration of CNTs is not as good as that at low CNT concentration [1]. It appears that the CNT dispersion pattern becomes worse, resulting in the formation of CNT bundles. In this work, we apply Monte Carlo simulations to investigate the keff at different weight fractions taking into account the bundle size and orientation, as well as the thermal boundary resistance. By validating with the experiment data, we found that the phonon transmission probability at the interface decreases by temperature. In addition, the poor enhancement of keff at high CNT concentration is because of the CNT-CNT contact resistance and because of the bundle geometry itself, which is equivalent to the presence of one low aspect ratio nanotube. References [1] Peters J. E.; Papavassiliou D.V; Grady B. P., Macromolecules 2008, 41, 7274-7277.

[1]DoE ER64239 0012293; DoD FA9550-10-1-0031

8:12AM V30.00002 Strain Engineering of the thermal conductance in Si nanowires , A. PAUL, K. MIAO, M. LUISIER, G. KLIMECK, Purdue University — Silicon nanowires (SiNWs) are promising semiconductor structures spanning a wide range of applications from CMOS devices to thermoelectric modules. Recently, SiNWs have shown tremendous potential as good thermoelectric materials with ZT coefficients larger than 1 [1]. This figure of merit can be further improved by tuning the thermal conductivity of the SiNWs. Here, we show that strain provides a natural way of tuning the thermal conductance of ultra-scaled SiNWs. We utilize a modified Valence Force Field (MVFF) model [2] to calculate the phonon dispersion in these SiNWs under strain and extract their thermal conductance using Landauer's approach. Our investigation shows that uniaxial tensile and hydrostatic compressive help reduce the thermal conductance of SiNWs. For example, a 3nm X 3nm, <100> oriented nanowire undergoing a 2% uniaxial tensile strain exhibits a thermal conductance reduced up to 2.6%, whereas a compressive hydrostatic strain of 2% gives a reduction of around 8%. Thus, strain engineering can prove beneficial in tuning the thermal conductance in Si nanowires and offers an efficient way to further improve the ZT figure of merit. Finanacial support from MSD, SRC, MIND and NSF, computational support from nanoHUB.org under NCN. Refs: [1] A. I. Hochbaum et al., 'Enhanced thermoelectric performance of rough silicon nanowires', Nature 451, no. 7175, pp. 163, 2008. [2] A Paul, M Luisier and G Klimeck, 'Modified valence force field approach for phonon dispersion: from zinc-blende bulk to nanowires.', arXiv:1009.6188v2[cond-mat.mes-hall].

8:24AM V30.00003 Thermal Conductivity of Metallic Nanowires near Room Temperature , N. STOJANOVIC, J. BERG, Texas Tech University, D.H.S. MAITHRIPALA, University of Peradeniya, M. HOLTZ, Texas Tech University — In metallic structures with nanoscale dimension both electrical and thermal conductivities are significantly different from their bulk counterparts. The total thermal conductivity is generally the sum of the electronic and phonon contributions. We examine electron and phonon heat transport in metals, in the temperature range near to or above the Debye temperature, where it is generally assumed that phonon component is negligible for metals, an assumption that has not been subjected to rigorous experimental verification, particularly at the nanoscale, due to difficulties in direct measurement of thermal conductivity. Experimental evidence suggests that the Wiedemann-Franz (W-F) law breaks down at the nanoscale. The neglected phonon component is one factor that has been cited as contributing to the apparent discrepancy in W-F. Another factor is inelastic electron-phonon scattering that influences transport due to a temperature gradient, but not due to an electric field. We report experimental results for Al nanowires and develop a model based on the Boltzmann transport equation for size dependence of electrical and thermal conductivity in nanowires. The model is validated with available data reporting direct measurements of thermal conductivity of nanowires, ribbons, and thin films. The W-F law and Lorenz factor are examined and a modified version of W-F is presented, corrected for these two factors and valid from macro- to nanoscale provided characteristic sizes exceed the phonon mean free path.

8:36AM V30.00004 Diffusion-induced dephasing and bistability of nanoresonators , JUAN ATALAYA, Chalmers University of Technology, MARK I. DYKMAN, Michigan State University, ANDREAS ISACSSON, Chalmers University of Technology — We study dephasing of an underdamped harmonic oscillator due to frequency fluctuations. The spectrum of the response to an external field is sensitive to the nature of the fluctuations. For nanomechanical resonators, if the dephasing is due to diffusion of adsorbed particles along the resonator, the spectrum varies from a single Lorentzian peak to two closely spaced peaks depending on the parameters. If the dephasing depends on the oscillator state, the oscillator can exhibit bistability of forced vibrations. We study this bistability for a nanomechanical resonator with diffusing adsorbed particles. The vibrations affect the particles by driving them toward the antinodes of the vibrational mode. Unexpectedly, even though diffusion is a random process, the bistability arises if it is sufficiently strong, i.e., fast compared to the vibrations decay time. For fast diffusion, we find the bistable response in the mean-field approximation. We also study, analytically and numerically, the rate of fluctuation-induced switching between the coexisting stable states.

8:48AM V30.00005 Electrical Detection of Resonance of ZnO nanowires using Harmonic Detection of Radiation , DEEPIKA SAINI, RAMAKRISHNA PODILA, MALCOLM SKOVE, APPARAO RAO, Clemson University — ZnO nanowires exhibit semiconducting and piezoelectric properties making them a technologically promising material. We have measured the mechanical resonance of cantilevered ZnO nanowires using the Harmonic Detection of Resonance (HDR) method.[1] The resonance is induced by an oscillating electric field and detected by second harmonic electric response of the ZnO nanocantilever. The diameter of the nanowires used was about 200 nm and length varied from 60 to 300 μm. Other mechanical properties of the cantilever, such as Young's modulus, are calculated from the observed resonance frequency.

[1]J. Gaillard, M.J. Skove, R. Ciocan and A.M. Rao, Rev. Sci. Instrum. 77, 073907(2006)

9:00AM V30.00006 Semiconducting nanowire electromechanics in the Coulomb blockade regime , HARI SOLANKI, SAJAL DHARA, ARNAB BHATTACHARYA, MANDAR DESHMUKH, Tata Institute, Mumbai, India — We fabricate and study Indium Arsenide (InAs) nanowire electromechanical resonators, in field effect transistor (FET) geometry, which allows us to tune the carrier density and tension in the wire at electromechanical resonance by tuning the dc gate voltage. At temperatures below 5K, quality factor (Q) of these resonators is $\sim$10000, two orders of magnitude larger than at room temperature, and the dynamic range reduces by an order of magnitude at low temperatures. Further in Coulomb blockade regime (charging energy $\sim$10 meV), using rectification technique, we have observed the modification in Coulomb diamond structure at the resonance frequency of the wire. Near the electromechanical resonance frequency, Coulomb peaks become broader symmetrically (independent of dc gate voltage and frequency sweep direction) and right at the resonance frequency their intensity is significantly reduced. This indicates a strong coupling between electron transport and mechanical vibration of the nanowire.

9:12AM V30.00007 Capacitive Spring Softening in Single-Walled Carbon Nanotube Nanoelectromechanical Resonators , CHUNG CHIANG WU, Department of EECS, University of Michigan — Due to their low mass density and high Young's modulus, single-walled carbon nanotubes (SWNTs) offer great promise as nanoelectromechanical (NEM) resonators with applications in ultrasmall mass and force sensing. Nanotube resonators can be actuated and detected simultaneously through electrostatic gate coupling. This gate induced frequency tuning of NEM resonators is known to be governed by two mechanisms: the elastic hardening effect and the capacitive softening effect. Although elastic hardening effect has been widely reported in SWNT resonators, the field-induced capacitive spring softening has rarely been observed. Here we report the capacitive spring softening effect observed in SWNT resonators. The nanotube resonators adopt dual-gate configuration with both bottom-gate and side-gate capable of tuning the resonance frequency through capacitive coupling. Interestingly, downward resonance frequency shifting is observed with increasing side-gate voltage, which can be attributed to the capacitive softening of spring constant. Furthermore, in-plane vibrational modes exhibit much stronger spring softening effect than out-of-plan modes. Our dual-gate design should enable the differentiation between these two types of vibrational modes, and open up new possibility for nonlinear operation of nanotube resonators. Other nonlinear effects in SWNT resonators will also be discussed.

9:24AM V30.00008 Vibrational Behaviour of Metal Nanowires under Tensile stress[1] , YASEMIN SENGUN, Department of Physics, Istanbul Technical University, Maslak, 34469, Istanbul, Turkey, SONDAN DURUKANOGLU, Faculty of Engineering and Natural Sciences, Sabanci University, Tuzla, 34956 Istanbul, Turkey — We present results of calculations on vibrational density of states (VDOS) of a thin Cu nanowire with <100> axial orientation and discuss on the effect of axial strain. The calculations are performed using real space Green's function method with the force constant matrix extracted from the interaction potentials based on the embedded atom method. It is shown that the characteristics of the VDOS of a strain-free nanowire are quite distinctive compared to that of a bulk atom. Among the striking features of this type nanowire is the existence of high frequency modes above the top of the bulk spectrum. From an examination of VDOS of local atoms it is seen that the corner and core atoms are the primary moderators for the anomalous increase in low frequency and high frequency modes, respectively. We, additionally, find that while the high frequency band above the top of the bulk phonon shifts to even higher frequencies, the characteristics at low frequencies remains almost the same upon stretching the nanowire along the axial direction.

[1]This work is supported by TUBITAK under Grant No. 109T105.

9:36AM V30.00009 Understanding and Controlling Intrinsic Dissipation in Driven Single Walled Carbon Nanotube Resonators[1] , RAJAMANI RAGHUNATHAN, P. ALEX GREANEY, JEFFREY C. GROSSMAN, Massachusetts Institute of Technology, Cambridge, MA 02139 — A "Phonostat" algorithm that can regulate total energy in a given internal degree of freedom within a molecular dynamics (MD) simulation is presented. The algorithm computes modal energies at every MD timestep, controls energy in a chosen vibrational mode with an external driving force and an internal damping. Using a test case of driven damped anharmonic oscillator, two different approaches of force correction are presented and various parameters that control the phonostat algorithm are analyzed. This algorithm is then employed to drive a chosen vibrational mode in carbon nanotube resonator to understand intrinsic dissipation under continuous driving, simultaneously computing its quality factor to mimic experimental conditions. The *gateway* modes that couple the driven mode to the thermal background are identified. Regulating these gateway modes hold the key to control intrinsic dissipation and improve quality factor for mass sensing application.

[1]The authors acknowledge funding from the Defense Threat Reduction Agency-Joint Science and Technology O?ce for Chemical and Biological Defense (Grant HDTRA1-09-1-0006).

9:48AM V30.00010 Anomalous Electromechanical Resonance Behavior of Single-walled Carbon Nanotubes under High Bias Voltages , MEHMET AYKOL, WILLIAM BRANHAM, ZUWEI LIU, MOH AMER, I-KAI HSU, ROHAN DHALL, SHUN-WEN CHANG, STEPHEN CRONIN, University of Southern California — By monitoring the nanoelectromechanical response of suspended individual carbon nanotubes (CNT), we observe the onset of optical phonon (OP) emission in these CNTs under high bias voltages. An abrupt upshift in the mechanical resonance frequency is observed at high voltage biases. The underlying cause of this behavior is the sudden increase in the lattice temperature of the CNT that causes contraction of the lattice due to the negative thermal expansion coefficient. This, in turn, results in increased tension in the suspended nanotube and an upshift in the mechanical resonance frequency. The sudden increase in temperature is explained by the OP emission in CNT. This effect is also observed in the Raman spectra of CNTs as a sudden downshift in the G band OP frequencies at high bias voltages.

10:00AM V30.00011 Transport in partially equilibrated inhomogeneous quantum wires[1] , ALEX LEVCHENKO, Argonne National Laboratory, TOBIAS MICKLITZ, Freie Universitat Berlin, JEROME RECH, Centre de Physique Theorique Marseille, KONSTANTIN MATVEEV, Argonne National Laboratory — We study transport properties of weakly interacting one-dimensional electron systems including on an equal footing thermal equilibration due to three-particle collisions and the effects of large-scale inhomogeneities. We show that equilibration in an inhomogeneous quantum wire is characterized by the competition of interaction processes which reduce the electrons total momentum and such which change the number of right- and left-moving electrons. We find that the combined effect of interactions and inhomogeneities can dramatically increase the resistance of the wire. In addition, we find that the interactions strongly affect the thermoelectric properties of inhomogeneous wires and calculate their thermal conductance, thermopower, and Peltier coefficient.

[1]This work at ANL was supported by the U.S. Department of Energy, Office of Science, under Contract No. DE-AC02-06CH11357.

10:12AM V30.00012 Energy loss of the electron system in individual single-walled carbon nanotubes[1] , DANIEL SANTAVICCA, JOEL CHUDOW, DANIEL PROBER, Yale University, MENINDER PUREWAL, PHILIP KIM, Columbia University — We characterize the energy loss of the non-equilibrium electron system in individual metallic single-walled carbon nanotubes at low temperature. Using Johnson noise thermometry, we demonstrate that, for a nanotube with ohmic contacts, the dc resistance at finite bias current directly reflects the average electron temperature. This enables a straightforward determination of the thermal conductance associated with cooling of the nanotube electron system. In analyzing the temperature- and length-dependence of the thermal conductance, we consider contributions from acoustic phonon emission, optical phonon emission, and hot electron outdiffusion [1]. In the same sample, we also characterize the radio frequency heterodyne response. Distinct responses are seen from bolometric detection and from the electrical nonlinearity due to non-ohmic contacts.

[1] D.F. Santavicca, J.D. Chudow, D.E. Prober, M.S. Purewal, and P. Kim, Nano Lett. 10, 4538 (2010).

[1]This work was supported by NSF-DMR and NSF-CHE.

10:24AM V30.00013 Heat pumping in nanomechanical systems[1] , LILIANA ARRACHEA, Universidad de Buenos Aires, CLAUDIO CHAMON, Boston University, EDUARDO MUCCIOLO, University of Central Florida, RODRIGO CAPAZ, Universidade Federal de Rio de Janeiro — We propose using phonon pumping mechanism to transfer heat from a cold to a hot body. The mechanism is based on inducing a traveling modulation of the acoustic phonon velocity along the medium connecting the two bodies. This phonon pumping can cool nanomechanical systems without the need for active feedback. We have derived an estimate of the lowest achievable temperature. We have also analyzed this mechanism in the framework of simple one-dimensional microscopic models, which can be exactly solved with non-equilibrium Green function techniques.

[1]J. S. Guggenheim Memorial Foundation

10:36AM V30.00014 Phonon spectrum in a CdSe nanowire[1] , CHRIS BARRETT, Material Science and Engineering Department, University of California at Berkeley, LIN-WANG WANG, Material Sciences Division — It is important to calculate the phonon spectrum of realistic nanowires, e.g. to understand its thermo conductivity or to calculate the electron-phonon interaction. In this talk, we will present results of phonon spectrum calculation using valence force field (VFF) method. An important issue is to construct the VFF to describe the surface atomic displacement. We have developed a general VFF formalism to fit our VFF result with the density functional theory (DFT) calculated surface atom displacement energies. In particular, the (10-10) CdSe surface is modelled with Cd-Se dimerization. We will discuss the quality of such VFF model. The phonon spectrum of the nanowire will be presented, and its implication on the phonon transport and electron-phonon coupling will also be discussed.

[1]This work is supported by U.S. Department of Energy BES, office of science, under Contract No. DE-AC02-05CH11231.

10:48AM V30.00015 Curvature-induced Effects on the Phonon Modes in Sub-nanometer Diameter Single-walled Carbon Nanotubes , RAMAKRISHNA PODILA, Clemson University, RAHUL RAO, Air Force Research Laboratory, Materials and Manufacturing Directorate, WPAFB, OH, CODRUTA LOEBICK, NAN LI, Yale University, JASON REPPERT, Clemson University, LISA PFEFFERLE, Yale University, APPARAO M. RAO, Clemson Univeristy — Sub-nanometer diameter single-walled carbon nanotubes (sub-nm SWNTs) are of great interest for fundamental studies due to the effect of large curvature on their properties. We have recently synthesized high quality, narrow diameter distribution sub-SWNTs using CoMn catalysts supported on MCM-41 silica templates in a thermal chemical vapor deposition process [1]. The high curvature in the sub-nm SWNTs leads an unusual S-like dispersion of the G-band frequency due to the strong electron–phonon coupling. In addition, we observe diameter-selective intermediate frequency modes (IFMs) that are as intense as the low frequency radial breathing modes (RBMs). The effect of large curvature in the sub-nm SWNTs is also evident in the lower phonon dispersion of the double resonant Raman features compared to SWNTs with larger diameters. The origin of previously unidentified IFM features (600-1100 cm^{-1}) and the dispersion of high frequency phonons (1650 – 2300 cm^{-1}) will be discussed.
[1] C. Z. Loebick *etal.*, *J. Am. Chem. Soc.*,132, 11125 (2010)

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V31 GERA: Energy Production: Combustion, Heat Engines, Solar Thermal and Thermoelectrics C145

8:00AM V31.00001 Electricity from Coal Combustion: Improving the hydrophobicity of oxidized coals , MOHINDAR SEEHRA, VIVEK SINGH, West Virginia University — To reduce pollution and improve efficiency, undesirable mineral impurities in coals are usually removed in coal preparation plants prior to combustion first by crushing and grinding coals followed by gravity separation using surfactant aided water flotation. However certain coals in the US are not amendable to this process because of their poor flotation characteristics resulting in a major loss of an energy resource. This problem has been linked to surface oxidation of mined coals which make these coals hydrophilic. In this project, we are investigating the surface and water flotation properties of the eight Argonne Premium (AP) coals using x-ray diffraction, IR spectroscopy and zeta potential measurements. The role of the surface functional groups, (phenolic -OH and carboxylic -COOH), produced as a result of chemisorptions of O_2 on coals in determining their flotation behavior is being explored. The isoelectric point (IEP) in zeta potential measurements of good vs. poor floaters is being examined in order to improved the hydrophobicity of poor floating coals (e.g. Illinois #6). Results from XRD and IR will be presented along with recent findings from zeta potential measurements, and use of additives to improve hydrophobicity. Supported by USDOE/CAST, Contract #DE-FC26-05NT42457.

8:12AM V31.00002 Electrorheology for Efficient Energy Production and Conservation , R. TAO, ENPENG DU, HONG TAO, XIAOJUN XU, Temple University, YUN LIU, NIST Center for Neutron Research — At present, most of our energy comes from liquid fuels. The viscosity plays a very important role in liquid fuel production and conservation. For example, reducing the viscosity of crude oil is the key for oil extraction and its transportation from off-shore via deep water pipelines. Currently, the dominant method to reduce viscosity is to raise oil's temperature, which does not only require much energy, but also impacts the environment. Recently, based on the basic physics of viscosity, we proposed a new theory and developed a new technology, utilizing electrorheology to reduce the viscosity of liquid fuels. The method is energy-efficient, and the results are significant. When this technology is applied to crude oil, the suspended nanoscale paraffin particle, asphalt particles, and other particles are aggregated into micrometer-size streamline aggregates, leading to significant viscosity reduction. When the temperature is below 0°C and the water content inside the oil becomes ice, the viscosity reduction can be as high as 75%. Our recent neutron scattering experiment has verified the physical mechanism of viscosity reduction. In comparison with heating, to reach the same level of viscosity reduction, this technology requires less than 1% of the energy needed for heating. Moreover, this technology only takes several seconds to complete the viscosity reduction, while heating takes at least several minutes to complete.

8:24AM V31.00003 Small angle neutron (SANS) and X-ray scattering (SAXS) investigation of microstructure and porosity with fractal properties of coal, shale, and sandstone from Indiana , NARAYAN CH DAS, HU CAO, H. KAISER, T.R. PRISK, PAUL E. SOKOL, Low Energy Neutron Source, Center for Exploration of Energy and Matter & Department of Physics, Indiana University, Bloomington, M. MASTALERZ, J. RUPP, Indiana Geological Survey, Indiana University, Bloomington — We have applied SAXS, SANS and adsorption isotherms to study the porosity, pore structure and interaction of confined fluids in the various Indiana rock samples. This study included a bituminous coal, a sandstone, and a grey shale from formations investigated as possible targets for CO2 sequestration. SAXS and SANS are demonstrated quantitative information about the microstructure and pore morphology of the coals and other rocks at length scale (1 nm to 0.3 micron) as well as the fractal nature of pore matrix interfaces. The different scattering cross sections of X-rays and neutrons provide information on the distribution of pore sizes in organic and inorganic components. Neutrons are relatively sensitive to the presence of either hydrocarbons or water in the pores, and always give a smaller Porod exponent that that for X-ray. Construction of LENS was supported by the NSF, the 21^{st} Century Science and Technology fund of Indiana, and the DOD. LENS operation is supported by Indiana University.

8:36AM V31.00004 Optimizing the performance of a heat engine: A simulation study , MULUGETA BEKELE, MEHARI BAYOU, YERGOU TATEK, MESFIN TSIGE — We performed a simulation study of a simple heat engine as it undergoes Carnot-type cyclic motion in a finite time over a wide range of piston speeds. There exists a specific piston speed at which the power delivered by the engine is maximum (P_{max}) and its corresponding efficiency is slightly larger than *half* of the Carnot efficiency (1/2 η_c). An optimization criterion leads to a trade-off between high power and high efficiency with respective values of 4/5 P_{max} and 3/4 η_c. In addition, we found the time taken at the optimized state to be twice the time taken when operating at maximum power.

8:48AM V31.00005 Analysis of Binary Cycle Efficiency Using Redlich-Kwong Equation of State , DEBORAH SAUNDERSON, ARIEF BUDIMAN, University of Calgary — Coal, natural gas and nuclear power plants operate using various forms of Rankine cycle. We present an efficiency maximization strategy of binary cycle, which has two Rankine cycles in tandem, using Redlich-Kwong equation of state for wide ranging working fluids: alkali metals, mercury, water, and ammonia. Binary cycle efficiency can approach the Carnot efficiency at a cost. The mercury/ammonia working fluid combination yields the highest efficiency for typical binary cycle conditions. We discuss practical implications given that mercury and ammonia create safety concerns, especially on finding other fluids having similar efficiency based on our simulations.

9:00AM V31.00006 Carbon dioxide adsorption on H_2O_2 treated single-walled carbon nanohorns[1] , ALDO MIGONE, VAIVA KRUNGLEVICIUTE, SHREE BANJARA, Department of Physics, Southern Illinois University Carbondale, MASAKO YUDASAKA, SUMIO IIJIMA, National Institute of Advanced Industrial Science and Technology, Japan — Carbon nanohorns are closed single-wall structures with a hollow interior. Unlike SWNTs, which assemble into cylindrical bundles, nanohorns form spherical aggregates. In our experiments we used dahlia-like carbon nanohorn aggregates. Our sample underwent treatment with H_2O_2 which opened access to the interior spaces of the individual nanohorns. We measured carbon dioxide adsorption at several temperatures between 167 and 195 K. We calculated the isosteric heat as a function of loading, and the binding energy values for CO_2 on the nanohorn aggregates from the isotherm data. Results on the H_2O_2-treated nanohorns will be compared with those obtained on other carbon substrates. We have also determined detailed equilibration profiles for CO_2 adsorption on the nanohorn aggregates; these results will also be presented.

[1]This work was supported by the NSF through grants DMR-1006428 and DMR-0705077.

9:12AM V31.00007 GOFs and ZIFs: Experimental Results and Analysis of Carbon Dioxide Sorption , JACOB BURRESS, JASON SIMMONS, NIST Center for Neutron Research, WEI ZHOU, University of Maryland, GADIPELLI SRINIVAS, JAMIE FORD, University of Pennsylvania, TANER YILDIRIM, NIST Center for Neutron Research — In recent years, growing concerns about global warming and the environment have spurred an accelerated development of materials technology for carbon dioxide (CO2) capture and storage. Two recent categories of materials being investigated for their CO2 storage capabilities are graphene oxide frameworks (GOFs) [1] and zeolitic imidazolate frameworks (ZIFs). We have synthesized graphene-oxide-frameworks (GOFs) by linking the OH groups on graphene oxide with benzene-boronic acids. Our initial GOF materials exhibit isosteric heats at low coverage of 32 kJ/mol for CO2. The nitrogen BET surface area of these initial materials is around 500 m2/g. Also, ZIFs are particularly useful for CO2 capture and storage due to high selectivities, CO2 uptakes and sample robustness. Neutron scattering and spectroscopic results of GOFs and select ZIFs with in-situ gas sorption will be presented. Neutrons are able to determine locations and strengths of binding sites. We will present detailed isotherms of carbon dioxide, methane and nitrogen at different temperatures of these interesting GOF and ZIF materials.
[1] J. W. Burress et al., Angewandte Chemie International Edition 49, 8902 (2010).

9:24AM V31.00008 Eutectics and Phase Diagrams of Molten Salts from Molecular Dynamics simulations , SAIVENKATARAMAN JAYARAMAN, ANATOLE VON LILIENFELD, AIDAN THOMPSON, Sandia National Laboratories — The use of alkali nitrate salt mixtures as heat transfer fluids in solar thermal power plants is limited by their relatively high melting point. Certain compositions of quaternary and higher dimensional mixtures of alkali and alkaline earth nitrates and nitrites have low melting points. However, the high dimensionality of the search space makes it difficult to find lowest melting compositions. Molecular simulations offer an efficient way to screen for promising mixtures. A molecular dynamics scheme general enough to identify eutectics of any HTF candidate mixture will be presented. The eutectic mixture and temperature are located as the tangent point between free energies of mixing for the liquid and a linear plane connecting the pure solid-liquid free energy differences. The free energy of mixing of the liquid phase is obtained using thermodynamic integration over "alchemical" transmutations sampled with molecular dynamics, in which particle identities are swapped gradually. Numerical results for binary and ternary mixtures of alkali nitrates agree well with experimental measurements.

9:36AM V31.00009 Energy Harvesting with Stochastic, Subharmonic and Ultraharmonic Vibrations[1] , JI-TZUOH LIN, BRUCE ALPHENAAR, University of Louisville — Non-linear bi-stable systems have been shown to provide improved efficiency for harvesting energy from random and broad band vibration sources. This paper explores the distinct frequency response in the broadened spectrum of a particular non-linear energy harvester, a piezoelectric cantilever with magnetic coupling. The cantilever response evolves dynamically with frequency around the main cantilever resonance. Both stochastic and multi-frequency vibration responses are observed, and account for some of the improved efficiency. In addition, sub-harmonics and ultra-harmonics of the main resonance, along with various combinations of these appear. Taken together, the sub-harmonic and ultra-harmonic response produces an average of four-fold increase in voltage production. For energy harvesting purposes, the mixtures of the stochastic and various harmonic features together with the un-damped resonant response enhances the performance well beyond that of a standard energy harvester. An analytical model of the bi-stable dynamics produces results consistent with those observed experimentally.

[1]The effort was funded by the U.S. Navy under Contract DAAB07-03-D-B010/TO-0198. Technical program oversight under Navy contract was provided by Naval Surface Warfare Center, Crane Division.

9:48AM V31.00010 Enhanced thermoelectric properties of n-type filled skutterudite Yb0.35Co4Sb12 by substitution on both the Co and Sb sites , TIANYI SUN, Boston College, GANG CHEN, MIT, ZHIFENG REN, Boston College — A dimensionless thermoelectric figure of merit (ZT) of about 1.2 was reported in Yb0.35Co4Sb12 at 550°C by ball milling and hot pressing. Through alloying on both the Co and Sb sites, we expect to achieve lower thermal conductivity while maintaining the power factor. The composition tuning is aimed for reducing the electrical conductivity and increasing the Seebeck coefficient, which will lead to a lower thermal conductivity, and ultimately higher ZT. In this report, we present the thermoelectric properties of skutterudites Yb0.35FexCo4-2xNixSb12 and Yb0.35Co4Sb12-yMy (M=Si, Ge, Sn, B, Al, Ga, In, etc.).

10:00AM V31.00011 Optimum Working Fluid Selection For Rankine Cycle Using Redlich-Kwong Equation of State , ARIEF BUDIMAN, DEBORAH SAUNDERSON, University of Calgary — Efficiency of Rankine cycle as a function of working fluid molecule is modeled using Redlich-Kwong equation of state. We have evaluated 12 molecules, ranging from water to ethylene glycol, and have parameterized their individual performance on several material parameters, including heat capacity and compressibility. This research aims to understand at the molecular level what drives some molecules to perform better at certain temperature and pressure range of the Rankine cycle. Immediate applications we are interested in are geothermal power, solar thermal energy conversion and waste heat recovery.

10:12AM V31.00012 Thermoelectric properties of correlated materials , JAN TOMCZAK, KRISTJAN HAULE, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA, TAKASHI MIYAKE, Nanosystem Research Institute, AIST, Tsukuba 305-8568, Japan, ANTOINE GEORGES, Centre de Physique Theorique, Ecole Polytechnique, CNRS, 91128 Palaiseau Cedex, France, GABRIEL KOTLIAR, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA — The discovery of large Seebeck coefficients in transition metal compounds such as FeSi, FeSb2, or the iron pnictides, has stirred renewed interest in the potential merits of electronic correlation effects for thermoelectric properties. The notorious sensitivity in this class of materials to small changes in composition (doping, chemical pressure) and external stimuli (temperature, pressure), makes a reliable and, possibly, predictive description cumbersome, while at the same time providing an arena of possibilities in the search for high performance thermoelectrics. Based on state-of-the-art electronic structure methods (density functional theory with the dynamical mean field theory) we here compute the thermoelectric response for several of the above mentioned exemplary materials from first principles. With the ultimate goal to understand the origin of a large thermoelectricity in these systems, we discuss various many-body renormalizations, and identify correlation controlled ingredients that are pivotal for thermopower enhancements.

10:24AM V31.00013 Electron correlation effect on temperature and magnetic-field dependences of thermopower[1] , MARI MATSUO, Japan Atomic Energy Agency and JST-CREST, SATOSHI OKAMOTO, Oak Ridge National Laboratory, WATARU KOSHIBAE, RIKEN, Japan, MICHIYASU MORI, SADAMICHI MAEKAWA, Japan Atomic Energy Agency and JST-CREST — We theoretically investigate the temperature T and the magnetic field dependences of thermopower. To focus on the strong electron correlation, the Hubbard model is solved in the dynamical mean field theory with the non-crossing approximation impurity solver. The thermopower shows a non-monotonic behavior as a function of T and asymptotes to the high-T values given by the Heikes formula, depending on the ratio of Coulomb repulsion and T. The large response to the magnetic-field, which is observed in the cobalt oxides [1], can be associated with the sharp quasiparticle peak intrinsic to the strongly correlated electron system. We discuss the effect of orbital degeneracy, which is another key factor to enhance the thermopower in the correlated system [2].

[1] Y. Wang *et al.*, Nature **423**, 425 (2003).
[2] W. Koshibae *et al.*, Phys. Rev. B **62**, 6869 (2000).

[1]SO was supported by the Materials Sciences and Engineering Division, Office of Basic Energy Sciences, U.S. DOE.

10:36AM V31.00014 Unusual Transport and Strongly Anisotropic Thermopower in $PtCoO_2$ and $PdCoO_2$, KHUONG ONG, Institute of High Performance Computing, DAVID SINGH, Oak Ridge National Laboratory, PING WU, Institute of High Performance Computing — Thermoelectrics provide a technology for producing electrical energy from solar and other heat sources. Thermoelectric performance requires materials with high thermopower, normally found in doped semiconductors, where the thermopower is generally nearly isotropic. We discovered using first principles calculations and Boltzmann transport theory that two oxides, $PtCoO_2$ and $PdCoO_2$, which are not semiconductors, but rather good metals, have exceptionally large thermopowers in one direction, and moreover that the thermopower in these materials is highly anisotropic. This places these compounds in a highly unusual transport regime. Besides providing a new direction for thermoelectric materials research, they may be very useful in probing the fundamental limits of conventional transport theory for metals.

10:48AM V31.00015 Analysis of Wind Forces on Roof-Top Solar Panel[1] , YOGENDRA PANTA, GANESH KUDAV, Department of Mechanical & Industrial Engineering, Youngstown State University, Youngstown, Ohio — Structural loads on solar panels include forces due to high wind, gravity, thermal expansion, and earthquakes. International Building Code (IBC) and the American Society of Civil Engineers are two commonly used approaches in solar industries to address wind loads. Minimum Design Loads for Buildings and Other Structures (ASCE 7-02) can be used to calculate wind uplift loads on roof-mounted solar panels. The present study is primarily focused on 2D and 3D modeling with steady, and turbulent flow over an inclined solar panel on the flat based roof to predict the wind forces for designing wind management system. For the numerical simulation, 3-D incompressible flow with the standard k-ε was adopted and commercial CFD software ANSYS FLUENT was used. Results were then validated with wind tunnel experiments with a good agreement. Solar panels with various aspect ratios for various high wind speeds and angle of attacks were modeled and simulated in order to predict the wind loads in various scenarios. The present study concluded to reduce the strong wind uplift by designing a guide plate or a deflector before the panel.

[1]Acknowledgments to Northern States Metal Inc., OH (GK & YP) and School of Graduate Studies of YSU for RP & URC 2009-2010 (YP).

Thursday, March 24, 2011 8:00AM - 10:36AM –
Session V32 FIAP: Photonics: Metamaterials, Nanotechnology and Sensors C144

8:00AM V32.00001 Topological photonic systems: from integer to fractional quantum Hall states[1] , MOHAMMAD HAFEZI, Joint Quantum Institute, University of Maryland, MIKHAIL LUKIN, EUGENE DEMLER, Harvard University, JACOB TAYLOR, Joint Quantum Institute, NIST — Topological properties of systems lead to remarkable robustness against disorder. The hallmark of such behavior is the quantized quantum Hall effect, where the electronic transport in two-dimensional systems is protected against scattering from impurities and the quantized Hall conductance is the manifestation of a topological invariance. Here we suggest an analogous approach to quantum Hall physics to create robust photonic devices. Specifically, we show how quantum Hall and quantum spin Hall Hamiltonians can be implemented with linear optics using coupled resonator optical waveguides (CROW) in two dimensions. Key features of quantum Hall systems could be observed via reflection spectroscopy, including the characteristic Hofstadter "butterfly" and edge state transport. Furthermore, the addition of an optical non- linearity to our proposed system leads to the possibility of implementing a fractional quantum Hall state of photons, where phenomenon such as non-abelian statistics may be observable.

[1]This research was partially supported by the U.S. Army Research Office MURI award W911NF0910406.

8:12AM V32.00002 Analytical and numerical analysis of a generic cloaking system[1] , PATTABHIRAJU MUNDRU, DENTCHO GENOV, Louisiana Tech University — We present a technique to realize a multi-shell generic cloaking system. By considering specific geometrical and material properties for the shells around the object, we were able to achieve a transparency conditions independent of object's optical properties in quasi-static regime. A complete suppression of dipolar scattering is demonstrated for an arbitrary object enclosed in such a system. We propose *tunable-low loss* realistic shell designs based on composite media and the effect of dispersion on the overall scattering cross-section is evaluated. Full wave analytical and numerical simulations based on the transparency conditions obtained in the quasi-static limit are performed. It is shown that strong reduction of the scattering by a factor of up to 10^3 can be achieved across the entire optical spectrum.

[1]NSF(2010)-PFUND-202. Louisiana Board of Regents under contract number LEQSF (2007-12)- ENH-PKSFI-PRS-01.

8:24AM V32.00003 Optical spin-orbit coupling and Darwin terms in epsilon-near-zero materials , ANDREW COOK, JENS NOECKEL, University of Oregon — In optical cavities formed from spatially inhomogeneous epsilon-near-zero (ENZ) metamaterials, optical spin-orbit coupling can be made nearly isospectral to relativistic electron spin-orbit coupling in atoms; the only difference is that the 3x3 classical spin-orbit operator shifts transverse fields by a different integer amount than the quantum operator. When the electric field is rescaled to account for unequal dispersive energy density in the electric and magnetic field quadratures, Maxwell's equations give a Darwin term with the same form as in quantum mechanical systems. These classical/QM similarities, combined with a pronounced importance of the Kerr nonlinearity, make ENZ materials ideal for coaxing electron-like behavior from light.

8:36AM V32.00004 Design of Optical Microcavities for Coupling to Nitrogen-Vacancy Centers in Diamond , JENNA HAGEMEIER, University of California Santa Barbara, California, USA, TOENO VAN DER SAR, Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands, SUSANNA THON, HYOCHUL KIM, DUSTIN KLECKNER, University of California Santa Barbara, California, USA, WOLFGANG PFAFF, Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands, ERWIN HEERES, TJERK OOSTERKAMP, Leiden Institute of Physics, Leiden University, The Netherlands, PIERRE PETROFF, Department of Materials and Department of ECE, University of California Santa Barbara, California, USA, RONALD HANSON, Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands, DIRK BOUWMEESTER, University of California Santa Barbara, California, USA and Leiden University, The Netherlands — Nitrogen-Vacancy (NV) centers in diamond have emerged as promising candidates for solid state qubits. When placed in a confined optical field, such as exists in an optical microcavity, the properties of single quantum emitters can be drastically modified. In the weak coupling regime, the rate of spontaneous light emission from the quantum emitter can be enhanced via the Purcell effect. We demonstrate deterministic coupling between single NV centers and photonic crystal microcavities in Gallium Phosphide (GaP). Designs of novel optical cavities for coupling to NV centers in diamond will also be discussed.

8:48AM V32.00005 Radiation Tuning of Optical Nanoantennas for Design of Nanofilter Elements , MARJAN SABOKTAKIN, BRIAN EDWARDS, NADER ENGHETA, CHERIE KAGAN, University of Pennsylvania, PROF. KAGAN COLLABORATION, PROF. ENGHETA COLLABORATION — We experimentally and numerically explore the radiation characteristics of optical nanoantennas. These nanoantennas are dipole antennas with dimensions on the order of several tens of nanometers that are fabricated to form lumped capacitance and Inductance through the use of sandwich structures made of dielectric and plasmonic-material layers. We then investigate tuning the response of these optical nanoantennas by varying the material and/or thickness of the dielectric layer. After each experiment, experimental results are compared with numerical simulations to verify the validity of the results. We then exploit these characteristics in building a "lumped" nanofiltering device, and thereby extending the concept of antennas and circuit elements such as filters from the microwave regime to the visible regime.

9:00AM V32.00006 Confined Three-Dimensional Plasmon Modes inside a Ring-Shaped Nanocavity on a Silver Film Imaged by Cathodoluminescence Microscopy[1] , XINLI ZHU, JIASEN ZHANG, JUN XU, DAPENG YU, Department of Physics, Peking University — The confined modes of surface plasmon polaritons in boxing ring-shaped nanocavities have been investigated and imaged by using cathodoluminescence spectroscopy. The mode of the out-of-plane field components of surface plasmon polaritons dominates the experimental mode patterns, indicating that the electron beam locally excites the out-of-plane field component of surface plasmon polaritons. Quality factors can be directly acquired from the spectra induced by the ultrasmooth surface of the cavity and the high reflectivity of the silver reflectors. Because of its three-dimensional confined characteristics and the omnidirectional reflectors, the nanocavity exhibits a small modal volume, small total volume, rich resonant modes, and flexibility in mode control.

[1]This work is supported by NSFC (10804003, 61036005 and 11074015), the national 973 program of China (2007CB936203, 2009CB623703), MOST and NSFC/RGC (N HKUST615/06).

9:12AM V32.00007 Novel meta-surfaces for wave manipulation , SHULIN SUN, National Taiwan University, QIONG HE, SHIYI XIAO, Fudan University, QIN XU, LEI ZHOU, Fudan University — Meta-materials are man-made electromagnetic (EM) materials composed by subwavelength local resonance structures of electric and/or magnetic type, and thus possess arbitrary values of permittivity and permeability dictated by such resonance structures. Many novel EM properties, such as the negative refraction, the superlensing effect, and even the invisibility cloaking were predicted or discovered based on meta-materials. By carefully designing metamaterials with appropriate EM wave properties, one can employ metamaterials to efficiently manipulate various properties of EM waves, including the wave propagation, polarization, and so on. Here, we present our latest theoretical and experimental efforts in designing novel meta-surfaces (ultra-thin metamaterials) with anomalous EM wave properties to allow efficiently manipulating wave propagation directions. Furthermore, our system can also convert propagating wave to surface plasmon polariton. Microwave experiments are performed on realistic structures to successfully realize the theoretical predictions, and the obtained results are in agreements with FDTD simulations.

9:24AM V32.00008 Percolation and polaritonic effects in periodic planar nanostructures evolving from holes to islands[1] , YUN PENG, TRILOCHAN PAUDEL, WEN-CHEN CHEN, WILLIE PADILLA, ZHIFENG REN, Boston College, KRIS KEMPER, Boston College, South China Normal University — We study interaction of the electromagnetic radiation with a series of thin film periodic nanostructures evolving from holes to islands. We show, through model calculations, simulations and experiments, that the responses of these structures evolve accordingly, with two topologically distinct spectral types for holes and islands. We find also, that the response at the transitional pattern is singular. We show that the corresponding effective dielectric function follows the critical behavior predicted by the percolation theory, and thus the hole-to-island structural evolution in this series is a topological analog of the percolation problem, with the percolation threshold at the transitional pattern.

[1]This work was supported in part by a grant from DOE (Grant No. DE-FG02-00ER45805) (ZFR). W.-C.C. and W.J.P. acknowledge support from the Office of Navel Research under U. S. Navy Contract No. N00014-07-1-0819.

9:36AM V32.00009 ABSTRACT WITHDRAWN –

9:48AM V32.00010 An XPS study of gas phase interaction with Au nanoparticles coated TiO_2 nanosprings[1] , I. NIRAULA, B.A. FOUETIO, D.N. MCILROY, Dept. of Physics, Univ. of Idaho, Moscow, ID 83844, T. TURBA, M.G. NORTON, School of Mech. and Mat. Eng., Washington St. Univ., Pullman, WA 99164 — The interaction of CO and O_2on the surface of the Au nanoparticles (NPs) supported on TiO_2(Au/TiO_2) nanosprings (NS) by x-ray photoelectron spectroscopy will be discussed. The Au NPs were coated onto the TiO_2NS by plasma enhanced chemical vapor deposition, where the average particle size is 7-8 nm. The gas interactions with the Au NPs is evaluated by examining binding energy shifts of the Au 4f, C 1s, Ti 2p and O 1s electron core level states. For both of the gases, all of the core levels shifted to higher binding energy. Temperature dependent desorption, or the lack thereof, as determined by XPS analysis, indicates that the gas-substrate interaction is chemisorption, as opposed to physisorption. A detailed discussion on the mechanism of adsorption, as well as the roles of the Au NP and the TiO_2 substrate, will be presented.

[1]Univ. of Idaho, BANtech

10:00AM V32.00011 Paper based Flexible and Conformal SERS Substrate for Rapid Trace Detection on Real-world Surfaces[1] , SRIKANTH SINGAMANENI, CHANG LEE, LIMEI TIAN, Washington University in St. Louis — One of the important but often overlooked considerations in the design of surface enhanced Raman scattering (SERS) substrates for trace detection is the efficiency of sample collection. Conventional designs based on rigid substrates such as silicon, alumina, and glass resist conformal contact with the surface under investigation, making the sample collection inefficient. We demonstrate a novel SERS substrate based on common filter paper adsorbed with gold nanorods, which allows conformal contact with real-world surfaces, thus dramatically enhancing the sample collection efficiency compared to conventional rigid substrates. We demonstrate the detection of trace amounts of analyte (140 pg spread over 4 cm^2) by simply swabbing the surface under investigation with the novel SERS substrate. The hierarchical fibrous structure of paper serves as a 3D vasculature for easy uptake and transport of the analytes to the electromagnetic *hot spots* in the paper. Simple yet highly efficient and cost effective SERS substrate demonstrated here brings SERS based trace detection closer to real-world applications.

[1]We acknowledge the financial support from Center for Materials Innovation at Washington University.

10:12AM V32.00012 Sensitive detection of nitro aromatic explosives using novel polythiophene nanoparticles , SOUMITRA SATAPATHI, University of Massachusetts Lowell, B. HARIHARA VENKATARAMAN, University of Massachusetts Amherst, AKSHAY KOKIL, University of Massachusetts Lowell, LIAN LI, US Army Natick Soldier Research, Development & Engineering Center, Natick,, DHANDAPANI VENKATARAMAN, University of Massachusetts Amherst, JAYANT KUMAR, University of Massachusetts Lowell, CENTER FOR ADVANCED MATERIALS TEAM, UNIVERSITY OF MASSACHUSETTS LOWELL TEAM, UNIVERSITY OF MASSACHUSETTS AMHERST COLLABORATION — Fluorescent polythiophene nanoparticles were fabricated by surfactant assisted mini emulsion technique. The size distribution of the synthesized nanoparticles was characterized using dynamic light scattering (DLS) and scanning electron microscopy (SEM). The synthesized nanoparticles were also characterized using UV-Vis and fluorescence spectroscopy. Strong two-photon induced fluorescence was observed from these nanoparticles using 800 nm pulses from a femto second laser. The fluorescence response of these nanoparticles to nitro-aromatic explosives 2,4-dinitrotoluene and 2,4,6-trinitrotoluene in solution was investigated at different concentrations of the analytes. Strong fluorescence quenching was observed using both one photon and two-photon excitation source. The Stern Volmer constant is also higher.

10:24AM V32.00013 A novel nanostructure for ultrasensitive volatile organic compound sensing[1] , HUAIZHOU ZHAO, BINOD RIZAL, ZHIFENG REN, MICHAEL J. NAUGHTON, THOMAS C. CHILES, DONG CAI, Boston College — We have developed an arrayed nanocoaxial structure for the ultrasensitive sensing detection and identification of volatile organic compounds (VOC) by dielectric impedance spectroscopy. VOC molecules are absorbed into porous dielectric material in the annulus between nanoscale coax electrodes. A theoretical expression for the basic adsorption mechanism agrees with the experimental results. Detection sensitivities at parts-per-billion levels were demonstrated for a variety of VOCs. A limit-of-detection of ethanol reached $\sim$100 parts-per-trillion, following a Freundlich power-law isotherm across four decades of ethanol concentration. A linear dependence on VOC dielectric constant was observed. Dielectric impedance nanospectroscopy was also performed by scanning frequency from 10 mHz to 1 MHz, with distinctive spectra of different VOCs discovered. These were utilized to conduct colorimetric identification of VOCs. The results suggest our novel nanocoaxial sensor can be used as a sensitive, broadband, and multimodal sensing platform for chemical detection.

[1]The National Cancer Institute CA137681, the Department of Navy, the National Science Foundation PHY-0804718, and the Seaver Institute. Emails: caid@bc.edu; naughton@bc.edu

Thursday, March 24, 2011 8:00AM - 10:24AM –

Session V33 DMP DCOMP: Focus Session: Dielectric, Ferroelectric, and Piezoelectric Oxides: Vortices and Novel Mechanisms C143/149

8:00AM V33.00001 Effect of A-site size difference on polar behavior in MBiScNbO$_6$ (M=Na, K, and Rb) perovskite: Density functional calculations , SHIGEYUKI TAKAGI, ALASKA SUBEDI, Oak Ridge National Laboratory and University of Tennessee, VALENTINO COOPER, DAVID SINGH, Oak Ridge National Laboratory — We investigated the effect of A-site size difference in the double perovskites BiScO$_3$-MNbO$_3$ (M=Na, K, and Rb) using first-principles calculations. The materials studied have increasing ionic radii at the A-site ($r_{\mathrm{Na}^+} < r_{\mathrm{K}^+} < r_{\mathrm{Rb}^+}$) but are otherwise chemically similar. We find that the polarization of these materials is 70-90 μC/cm^2 along the rhombohedral direction, which increases as the A-site size difference becomes larger. The main contribution to the high polarization comes from large off-centerings of Bi ions, which are strongly enhanced by the suppression of octahedral tilts as the M-ion size increases. A high Born effective charge of Nb also contributes to the polarization and this contribution is also enhanced by increasing the M-ion size. This work was supported by ONR and DOE, BES, Materials Sciences and Engineering.

8:12AM V33.00002 First Principles Study of Flexoelectricity , JIAWANG HONG, DAVID VANDERBILT, Rutgers University — Flexoelectricity is the linear response of polarization to a strain gradient. Because strain gradients break inversion symmetry, flexoelectricity allows for charge to be extracted from deformations even in materials that are not piezoelectric. The flexoelectric effect is negligible on conventional length scales, but it becomes very strong at the nanoscale where large strain gradients can significantly affect the functional properties of dielectric thin films and superlattices. We present first-principles calculations of flexoelectric effects in nonpiezoelectric materials by introducing the strain gradient artificially in a slab geometry and obtain the flexoelectric coefficients. Furthermore, we model the results in terms of quantities, such as dynamical charges and higher[1] multipole moments that can be computed in the bulk, bringing us closer to a full theory of flexoelectricity.

[1]R. Resta, Phys. Rev. Lett. **105**, 127601 (2010).

8:24AM V33.00003 Coexistence of ferroelectricity and octahedral rotations in ABX$_3$ perovskites , NICOLE BENEDEK, CRAIG FENNIE, School of Applied and Engineering Physics, Cornell University — Nearly all cubic perovskite materials are unstable to energy-lowering structural distortions. The most intensively studied distortions are those that induce ferroelectricity and tilts or rotations of the anion octahedra. The phonon dispersion curves of many perovskites contain both types of instability, although competition between the different types of distortions usually leads to ground-state structures in which one type of instability has been eliminated. Hence, whereas there are many perovskites that are *either* ferroelectric or have rotated octahedra, there are very few perovskites that are *both* ferroelectric and have rotated octahedra. We use a combination of Density Functional Theory, group theoretical techniques and crystal chemistry arguments to study the competition between ferroelectric and octahedral rotation distortions in a family of ferroelectric perovskite fluorides and oxides. By considering both "long-range" distortions (phonons) and the local bonding environment of each ion, we are able to build up a picture of which factors favor one type of distortion over the other.

8:36AM V33.00004 Vortex Domains in Ferroelectric Nano-Structures

, JAMES F. SCOTT, Cambridge University — Recently the study of submicron-diameter ferroelectric disks and squares and rectangles fabricated from films of ca. 100-300 nm thick have revealed usual domain patterns, qualitatively different from the stripe domains commonly studied in macroscopic specimens in the past. These include doughnut-shaped domains, four-fold vertex closure domains, and fractal domains. The static configurations offer a variety of puzzles, and the structures differ from those in magnetic vortex domains, presumably due to the much larger anisotropy in ferroelectrics, which generally prohibits true vortex configurations with polarization forced out of plane. The dynamics also differ qualitatively from early studies: For decades ferroelectrics were thought to be highly Ising-like, but recent data and theoretical simulations favor Bloch walls and more Heisenberg-like kinetics. This talk will include data from Alina Schilling and Marty Gregg in Belfast, Marin Alexe in Halle, and modeling from Hlinka and Marton in Prague and Bellaiche and Prosandeev in Arkansas.

9:12AM V33.00005 Multiferroic Vortices and Graph Theory

, SANG-WOOK CHEONG, S.C. CHAE, Y. HORIBE, Rutgers Center for Emergent Materials, D.Y. JEONG, Department of Mathematics, Soongsil University, Korea , N. LEE, S. RODAN, T. CHOI, Rutgers Center for Emergent Materials — Hexagonal $REMnO_3$ (RE= rare earths) with RE=Ho-Lu, Y, and Sc, is an improper ferroelectric where the size mismatch between RE and Mn induces a trimerization-type structural phase transition, and this structural transition leads to three structural domains, each of which can support two directions of ferroelectric polarization. We reported that domains in h-$REMnO_3$ meet in cloverleaf arrangements that cycle through all six domain configurations, Occurring in pairs, the cloverleafs can be viewed as vortices and antivortices, in which the cycle of domain configurations is reversed. Vortices and antivortices are topological defects: even in a strong electric field they won't annihilate. Recently we have found intriguing, but seemingly irregular configurations of a zoo of topological vortices and antivortices in h-$REMnO_3$. These configurations can be neatly analyzed in terms of graph theory.

9:24AM V33.00006 Hidden Roto Symmetries in Crystals and Handed Structures[1]

, VENKATRAMAN GOPALAN, DANIEL LITVIN, Pennsylvania State University — Symmetry is a powerful framework to perceive and predict the physical world. The structure of materials is described by a combination of rotations, rotation-inversions and translational symmetries. By recognizing the reversal of static structural rotations between clockwise and counterclockwise directions as a distinct symmetry operation, here we show that there are many more structural symmetries than are currently recognized in right- or left-handed handed helices, spirals, and in antidistorted structures composed equally of rotations of both handedness. For example, though a helix or spiral cannot possess conventional mirror or inversion symmetries, they can possess them in combination with the rotation reversal symmetry. Similarly, we show that many antidistorted perovskites possess twice the number of symmetry elements as conventionally identified. These new symmetries, referred to as "roto" symmetries, predict new forms for roto properties that relate to static rotations, such as rotoelectricity, piezorotation, and rotomagnetism. They also enable a symmetry-based search for new phenomena, such as multiferroicity involving a coupling of spins, electric polarization and static rotations. This work is relevant to structure-property relationships in all material structures with static rotations.

[1]We acknowldege funding from the National Science Foundation.

9:36AM V33.00007 Spontaneous Vortex Nanodomain Arrays at Ferroelectric Heterointerfaces

, XIAOQING PAN, CHRISTOPHER NELSON, YI ZHANG, Dept. of Mater. Sci. & Eng., Univ. of Michigan, Ann Arbor, MI, BENJAMIN WINCHESTER, LONG-QING CHEN, Dept. of Mater. Sci. & Eng., Penn State Univ., University Park, PA, COLIN HEIKES, CAROLINA ADAMO, ALEXANDER MELVILLE, DARRELL SCHLOM, Dept. Sci. & Eng., Cornell Univ., Ithaca, NY, CHAD FOLKMAN, CHANG-BEOM EOM, Dept. of Mater. Sci. & Eng., Univ. of Wisconsin-Madison, Madison, WI — The polarization of $BiFeO_3$ subjected to different electrical boundary conditions by hetero-interfaces is imaged with atomic resolution using a Cs-corrected transmission electron microscope. Unusual nanodomains are seen and their role in providing polarization closure is understood through phase-field simulations. Hetero-interfaces are key to the performance of ferroelectric devices and this first observation of vortex arrays at ferroelectric hetero-interfaces reveals properties unlike the surrounding film including mixed Ising-Néel domain walls, which will affect switching behavior, and a drastic increase of in-plane polarization. Imaging this magnetic analogous effect at ferroelectric hetero-interfaces provides the ability to see device-relevant interface issues.

9:48AM V33.00008 Helical strain patterns and charge ordering in $YbFe_2O_4$

, ALEXANDER HEARMON, PAOLO RADAELLI, PRABHAKARAN DHARMALINGAM, Clarendon Laboratory, Oxford University, MATTHIAS GUTMANN, ISIS Facility, Rutherford Appleton Laboratory, FEDERICA FABRIZI, Clarendon Laboratory, Oxford University, DAVE ALLAN, Diamond Light Source Ltd — The RFe_2O_4 compounds exhibit simultaneously charge ordering (CO) of the Fe^{2+} and Fe^{3+} ions,[1] together with magnetic ordering of the Fe spins[2] and possible multiferroic behavior.[3] Synchrotron data collected below the 3D CO transition show intensity concentrated around peaks separated by $\sim 1/3$ c^* but slightly displaced in the (a^*, b^*) plane. Calculations modelling an oxygen displacement pattern are in excellent agreement with the data, suggesting an incommensurate charge ordering of the Fe ions close to the commensurate $\sqrt{3} \times \sqrt{3}$ structure, associated with a helical strain pattern. At high temperature, ordering wavevectors corresponding to many different displacement patterns are simultaneously populated by the system, leading to diffuse but highly structured features in reciprocal space.

[1]Ikeda *et al*, Nature **436** 1136 (2005)
[2]Christianson *et al*, PRL **100** 107601 (2008)
[3]S-W Cheong *et al*, Nat. Mater. **6** 13 (2007)

10:00AM V33.00009 Three-dimensional distribution of ferroelectric vortices in multiferroic hexagonal $YMnO_3$

, MANFRED FIEBIG, HISKP, University of Bonn, Germany, ELISABETH SOERGEL, TOBIAS JUNGK, IAP, University of Bonn, Germany, NICOLA A. SPALDIN, Dept. Materials, ETH Zurich, Switzerland, KRIS DELANEY, MRL, UC Santa Barbara, USA — Multiferroics are a rich source for "unusual" forms of ferroelectric order. The spontaneous polarizations is induced by magnetism, charge order, geometric effects, etc., and may lead to novel domain states and functionalities. Recently it was shown that ferroelectric domains in hexagonal multiferroic $YMnO_3$ form vortex-like structures around the direction of polarization [1]. It was assumed that the sixfold character of the domain vortices reflects the uniaxial hexagonal structure. Here we show by piezoresponse force microscopy that high densities of sixfold vortices are also present *perpendicular* to the direction of the spontaneous polarization in spite of the merely twofold rotation-inversion symmetry in this direction [2]. We present a simple geometric explanation for this unexpected result and discuss the principal difference between the present case and vortex formation in discommensurate systems.

[1] T. Choi et al., Nature Mater. **9**, 253 (2010)
[2] T. Jungk et al., Appl. Phys. Lett. **97**, 012904 (2010)

10:12AM V33.00010 Cloverleaf domain patterns in multiferroic $RMnO_3$ (R = Ho, Er, and Lu)

, Y. HORIBE, S.C. CHAE, N. LEE, S-W. CHEONG, Rutgers Center for Emergent Materials and Department of Physics & Astronomy, Rutgers University — Hexagonal $RMnO_3$ (R=rare earths) exhibits a unique improper ferroelectricity induced by structural trimerization. Intriguing domain pattern associated with ferroelectricity and trimerization, so-called "cloverleaf" domain pattern, has been reported in $YMnO_3$ [1] In this talk, we will report the domain structures in a series of $RMnO_3$ with different rare earth elements, obtained from the results of our transmission electron microscopy. Characteristic cloverleaf domain patterns are clearly observed in $RMnO_3$ (R = Ho, Er, and Lu). The results imply that the cloverleaf domain pattern is a common domain feature in the hexagonal manganites.

[1] T. Choi et al., Nature Materials 9, 818 (2010)

Thursday, March 24, 2011 8:00AM - 11:00AM –
Session V35 DCMP: Topological Insulators: ARPES & STM C140

8:00AM V35.00001 Local probing of Quantum Spin Hall edge states , MARKUS KÖNIG, ANDREI GARCIA, MATTHIAS BAENNINGER, Stanford University, CHRISTOPH BRÜNE, HARTMUT BUHMANN, LAURENS MOLENKAMP, University of Wuerzburg, DAVID GOLDHABER-GORDON, Stanford University — Since their recent experimental discovery, topological insulators have attracted a lot of interest. The two-dimensional manifestation of a topological insulator, the Quantum Spin Hall (QSH) state, is characterized by counter- propagating edge states with opposite spin-polarization, while the bulk is insulating. We use Scanning Gate Microscopy to demonstrate the edge state nature of transport in the QSH state. Utilizing the high spatial resolution of this technique, we gain insight into the spatial properties of the edge states. Furthermore, the experiments can yield information regarding the sensitivity of the QSH edge states to local perturbations, which can be useful for future applications.

8:12AM V35.00002 Visualizing Strong Scattering of Topological Surface States from Magnetic Impurities in Bi_2Te_3[1] , HAIM BEIDENKOPF, PEDRAM ROUSHAN, JUNGPIL SEO, LINDSAY GORMAN, Y.S. HOR, R.J. CAVA, ALI YAZDANI, Physics Department, Princeton University — Bi_2Te_3 is a topological insulator with a single Dirac cone in the band structure of its helical surface states. The associated spin texture protected by time reversal symmetry (TRS) is thought to suppress scattering off non-magnetic defects. We tested this using scanning tunneling microscopy and spectroscopy. At high energies, far above the Dirac point, backscattering off non-magnetic defects, such as step-edges, is facilitated by quasi-nesting conditions brought about by the hexagonal warped surface band. At lower energies at which the surface dispersion is linear backscattering is highly suppressed by the helical spin texture protected by TRS. In contrast, in Mn-doped Bi_2Te_3 the measured quasi- particle interference pattern shows the onset of strong scattering both in the warped region as well as in the conic one. The scattering processes involved are affected both by the spin texture as well as by the geometry of the scattering potential. Furthermore, close to the Dirac point the increased scattering in Mn-doped Bi_2Te_3 seems to promote localization of the surface states.

[1]Supported by NSF-DMR, and MRSEC through PCCM. Infrastructure at Princeton Nanoscale Microscopy Laboratory are also supported by grants from DOE, and the W.M. Keck foundation.

8:24AM V35.00003 Magnetic Versus Non-magnetic Scattering of Topological Surface States in Bi_2Te_3[1] , LINDSAY GORMAN, HAIM BEIDENKOPF, PEDRAM ROUSHAN, JUNGPIL SEO, Department of Physics, Princeton University, YEW SAN HOR, ROBERT CAVA, Department of Chemistry, Princeton University, ALI YAZDANI, Department of Physics, Princeton University — Due to their novel spin texture, the surface states of topological insulators are predicted to be impervious to backscattering from non-magnetic disorder. For impurities which break time-reversal symmetry, however, such backscattering is not forbidden by the topological character of the states. Here we use scanning tunneling microscopy to study scattering from impurities in doped Bi_2Te_3. In Mn-doped Bi_2Te_3, we have observed an interference pattern from the surface states throughout a broad range of energies, even in the region of linear dispersion near the Dirac point. We contrast these findings of the scattering of topological surface states from magnetic defects with similar measurements on Ca-doped Bi2Te3 using spectroscopic mapping. We will use the results of these experiments to probe whether the presence of magnetic impurities gives rise to backscattering in topological surface states.

[1]Supported by NSF-DMR, MRSEC through PCCM. Infrastructure at PNML also supported by DOE, and the W.M. Keck foundation.

8:36AM V35.00004 Scanning tunneling spectroscopic (STS) studies of MBE-grown topological insulators of Bi_2Se_3 epitaxial films on Si(111) , N.-C. YEH, M.L. TEAGUE, W.-H. LIN, H. CHU, Dept. of Physics, Caltech, Pasadena, CA 91125, F.X. XIU, L. HE, K.L. WANG, UCLA, Los Angeles, CA 90095 — We report STS studies of MBE-grown Bi_2Se_3 epitaxial films on Si(111) with varying thicknesses. The films were atomically flat on the scale of hundreds of nanometers, with occasional atomic steps of one c-axis lattice constant. In the case of thick Bi_2Se_3 films, the tunneling spectra were consistent with those found in single crystalline Bi_2Se_3, except that the Dirac point ($E_{Dirac} = -50 \sim$ -100 meV) of the MBE-film is generally much closer to the Fermi level ($E = 0$), in contrast to the large downshift of E_{Dirac} (= -400 $\sim$ -200 meV) commonly found in single crystalline bulk grown Bi_2Se_3. The STS spectra of the thinner films deviate from those of the thicker samples, probably the result of strain. Fourier transformed (FT) STS data as a function of energy reveals several quasiparticle scattering interference wave-vectors that are consistent with the topologically protected surface states with chiral spin texture, although the overall FT-STS maps are simpler than those reported on the $Bi_{0.92}Sb_{0.08}$ (111) surface due to simpler electronic band-structures of Bi_2Se_3. The effect of time reversal symmetry breaking on the FT-STS will be investigated by either magnetic doping or application of magnetic fields. This work was supported by a grant from FENA of FCRP and DARPA.

8:48AM V35.00005 Electron interference in the 3D topological insulator Bi_2Se_3 probed by scanning tunneling microscope , MAO YE, A. KIMURA, S. KIM, K. KURODA, Hiroshima University, E.E. KRASOVSKII, E.V. CHULKOV, Universidad del Pais Vasco, K. MIYAMOTO, M. NAKATAKE, T. OKUDA, Hiroshima University, Y. UEDA, Kure National College of Technology, H. NAMATAME, Hiroshima University, M. TANIGUCHI — Three-dimensional topological insulators (TIs) have aroused great attention to the new state of quantum matter originating from the surface state that forms a massless Dirac cone. Among the recently discovered TIs, Bi_2Se_3 is regarded as the most promising candidate [1]. However, recent magnetotransport measurements showed that the bulk conductance dominates even in low carrier samples [2], which raises the question of possible scattering channels responsible for the reduced surface mobility. Band structure calculations predict the Dirac point of the surface state to be located close to the bulk valence band maximum [1]. In order to clarify the surface state scattering feature, we have performed differential tunneling conductance mapping for the surface of Bi_2Se_3. The fast Fourier transformation image shows an electron interference pattern near the Dirac node, which provides the evidence of near-surface scattering of the spin polarized surface electrons at the Dirac point in Bi_2Se_3 into the spin-degenerate bulk continuum states.

[1] Y. Xia et al., Nat. Phys. **5**, 398 (2009).
[2] N. P. Butch, Phys. Rev. B **81**, 241301(R) (2010).

9:00AM V35.00006 Power laws and STM image of standing wave of the topological surface states[1] , BANG-FEN ZHU, JING WANG, WEI LI, PENG CHENG, CANLI SONG, TONG ZHANG, XI CHEN, Department of Physics, Tsinghua University, XUCUN MA, KE HE, Institue of Physics, Chinese Academy of Science, JIN-FENG JIA, QI-KUN XUE, Department of Physics, Tsinghua University — We have theoretically and experimentally studied the quasiparticle interference pattern caused by scattering off the step edges of topological surface states in Bi_2Te_3 and Bi_2Se_3. We propose a general formalism to identify the power law that governs the decaying spatial oscillations of standing wave of the quasiparticle. With strong hexagonal warping of the surface states in Bi_2Te_3, the standing wave will have different decay index as the Fermi energy varies; while in Bi_2Se_3, the standing wave has only a single decay index due to weak warping effect. Using a scanning tunneling microscope, we directly observe the standing waves in the local density of states on both surfaces, which together with the analysis of such oscillations at different voltage confirms our theoretical predictions. We further show that, the characteristic scattering wavevectors of the standing wave of surface states caused by scattering off the nonmagnetic impurity in both Bi_2Te_3 and Bi_2Se_3can also be well explained by this general formalism.

[1]This work was supported by the NSFC and the Basic Research Program of China.

9:12AM V35.00007 Multifunctional electronic structure in a topological insulator class , SUYANG XU, ZAHID HASAN, Princeton University — The discovery of topological properties in three dimensional bulk solids have opened up many new research avenues in condensed matter physics. Only a very few compounds have been identified to be topological insulators to this date. However, none of them is proven to be suitable for the majority of experimental configurations including giant magnetoelectric and anomalous optical rotation, unusual exciton condensation, or the neutral half-fermions and interface superconductivity. In fact the realization of even any one of these proposals requires a number of multiply-connected topological compounds with modulated surface band dispersions and naturally tuned in-gap Fermi level, as well as spin variations in the presence of long life-time of the surface states. Here, using conventional and spin-sensitive probes, we report the discovery of several classes of positive band-gap high figure of merit topological insulators with critically important functional properties such as high degree of bulk resistivity and insulation, electronic structure with both in-gap Dirac point and Fermi level crossing, long surface state life-times, as well as chirality inversion through the Dirac node. The unprecedented combinations of electronic, spin, life-time and resistive bulk transport featured by the topological insulators uncovered here not only provide a new platform for research on topological quantum phenomena but also pave the way for functional devices.

9:24AM V35.00008 Observation of novel interference patterns in BixFe1-xTe3 by Fourier transform scanning tunneling spectroscopy (FT-STS) , YOSHINORI OKADA, Boston College, CHETAN DHITAL, WEN-WEN ZHOU, HSIN LIN, SUSMITA BASAK, ARUN BANSIL, YAOBO HUANG, HONG DING, ZIQIANG WANG, STEPHEN WILSON, VIDYA MADHAVAN — We utilize Fourier transform scanning tunneling spectroscopy (FT-STS) to probe the surface of the magnetically doped TI, Bi2-xFexTe3. Our measurements show the appearance of a hitherto unobserved channel of electronic backscattering along the surface q-vector. By referencing the FT-STS with angle-resolved photoemission spectroscopy (ARPES) data, we formulate a simple model showing that these new vectors are fully consistent with spin-flip scattering. Our combined data therefore present compelling evidence for the first momentum resolved measurement of enhanced backscattering due to magnetic impurities in a prototypical TI.

9:36AM V35.00009 Local interaction of magnetic impurities and topological surface states[1] , WARREN MAR, KENJIRO K. GOMES, WONHEE KO, HARI C. MANOHARAN, Stanford University — Topological insulators have garnered much attention as a vehicle to explore exotic Dirac physics through the projection of unpaired Dirac cones into conducting surface states wrapping a spin-orbit twisted bulk band structure. We use an ultrahigh-vacuum low-temperature scanning tunneling microscope (STM) to gain access to and manipulate the chiral Dirac particles present on the Sb(111) surface. Understanding the interplay between local spins and Dirac fermions represents a key foundation to the development of new spintronic applications. Magnetic moments break time-reversal symmetry and provide an additional local quantum degree of freedom to engineer topological states. By dosing magnetic impurities of varying concentration and species, we show how STM can atomically manipulate individual magnetic adatoms on topological surfaces, and in the process gain insight into the physical bonding arrangement of magnetic impurities on top of and embedded inside the host crystal lattice. Using scanning tunneling spectroscopy, we map in real and momentum space how local spins interact with the chiral surface Dirac carriers.

[1]Supported by the Department of Energy, Office of Basic Energy Sci- ences, Division of Materials Sciences and Engineering under contract DE-AC02-76SF00515

9:48AM V35.00010 Visualizing spin-vortex evolution of a topological insulator[1] , YIHUA WANG, DAVID HSIEH, DAN PILON, MIT, LIANG FU, Harvard, DILLON GARDNER, YOUNG LEE, NUH GEDIK, MIT — Charge carriers on the surface of a topological insulator are predicted to form a spin-vortex in momentum space with the direction of spin rotation determined by whether the carriers are electron-like or hole-like. We show that the angular momentum of photon is extremely sensitive to the spin of carriers by performing time-of-flight based angle-resolved-photoelectron spectroscopy (TOF-ARPES) with photons of different helicity. We demonstrate the first reciprocal space volumetric mapping of the vectorial spin-texture of the surface states of Bi_2Se_3 and directly observe spin-vortex evolution from electron-like to hole-like states and the departure from perpendicular momentum-spin locking.

[1]This work is supported by DOE award number DE-FG02-08ER46521, ARO-DURIP award number W911NF-09-1-0170 and MIT Center for Materials Science and Engineering

10:00AM V35.00011 Spin and angular reoslved photoemission studies of Bi2Se3[1] , ZHIHUI PAN, E. VESCOVO, G.D. GU, Brookhaven National Laboratory, D. GARDNER, S. CHU, Y. LEE, Massachusetts Institute of Technology, A.V. FEDOROV, Lawrence Berkeley National Laboratory, T. VALLA, Brookhaven National Labroatory — Topological insulators (TL) have attracted much attention because of their exotic properties. Bi_2Se_3 is a model TL with a relative large bulk gap and a simple surface state structure. By depositing various non-magnetic and magnetic impurities on the surface, we were able to fill the topological surface state and higher lying Rashba splitting surface states. The spin texture of the surface electronic structure was determined in spin resolved photoemission measurement.

[1]This work was supported by DOE

10:12AM V35.00012 Surface states never die by surface impurities in topological insulators[1] , HAN-JIN NOH, Department of Physics Chonnam National University, JINWON JEONG, EN-JIN CHO, Dep. of Phys. Chonnam National University, HAN-KOO LEE, HYEONG-DO KIM, Pohang Accelerator Laboratory Pohang University of Science and Technology — The metallic surface states in topological insulators are one of the most distinguished features among the characters of this newly discovered quantum state of matter. These states, if properly exploited, may open a new era in spintronics and quantum computing. However, full characterization and understanding of the surface states toward these goals are still far from satisfactory. Here, we focus on the robustness of the metallic surface states in a topological insulator $Bi_{0.9}Sb_{0.1}$, and demonstrate their durability over magnetic/non-magnetic surface impurities by measuring the scattering rates of the quasiparticles via angle-resolved photoemission spectroscopy.

[1]This work was supported by the National Research Foundation (NRF) of Korea Grant funded by the Korean Government (MEST) (Nos. 2008-0059108, 2010-0010771, and 2010-0028064)

10:24AM V35.00013 Experimental Realization of Three-dimensional Topological Insulator in Ternary Chalcogenides , K. KURODA, M. YE, A. KIMURA, Hiroshima Univ., Y. UEDA, Kure Nat. Coll. Tec., S.V. EREMEEV, Tomsk State Univ., E.E. KRASOVSKII, E.V. CHULKOV, DIPC, K. MIYAMOTO, T. OKUDA, K. SHIMADA, H. NAMATAME, M. TANIGUCHI, Hiroshima Univ. — Three-dimensional topological insulators (TIs) featured with spin-helical massless surface state have attracted a great attention. Up to now, the experimentally confirmed topological insulators are limited to some binary compounds, such as Bi_2Te_3, Bi_2Se_3 and so on. Recently, several ternary chalcogenides have been proposed as a new family of TI. In contrast to the layered binary chalcogenides, in ternary chalcogenides with a more substantial three dimensional character, the surface state depends on the topmost layer because the broken bonds at the surface may give rise also to trivial surface state. Therefore, the experimental realization of non-trivial surface state in TI has been strongly required. In this work, we have performed an angle resolved photoemission spectroscopy by using synchrotron radiation to prove the surface state in the ternary compounds. Especially, for one of the candidate materials, $TlBiSe_2$, two important aspects have been revealed: (i) The Dirac cone is more ideal than that of Bi_2Se_3. (ii) There are no bulk continuum states that energetically overlap with the Dirac point. This means that the scattering channel from the topological surface state to the bulk continuum is strongly suppressed in $TlBiSe_2$.

10:36AM V35.00014 STM/STS studies of the surface of Bi2Se3[1] , MEGAN ROMANOWICH, STUART TESSMER, Michigan State University, SERGEI URAZHDIN, West Virginia University, DUCK-YOUNG CHUNG, JUNG-HWAN SONG, MERCOURI KANATZIDIS, Northwestern University — Building upon previous work,[2] we apply scanning tunneling microscopy/spectroscopy to characterize the surface of the topological insulator Bi2Se3. We see clover-like defect states in the topographic scans and a residual image that appears in conductance scans, which we attribute to Bi substitutions in Se lattice sites. Spectroscopy reveals features in the density of states consistent with the topological surface state, with the defect states appearing as an additional enhancement. We will discuss the interaction of the topological surface state with the defect states.

[1]Supported by NSF DMR-0906939.

[2]Urazhdin S. et al. Physical Review B 69, 085313 (2004); Physical Review B 66, 161306(R) (2002).

10:48AM V35.00015 Scattering on Magnetic and Non-Magnetic Impurities on a Surface of a Topological Insulator[1] , T. VALLA, Z.-H. PAN, Brookhaven National Laboratory, D.R. GARDNER, S. CHU, Y.S. LEE, Massachusetts Institute of Technology — Dirac-like surface states on surfaces of topological insulators have a chiral spin structure that supresses back-scattering and protects the coherence of these states in the presence of potential scatterers. In contrast, magnetic scatterers are expected to open the back- scattering channel via the spin-flip processes and to degrade the state's coherence. We present angle-resolved photoemission spectroscopy studies of the electronic structure and the scattering rates upon adsorption of various magnetic and non-magnetic impurities on the surface of Bi_2Se_3, a model topological insulator. We uncovered an unusual insensitivity of the topological surface state to both non-magnetic and magnetic impurities. The electrons donated by the impurities fill the topological surface state and pairs of higher lying spin-orbit split surface bands, preserving the non-trivial spin texture of the surface.

[1]This work was supported by DOE.

Thursday, March 24, 2011 8:00AM - 10:12AM –
Session V36 DCMP: Graphene: Optical Properties I C142

8:00AM V36.00001 Imaging stacking order in few-layer graphene , CHUN HUNG LUI, ZHIQIANG LI, ZHEYUAN CHEN, PAUL V. KLIMOV, LOUIS E. BRUS, TONY F. HEINZ, Columbia University — Few-layer graphene (FLG) has been predicted to exist in various crystallographic stacking sequences, which can strongly influence the material's electronic properties We demonstrate an accurate and efficient method of characterizing stacking order in FLG using the distinctive features of the Raman 2D-mode. Raman mapping allows us to visualize directly the spatial distribution of Bernal (ABA) and rhombohedral (ABC) stacking in tri- and tetra-layer graphene. We find that ∼15% of exfoliated graphene tri- and tetra-layers is comprised of micron-sized domains with rhombohedral stacking, rather than the Bernal stacking. These domains are stable and remain unchanged for annealing to temperatures exceeding 800 °C.

8:12AM V36.00002 Electric-field induced changes in the band structure of trilayer graphene: The effect of crystallographic stacking order , ZHIQIANG LI, CHUN HUNG LUI, KIN FAI MAK, Columbia University, EMMANUELE CAPPELLUTI, Institute for Complex Systems, TONY F. HEINZ, Columbia University — We have studied by means of infrared spectroscopy the influence of a strong perpendicular electric-field on the band structure of graphene trilayers with two different types of crystallographic stacking: ABA (Bernal) and ABC (rhombohedral) stacking. The symmetries of the two crystallographic structures are different, the former having mirror symmetry and the latter inversion symmetry. Distinct infrared response was observed when breaking their respective symmetries by the application of the electric field. We observed an electrically tunable band gap of over 100 meV in ABC trilayers, while no band gap was found for ABA trilayers. Our results will be compared to the induction of a band gap in AB bilayer graphene [K. F. Mak *et al*, PRL **102**, 256405 (2009); Y. Zhang *et al*, Nature **459**, 820 (2009)]

8:24AM V36.00003 Photoluminescence in highly doped graphene , BAISONG GENG, CHI-FAN CHEN, LIANG ZHENG TAN, Department of Physics, University of California at Berkeley, Berkeley, CA 94720, USA, BRYAN W. BOUDOURIS, Department of Chemistry, University of California at Berkeley, Berkeley, CA 94720, USA, JASON HORNG, CAGLAR GIRIT, ALEX ZETTL, MICHAEL F. CROMMIE, Department of Physics, University of California at Berkeley, Berkeley, CA 94720, USA, RACHEL SEGALMAN, Department of Chemistry, University of California at Berkeley, Berkeley, CA 94720, USA, STEVE G. LOUIE, FENG WANG, Department of Physics, University of California at Berkeley, Berkeley, CA 94720, USA — Pristine graphene is a zero-bandgap semiconductor. Usually no photoluminescence can be observed from such zero-bandgap material upon laser excitation. In highly doped graphene, however, we observed a strong broadband photoluminescence. We will discuss the mechanism of this photoluminescence in graphene, which arises from new recombination pathways enabled by strong electrical doping. We will also describe the polarization dependence of this newly observed photoluminescence.

8:36AM V36.00004 Response of graphene to intense optical irradiation , ADAM ROBERTS, College of Optical Science, University of Arizona, COLLIN REYNOLDS, DANIEL HEMMER, BRIAN LEROY, ARVINDER SANDHU, Department of Physics, University of Arizona — We investigate the modification of graphene under intense ultrashort laser irradiation. Our observations indicate that the graphene structure is very resilient and exhibits a high damage threshold, which is promising for high order non-linear applications. In the case of epitaxially grown samples, we find that single-shot damage threshold is $5x10^{10}Wcm^{-2}$ for 50 fs pulse duration. Raman and optical microscopy measurements of irradiated samples show that the carbon lattice completely disappears from the region where the laser intensity exceeds the threshold without leaving any visual or spectroscopic signature. Below the threshold, single-shot irradiation does not exhibit a significant defect formation. However, repeated laser irradiation below the threshold leads to formation of defects. The mechanisms underlying the defect formation and lattice reduction will be discussed.

8:48AM V36.00005 Mid Infrared Near Field Study of Monolayer Graphene , Z. FEI, G.O. ANDREEV, University of California - San Diego, W. BAO, University of California - Riverside, L.M. ZHANG, Boston University, Z. ZHAO, University of California - Riverside, G. DOMINGUEZ, M. THIEMENS, M.M. FOGLER, University of California - San Diego, C.N. LAU, University of California - Riverside, F. KEILMANN, Max-Planck-Institute of Quantum Optics, D.N. BASOV, University of California - San Diego — We have performed near-field spectroscopic studies of both monolayer suspended graphene (SG) and graphene on SiO_2/Si substrate (GOS) using scattering-type scanning near-field optical microscope (s-SNOM). Our data show that SG produces reliable near-field signal in mid-infrared frequencies. Images taken with high spatial resolution ($\sim$20nm) show nanoscopic features such as ripples and electronic inhomogeneities. The SiO_2/Si substrate contributes a phonon resonance in the near-field signal around 1130 cm^{-1}. This resonance is remarkably strengthened and broadened by just a single layer of graphene in the case of GOS. By probing the resonance spectrum we find over 400% contrast in near field signal between GOS and the bare substrate. The detailed analysis of the contrast suggests that GOS is slightly doped. This study therefore provides much needed insight into the thickness resolution of the s-SNOM technique, proving it can be sensitive to just a single layer of atoms, and advances the fundamental understanding of graphene-light interactions by probing in the near-field regime.

9:00AM V36.00006 Terahertz and Infrared Conductivity of Large-Area Graphene , LEI REN, QI ZHANG, TAKASHI ARIKAWA, LAYLA G. BOOSHEHRI, JUNICHIRO KONO, Department of Electrical and Computer Engineering, Rice University, ZHONG JIN, ZHENGZONG SUN, ZHENG YAN, JAMES M. TOUR, Department of Chemistry, Rice University — Graphene is predicted to offer new opportunities for terahertz (THz) science and technology. Its zero-gap linear band dispersion is expected to lead to exotic nonlinear electromagnetic properties, which can be probed through frequency-dependent conductivity measurements. Here, we use THz time-domain spectroscopy and Fourier-transform infrared spectroscopy to investigate carrier dynamics in large-area graphene grown by chemical vapor deposition. We studied both nitrogen-doped and nominally-undoped graphene; the latter had accidental doping presumably through air and acid exposure. Absorption increased with the number of graphene layers and was larger in the nominally-undoped samples especially in the 0.2-2.2 THz range. For the highest-mobility samples, we observed Drude-like frequency dependence in the THz range. Further measurements in a wider spectral range are in progress to understand the differences between these samples and the interplay between intra-band and inter-band dynamics.

9:12AM V36.00007 Carrier Cooling in Graphene Measured by THz Time-Domain Spectroscopy , JARED STRAIT, HAINING WANG, SHRIRAM SHIVARAMAN, VIRGIL SHIELDS, CARLOS RUIZ-VARGAS, JIWOONG PARK, MICHAEL SPENCER, FARHAN RANA, Cornell University — We present results on the ultrafast relaxation dynamics of photoexcited electrons and holes in graphene using optical-pump terahertz-probe spectroscopy. Measurements done at different temperatures show that the measured differential transmission as a function of the probe delay decays on time scales that become very long at low temperatures with decay times exceeding $\sim$150 ps at temperatures lower than $\sim$50K. We interpret these transients as carrier cooling due to a combination of electron-optical phonon and electron-acoustic phonon scattering. When the carrier temperature goes below $\sim$250 K, optical-phonon scattering ceases to effectively cool the carriers given the large optical phonon energies in graphene. Since acoustic phonon scattering is not efficient in removing the heat from the carriers, the carrier distribution cools very slowly. Our data is in agreement with the theoretical predictions [1].

[1] Phys. Rev. B 79, 235406 (2009) and Phys. Rev. Lett., 102, 206410 (2009).

9:24AM V36.00008 Ultrafast electron dynamics in freely suspended graphene , LEANDRO MALARD, KIN FAI MAK, TONY F. HEINZ, Columbia University — The optical conductivity of free-standing graphene under the non-equilibrium conditions was investigated by femtosecond pump-probe spectroscopy. The conductivity transient exhibited a strong dependence on pump fluence, with a crossover from enhanced to reduced absorbance occurring with increasing pump fluence. The observed phenomena can be understood by taking into account both the induced intra- and inter-band optical response. Intra-band transitions dominate the transient at low pump fluence (and electronic temperature) and inter-band transitions dominate at high pump fluence (and electronic temperature). Analysis within a model incorporating these two responses allows us to infer the variation of carrier scattering rate with electronic temperature. The temporal evolution of the conductivity transient is controlled by the anharmonic decay of the optical phonons; a lifetime of $\sim$1.4 ps was inferred for intrinsic, suspended graphene.

9:36AM V36.00009 Ultrafast dynamics of highly-excited Dirac fermions in monolayer graphene[1] , JUNHUA ZHANG, JÖRG SCHMALIAN, TIANQI LI, JIGANG WANG, Ames Laboratory and Department of Physics and Astronomy, Iowa State University — One of the striking optical properties of single-layer graphene is the universal absorbance in the near-infrared-to-visible spectral range due to the Dirac spectrum of the low-energy electronic structure. High-fluence laser pump can produce superdense Dirac-fermionic excitations at the order of 10 femtoseconds so to reach the non-linear saturation of absorption. We construct a simple model for the transient state of the photo-excited graphene to explore the non-linear saturation of photoexcitations and the transport property of carries. The comparison of our model calculations with the experimental results shows good agreements.

[1]Research supported by the U. S. DOE, office of BES, Materials Science and Engineering Division.

9:48AM V36.00010 Ultrafast relativistic response of Photo-excited Carriers in Graphene[1] , J. LEE, K.M. DANI, CINT, Los Alamos National Laboratory, R. SHARMA, Theoretical Division, Los Alamos National Laboratory, A.D. MOHITE, A.M. DATTELBAUM, H. HTOON, A.J. TAYLOR, R.P. PRASANKUMAR, CINT, Los Alamos National Laboratory, C.M. GALANDE, P.M. AJAYAN, Dept. of Mechanical Engineering and Materials Science, Rice University — Understanding the ultrafast non-equilibrium dynamics of photocarriers in graphene's unique relativistic band structure is important for the development of such high-speed, graphene-based photonic devices and also from a fundamental point of view. Here, we directly demonstrate the relativistic nature of a non-equilibrium gas of electrons and holes photogenerated in a graphene monolayer as early as 100 femtoseconds (fs) after photoexcitation. We photoexcited carriers in graphene and then measured the time-resolved, pump-induced change in reflection at various visible probe photon energies. We observe a nonlinear scaling in the Drude-like optical conductivity of the photocarriers with respect to their density, in striking contrast to the linear scaling expected from conventional materials with parabolic dispersion relations.

[1]Supported by University of California President's (UCOP) program on Carbon Nanostructures.

10:00AM V36.00011 Carrier Dynamics in Colloidal Graphene Quantum Dots , CHENG SUN, Michigan State University, XIN YAN, LIANG-SHI LI, Indiana University, JOHN A. MCGUIRE, Michigan State University — We describe carrier dynamics for single and multiple excitons in colloidal graphene quantum dots (GQDs). Strong confinement and corresponding size-tunable electronic structure make GQDs potentially useful sensitizers in photovoltaic devices. We have studied the optical response of GQDs consisting of 132 and 168 sp^2 hybridized carbon atoms dissolved in toluene with HOMO-LUMO transitions of 1.4-1.6 eV. From measurements of ultrafast ($\sim$100 fs) transient absorption over nanosecond timescales, we extract the single-photon absorption cross-section and observe carrier-induced Stark shifts of the order of 0.1 eV indicating strong carrier-carrier interactions, as expected for the relatively weak screening of a two-dimensional nanostructure. Multiexcitons are observed to decay nonradiatively on $\sim$1 to 20 ps timescales, while single excitons display dynamics on multiple timescales due to carrier cooling, singlet-to-triplet intersystem crossing, and, on nanosecond to microsecond timescales, radiative recombination.

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V37 DMP: Focus Session: Graphene Growth, Characterization, and Devices: Transport

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8:00AM V37.00001 Electronic Transport Properties of Graphene on Aluminum Nitride[1] , LIANG LI, JUN YAN, Center for Nanophysics and Advanced Materials, University of Maryland, College Park, MD 20742-4111, USA, R.D. VISPUTE, Blue Wave Semiconductors, Inc., MICHAEL FUHRER, Center for Nanophysics and Advanced Materials, University of Maryland, College Park, MD 20742-4111, USA — We have fabricated graphene field-effect transistors on aluminum nitride (AlN) gate dielectric over silicon back gates. AlN thin films are prepared on Si by pulsed laser deposition, and exfoliated graphene on SiO2 is transferred onto the AlN/Si surface by using thermal tape as a transfer medium. After transfer, Raman spectra and AFM measurement have been performed to confirm the quality of graphene on AlN. Electron transport measurements will be reported.

[1]This work is supported by the Laboratory for Physical Sciences

8:12AM V37.00002 Exploring Transport Effects in Nanoscale Graphene Devices , JEFF WORNE, CHARUDATTA GALANDE, HEMTEJ GULLAPALLI, PULICKEL AJAYAN, DOUGLAS NATELSON, Rice University — Graphene, the single- to few-atomic layers cousin to graphite, has become a very interesting topic of research owing to its unique mechanical, optical, thermal and electrical properties. Many of the properties of graphene can be traced to its structural uniformity, allowing both electrons and holes to travel long distances (up to several microns) before scattering. However, studying graphene on the micron level can mask its true nanoscale behavior. Using very short length scales allows for the investigation of the behavior of charge impurities, contact effects and ballistic transport. In this work, we fabricate sub-30 nanometer suspended graphene 3-terminal devices on gold and platinum electrodes. We present data from electrical measurements on charge impurities that are apparent at this length scale and the effect of electrode work function on contact resistance. We compare this to mechanically exfoliated graphene on a silicon/SiO2 substrate with gold electrodes.

8:24AM V37.00003 Electrical transport study of suspended graphene nanoribbons near the Dirac point[1] , MING-WEI LIN, CHENG LING, YIYANG ZHANG, HYEUN JOONG YOON, MARK MING-CHENG CHENG, ZHIXIAN ZHOU, Wayne State University — We have fabricated graphene nanoribbon Field-effect transistors from high-quality graphene nanoribbons produced by sonicating multiwall carbon nanotubes in an organic solvent. To minimize the influence of the underlying substrate, individual nanoribbons in the devices were suspended by removing the underneath silicon oxide using a wet etching method. Subsequently, in situ current annealing was carried out in high vacuum to further reduce the impurities adsorbed to the ribbon surfaces. The electrical transport properties of the devices were measured for a wide range of temperatures, revealing a range of unusual phenomena pertinent to the competing effects of improved overall charge homogeneity and reduced charge puddle sizes when the graphene nanoribbons are tuned close to the Dirac point. The electrical transport results on suspended graphene nanoribbon with varying disorder will be presented and discussed.

[1]ZZ acknowledges the support of the WSU new faculty startup funds.

8:36AM V37.00004 Effects of disorder on the transport properties of chemically derived graphene , GOKI EDA, JAMES BALL, YE XIAO, ROBERT MAHER, LESLEY COHEN, THOMAS ANTHOPOULOS, MANISH CHHOWALLA, Imperial College London — Transport properties of chemically derived graphene (CDG) are strongly influenced by the concentration of defects that are introduced during synthesis. We present a comprehensive transport study on a range of CDG films with varying degrees of disorder. The electric properties of CDG were found to be tunable over several orders of magnitude via controlled oxidation and reduction. The structural properties of CDG were monitored by analyzing the defect-related features in the Raman spectra and correlated with transport. The temperature dependence of the resistivity of these samples indicate that the conduction mechanism evolves from tunneling to hopping for strongly disordered samples and to activated transport for weakly disordered samples. Strong disorder causes localization of carriers and field-dependent modulation of hopping conduction. We discuss the temperature- and gate-bias-dependence of the resistivity of weakly disordered samples in terms of scattering dominated by midgap states, as is the case in ion irradiated graphene [2].

[1] G. Eda et al., J. Phys. Chem. C, 113, 15768 (2009).
[2] J.-H. Chen et al. Phys. Rev. Lett. 102, 236805 (2009)

8:48AM V37.00005 Influence of Strain on Quantum Transport in Graphene , MD HOSSAIN, UIUC — Strain is unavoidable in graphene, either suspended or supported on a dielectric substrate such as SiO2. It is therefore crucial to identify the role of strain on transport properties in graphene. Experimentally, it is shown that local strain in graphene on a SiO2 substrate can modify graphene's conductance near the Fermi energy. The modification is attributed to the coupling of strain and phonon-mediated inelastic tunneling effects. However, conductance on the dielectric substrate is not ballistic and isolating the influence of strain is a difficult task. In this study, strain effects on ballistic conductance, an experimentally attainable transport property for suspended graphene, is studied using a combination of density functional theory and the Landauer-Buttiker formalism. It is found that, unlike in a CNT, regardless of the applied strain graphene's conductance at the Fermi energy is 0.21G0. Furthermore, for conducting electrons with energies higher or lower than the Fermi energy of the system, tensile hydrostatic strain is found to increase conductance but compressive hydrostatic strain decreases conductance. For an 8% compressive hydrostatic strain, conductance increases by as large as 30%. Surprisingly, for uni-axial strain, if the energy of the conducting electrons is higher than the Fermi energy, conductance remains approximately unchanged, whereas conductance by electrons less than the Fermi energy decreases (increases) with compressive (tensile) strain along the transport direction.

9:00AM V37.00006 ABSTRACT WITHDRAWN –

9:12AM V37.00007 Thermal and Electronic Transport Properties of Graphene Nanoribbons with Defects , JUSTIN HASKINS, Department of Chemical Engineering, Texas A&M University, ALPER KINACI, Department of Material Science, Texas A&M University, CEM SEVIK, TAHIR CAGIN, Department of Chemical Engineering, Texas A&M University — The interplay between graphene nanoribbon (GNR) structure and conductivity, both thermal and electrical, is probed with molecular dynamics and tight binding models. A variety of randomly oriented defects, vacancies and Stone-Wales, as well as edge terminations, zig-zag, armchair, and roughened, are studied in experimental sized systems (>100 nm long and >15 nm wide). It is found that GNR thermal conductivity responds similarly to edge roughness and moderate defect concentrations (0.0023) with a drastic reduction (81%) in lattice thermal conductivity, compared to pristine GNR value. Conversely, the presence of randomly oriented defects completely erodes the ballistic nature of the electrons, reducing conductance by two orders of magnitude, while edge roughened structures leave the electrical conductance intact.

9:24AM V37.00008 First principles study of transport properties of pristine and passivated bilayer graphene nanoribbons , XIAOLIANG ZHONG, RAVINDRA PANDEY, Michigan Technological University, SHASHI KARNA, Army research Laboratory — Transport properties of pristine and hydrogen passivated bilayers of zigzag-edged graphene nanoribbons (ZGNRs) coupled with gold electrodes are investigated using first-principles methods based on density-functional theory. The calculated ground state of the passivated bilayer 6-ZGNRs is non-magnetic and the antiferromagnetic coupling is energetically preferred for the pristine counterpart. The results of the bias and spin-dependent electron transmission and current calculated using the nonequilibrium Green's function formalism will be presented. The role of interlayer interaction in determining the I-V characteristics of bilayer graphene nanoribbons will also be discussed.

9:36AM V37.00009 1/f noise as a probe to investigate the band structure of graphene , ATINDRA NATH PAL, ARINDAM GHOSH, Department of Physics, Indian Institute of Science, Bangalore 560012, India — The flicker noise or low frequency resistance fluctuations in graphene depend explicitly on its ability to screen external potential fluctuations and more sensitive compared to the conventional time average transport. Here we show that the flicker noise is a powerful probe to the band structure of graphene that vary differently with the carrier density for the linear and parabolic bands. We have used different types of graphene field effect devices in our experiments which include exfoliated single and multilayer graphene on oxide substrate, freely suspended single layer graphene, and chemical vapor deposition (CVD)-grown graphene on SiO_2.We find this difference to be robust against disorder or existence of a substrate. Also, an analytical model has been developed to understand the mechanism of graphene field effect transistors. Our results reveal the microscopic mechanism of noise in Graphene Field Effect Transistors (GraFET), and outline a simple portable method to separate the single from multi layered graphene devices. References A. N. Pal and A Ghosh, Phys Rev. Lett 102, 126805 (2009). A. N. Pal and A. Ghosh, Appl. Phys. Lett., 95, 082105 (2009). A. N. Pal, A. A. Bol, and A. Ghosh, Appl. Phys. Lett. 97, 133504 (2010). A. N. Pal et al., arXiv: 1009.5832v2.

9:48AM V37.00010 Charge Trapping and Transport in Epitaxial Graphene , DAMON FARMER, IBM T.J. Watson Research Center — A thorough characterization of the electronic transport behavior of charge carriers in graphene that is epitaxially grown on the silicon face of 6H(0001) SiC is presented. A nonlinear temperature dependence of the carrier density is observed, and is attributed to the presence of charge traps in the material. Observation of this trapping effect has been previously unidentified, and gives critical information about the material properties of epitaxially grown graphene. The nature of the electrostatic screening associated with these traps is evaluated using zero screening, full screening, and RPA screening approximations, and it is found that the zero screening approximation best describes the measurements. Electrostatic homogeneity of this material allows for exceptionally low carrier densities to be attained, where the carrier mobility sharply increases. The entire mobility profile can be phenomenologically simulated assuming Coulomb and short-range scattering as the dominant scattering mechanisms at low temperatures. Based on this result, the temperature independent residual impurity concentration of this material can be directly extrapolated.

10:24AM V37.00011 ABSTRACT WITHDRAWN –

10:36AM V37.00012 Transport Through Andreev Bound States in a Graphene Quantum Dot , TRAVIS DIRKS, TAYLOR L. HUGHES, SIDDHARTHA LAL, BRUNO UCHOA, YUNG-FU CHEN, CESAR CHIALVO, PAUL M. GOLDBART, NADYA MASON, University of Illinois at Urbana-Champaign — We have performed transport measurements on a graphene-insulator-superconductor junction, and report the direct observation of sharp, gate-tunable Andreev bound states (ABS) in a graphene quantum dot (QD)[1]. The quantum dot is formed underneath the superconducting lead by local gating due to a work-function mismatch. We show that the ABS form when the discrete QD levels are proximity coupled to the superconducting contact. We find subgap resonant features which are remarkably narrow, can be tuned to zero energy by gating, and show a striking pattern as a function of applied bias and gate voltage.

[1] T. Dirks et al.,arXiv:1005.2749 (2010)

10:48AM V37.00013 Transport Properties of Graphene on Strontium Titanate[1] , RYUICHI TSUCHIKAWA, MASA ISHIGAMI, Department of Physics and Nanotechnology Center, University of Central Florida — We have investigated transport properties of mechanically exfoliated graphene on strontium titanate(STO) in ultra high vacuum at cryogenic temperatures. Field- and temperature-dependent dielectric constant of STO is used to measure the impact of substrate-induced screening on transport properties of graphene.

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

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V38 DCP DBP: Focus Session: The Physics of Evolution II A130/131

8:00AM V38.00001 Natural Selection in Large Populations , MICHAEL DESAI, Harvard University — I will discuss theoretical and experimental approaches to the evolutionary dynamics and population genetics of natural selection in large populations. In these populations, many mutations are often present simultaneously, and because recombination is limited, selection cannot act on them all independently. Rather, it can only affect whole combinations of mutations linked together on the same chromosome. Methods common in theoretical population genetics have been of limited utility in analyzing this coupling between the fates of different mutations. In the past few years it has become increasingly clear that this is a crucial gap in our understanding, as sequence data has begun to show that selection appears to act pervasively on many linked sites in a wide range of populations, including viruses, microbes, *Drosophila*, and humans. I will describe approaches that combine analytical tools drawn from statistical physics and dynamical systems with traditional methods in theoretical population genetics to address this problem, and describe how experiments in budding yeast can help us directly observe these evolutionary dynamics.

8:36AM V38.00002 Understanding Biological Fitness From First Principles , EUGENE SHAKHNOVICH, Harvard University — This abstract not available.

9:12AM V38.00003 Geometry Genetics and Evolution[1] , ERIC SIGGIA, Rockefeller University — Darwin argued that highly perfected organs such as the vertebrate eye could evolve by a series of small changes, each of which conferred a selective advantage. In the context of gene networks, this idea can be recast into a predictive algorithm, namely find networks that can be built by incremental adaptation (gradient search) to perform some task. It embodies a "kinetic" view of evolution where a solution that is quick to evolve is preferred over a global optimum. Examples of biochemical kinetic networks were evolved for temporal adaptation, temperature compensated entrainable clocks, explore-exploit trade off in signal discrimination, will be presented as well as networks that model the spatially periodic somites (vertebrae) and HOX gene expression in the vertebrate embryo. These models appear complex by the criterion of 19th century applied mathematics since there is no separation of time or spatial scales, yet they are all derivable by gradient optimization of simple functions (several in the Pareto evolution) often based on the Shannon entropy of the time or spatial response. Joint work with P. Francois, Physics Dept. McGill University.

[1]With P. Francois, Physics Dept. McGill University

9:48AM V38.00004 TBD , TANJA KORTEMME, UCSF — This abstract not available.

10:24AM V38.00005 Dynamical Mueller's Ratchet: Population Size Dependence of Evolutionary Paths in Bacteria , DIRK LORENZ, Department of Physics and Astronomy, Rice University, JEONG-MAN PARK, Department of Physics, The Catholic University of Korea, MICHAEL DEEM, Departments of Physics and Astronomy and Bioengineering, Rice University, MICHAEL DEEM TEAM — Experimental evolution has recently enabled the complete quantitative description of small-dimensional fitness landscapes. Quasispecies theory allows the mathematical modeling of evolution on such a landscape. Typically, analytic solutions for these models are only exactly solvable for the case of an infinite population. Here we use a functional integral representation of population dynamics and solve it using the Schwinger Boson method. This allows us to compute the first-order correction to the average fitness for finite populations. We will use these results to explain the experimental observations of dynamics of evolution in finite populations.

10:36AM V38.00006 At the crossroads of biophysics and evolution: protein robustness and evolvability[1] , WOUTER HOFF, MASATO KUMAUCHI, Department of Microbiology and Molecular Genetics, Oklahoma State University — Proteins consist of only 20 different amino acids with modest chemical reactivity, but perform a breathtaking range of functions. How do proteins achieve such functional versatility? Novel insights are emerging from research at the interface of protein biophysics and molecular evolution. Proteins are robustness against point mutations: most mutations do not abolish function. How can such robustness be reconciled with the effective evolution of protein function? We examine these issues using photoactive yellow protein (PYP), a prototype of the PAS domain superfamily. High-throughput biophysical measurements of active site properties, functional kinetics, stability, and production level on libraries of PYP mutants reveal that almost all mutants retain photocycle activity, but that the majority of substitutions significantly alter functional properties. Thus, PYP combines robustness with evolvability. The data also reveal the mysterious role of the conserved residues that define protein superfamilies: most PAS-conserved residues are required for maintaining protein production. Asn43, the most conserved residue in PAS domains, regulates PYP signaling kinetics. This residue is often substituted by Ser, Asp, and Thr in PAS domains while retaining two side chain hydrogen bonds. Thus, not residue identity at position 43 but the pattern of side chain hydrogen bonds is conserved.

[1]WDH was supported by NIH GM063805 and OCAST HR07-135S.

10:48AM V38.00007 Deciphering evolutionary instructions for specifying protein fold and function , WALRAJ GOSAL, RAMA RANGANATHAN, UT Southwestern Medical Center — Classical studies show that proteins have evolved to fold into functional native states that are, at best, only marginally stable through weak non-covalent interactions encoded by their primary sequences. How such fold and functional information is stored in a single amino acid sequence remains elusive. Using the statistical analysis of covariation between pairs of amino acids at all positions in a protein, here we identify groups of a few key physically-interconnected residues, which we term sectors. What information about the fold and function is captured by sectors? Using simulated-annealing Monte Carlo, we introduce variation in the sequence of a single member of the PDZ family in a manner that either preserves or disrupts sector correlations. Experimentally we show that function is specifically retained in designed proteins that obey sector correlations, and strikingly, even in the absence of a native state. Thus, we suggest that native-state stability is not a fundamental requirement for function, and is encoded in the sequence in an idiosyncratic manner in the PDZ family.

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V39 DBP: Cellular Biomechanics A124/127

8:00AM V39.00001 Three-dimensional traction force distribution in migrating amoeboid cells , BEGONA ALVAREZ, JUAN C. DEL ALAMO, RUDOLF MEILI, BALDOMERO ALONSO-LATORRE, RICHARD A. FIRTEL, JUAN C. LASHERAS — We have studied the 3D traction forces exerted by migrating *Dictyostelium* cells moving over flat elastic substrates. For that purpose, we have developed a method to calculate both vertical and tangential cell traction forces from measurements of 3D substrate deformation, based on the solution of the elastostatic equation for a linearly elastic medium. 3D substrate deformation is measured by applying correlation techniques to a volume of substrate containing fluorescent markers. We have performed experiments for wild-type (WT) and mutant cell lines with crosslinking defects to study how cytoskeletal organization affects the overall distribution of traction forces. We find that cells push the substrate downwards near their center and pull upwards at their periphery with forces of comparable magnitude. Our initial findings show that the effect of the crosslinking mutations on the tangential forces do not necessarily predict the effect on the vertical forces. For instance, myosin II-null cells show a significant reduction of the front-back organization of the tangential traction forces, while the distribution of vertical forces basically remains unaffected.

8:12AM V39.00002 The Physics Of Cell Crawling In Elastic Media , ELNAZ BAUM-SNOW, CHARLES WOLGEMUTH, University of Connecticut, Health Center — Understanding the motion of cells through deformable media, such as the extra-cellular matrix (ECM), is important for understanding many biological processes, such as cancer metastasis, wound healing, and organismal development. We propose a model to understand the cells' movements through ECM, described by an elastic medium. The deformations and the stress tensor are then calculated for different values of Young's modulus and Poisson's ratio. The results are then compared to the values measured experimentally.

8:24AM V39.00003 How Deep Cells Feel , AMNON BUXBOIM, EDWARD C. ECKELS, DENNIS E. DISCHER, University of Pennsylvania — Lacking eyes to see and ears to hear, cells can still sense their microenvironment by physically touching and deforming, thus sensing not only their immediate surroundings but also feeling beyond the cell-matrix interface. To elucidate how deeply cells feel we cultured mesenchymal stem cells on gels-made microfilms with controlled elasticity (E) and thickness (h). After 36hrs in culture cells spread area was smaller on thick and on soft than on thin and on stiff films, respectively, and correlated with nuclei morphology. Transition in spread area was obtained at <5 microns gel thickness. Transcription levels of Lamin-A predominantly decreased with E and in a similar fashion to Lamin-A expression levels increased with h. RNA levels of histones and of chromatin-remodeling enzymes were similar for stiff gels and for soft but thin films but suppression of cell contractility resulted in transcriptional profiles that were uncorrelated with matrix-emerging cues. We conclude that cells actively sense up to 20 microns into soft, adipose-like matrix. Cellular response to E and h includes cytoskeletal reorganization, NE remodeling with evidence of coupling between matrix-emerging signals and regulation of gene expression

8:36AM V39.00004 Delineating cell-matrix interaction at high resolution[1] , SHANG YOU TEE, JOHN CROCKER, PAUL JANMEY, University of Pennslyvania — It is increasingly evident that mechanic cues affect a wide variety of cells and can sometimes override biochemical cues to control cell division, cell death and even specify stem cell differentiation lineage. To understand how cells interact physically with their surrounding matrix, it is imperative to investigate the spatiotemporal distribution of forces and molecular players as cells undergo contractile activity. We examine human mesenchymal stem cell contractility at high temporal and spatial resolution on soft and hard substrates.

[1]We acknowledge NIH 5R01GM083272-03 funding.

8:48AM V39.00005 How substrate rigidity regulates the cellular motility , ALIREZA SARVESTANI, University of Maine — Mechanical stiffness of bio-adhesive substrates has been recognized as a major regulator of cell motility. We present a simple physical model to study the crawling locomotion of a contractile cell on a soft elastic substrate. The mechanism of rigidity sensing is accounted for using Schwarz's two spring model (Schwarz et al. (2006) BioSystems 83, 225-232). The predicted dependency between the speed of motility and substrate stiffness is qualitatively consistent with experimental observations. The model demonstrates that the rigidity dependent motility of cells is rooted in the regulation of actomyosin contractile forces by substrate deformation at each anchorage point. On stiffer substrates, the traction forces required for cell translocation acquire larger magnitude but show weaker asymmetry which leads to slower cell motility. On very soft substrates, the model predicts a biphasic relationship between the substrate rigidity and the speed of locomotion, over a narrow stiffness range, which has been observed experimentally for some cell types.

9:00AM V39.00006 Local nano-mechanical properties in cancer metastasis , LYNDON BASTATAS, Physics, Texas Tech University, RAUL MARTINEZ-ZAGUILAN, SOUAD SENNOUNE, Cell Physiology and Molecular Biophysics, Texas Tech University Health Sciences, SOYEUN PARK[1], Physics, Texas Tech University — We investigated whether the local nano-mechanical properties of cells can represent metastatic potential using the Atomic Force Microscope. As models, we used the lowly (LNCaP) and highly (CL1) metastatic prostate cancer cells. By varying the applied forces, we determined the heterogeneity in the local elastic properties of cells in the vertical direction. We also obtained the 2D array of the force-distance curves over the entire region of cells to investigate the lateral heterogeneity of local elastic moduli. By analyzing the force-distance curves using the Hertz and the advanced models, we delineated the 2D maps of elastic moduli and adhesiveness of cells. We found that the CL1 is more heterogeneous in the local elastic moduli compared to LNCaP. We also found that the CL1 adheres much better on the substrates than the LNCaP. The enhanced adhesion generates the tensional force and thus results in higher elastic moduli. We conclude that there is an optimal range of elastic moduli to make cells actively elicit the directional movements, leading to the enhance metastasis. We will discuss our results correlated with our intercellular calcium transit.

[1]Corresponding Author

9:12AM V39.00007 Cell Shape Dynamics: From Waves to Migration , MEGHAN DRISCOLL, University of Maryland, COLIN MCCANN, University of Maryland and National Cancer Institute, National Institutes of Health, RAEL KOPACE, TESS HOMAN, JOHN FOURKAS, University of Maryland, CAROLE PARENT, National Cancer Institute, National Institutes of Health, WOLFGANG LOSERT, University of Maryland — We analyzed the dynamic shape of migrating Dictyostelium discoideum cells. We found that regions of high boundary curvature propagate from the front to the back of cells in an organized fashion. These waves of high curvature are stabilized by surface contact, and so, at the sides of cells, are stationary relative to the surface. The initiation of curvature waves, though, which usually occurs at the front of cells, is associated with protrusive motion. The protrusion location shifts rapidly in a ballistic manner at speeds nearly double that of cellular migration. To examine curvature waves in the absence of surface contact, we guided cells to extend over the edge of micro-cliffs. The curvature wave speed of cells extended over a cliff was triple the wave speed of cells migrating on a surface, which is consistent with the higher wave speeds observed near the non-adherent leading edge of cells.

9:24AM V39.00008 Self-organized cell motility , XINXIN DU, KONSTANTIN DOUBROVINSKI, Princeton University — Cell migration plays a key role in a wide range of biological phenomena, such as morphogenesis, chemotaxis, and wound healing. Cell locomotion relies on the cytoskeleton, a meshwork of filamentous proteins, intrinsically out of thermodynamic equilibrium and cross-linked by molecular motors, proteins that turn chemical energy into mechanical work. In the course of locomotion, cells remain polarized, i.e. they retain a single direction of motion in the absence of external cues. Traditionally, polarization has been attributed to intracellular signaling. However, recent experiments show that polarization may be a consequence of self-organized cytoskeletal dynamics. Our aim is to elucidate the mechanisms by which persistent unidirectional locomotion may arise through simple mechanical interactions of the cytoskeletal proteins. To this end, we develop a simple physical description of cytoskeletal dynamics. We find that the proposed description accounts for a range of phenomena associated with cell motility, including spontaneous polarization, persistent unidirectional motion, and the co-existence of motile and non-motile states.

9:36AM V39.00009 Differentiation and Behavior of Dental Pulp Stem Cells in Hydrogel Scaffolds of Various Stiffnesses , DIVYA BHATNAGAR, VLADIMIR JURUKOVSKI, MIRIAM RAFAILOVICH, MARCIA SIMON, Stony Brook University — Dental Pulp Stem Cells (DPSCs) are known to differentiate in bone, dentine, or nerve tissue through different environment signals. This work investigates whether differentiation could occur in the absence of chemical induction and through mechanical stimuli only. For this study, we chose enzymatically cross-linked gelatin hydrogels as our substrates. Rheological studies carried out by oscillatory shear rheometry indicated that the modulus of the hardest hydrogel was of the order of 8kPa where as the medium and the softest hydrogel had modulus of the order of 1kPa and 100Pa respectively. DPSC were then plated on all three substrates and cultured with and without dexamethasone induction media. After 21 days of incubation, SEM analysis indicated that the cells cultured in the induction media produced biomineralized deposits on hard, medium as well as soft hydrogels. On the other hand, the cells cultured without the induction media also produced large amounts of biomineralized deposits.The modulus of the cells was also measured using AFM. En mass cell migration was also studied to determine the average velocity of migration of DPSCs. We also investigated whether stem cells that are induced to differentiate by their scaffold environment would continue to differentiate and biomineralize when removed from the inducing scaffold.

9:48AM V39.00010 Model of myosin recruitment to the cell equator for cytokinesis: feedback mechanisms and dynamical regimes , ALEXANDER VEKSLER, Rice University, DIMITRIOS VAVYLONIS, Lehigh University — The formation and constriction of the contractile ring during cytokinesis, the final step of cell division, depends on the recruitment of motor protein myosin to the cell's equatorial region. During animal cell cytokinesis, cortical myosin filaments (MF) disassemble at the flanking regions and concentrate in the equator [1]. This recruitment depends on myosin motor activity and the Rho proteins that regulate MF assembly and disassembly. Central spindle and astral microtubules help establish a spatial pattern of differential Rho activity [2]. We propose a reaction-diffusion model for the dynamics of MF recruitment to the equatorial region. In the model, the central spindle and mechanical stress [3] promote self-reinforcing MF assembly. Negative feedback is introduced by MF-induced recruitment of inhibitor myosin phosphatase. Our model yields various dynamical regimes and explains both the recruitment of MF to the cleavage furrow and the observed damped MF oscillations in the flanking regions [1], as well as steady MF assembly [4]. Space and time parameters of MF oscillations are calculated. We predict oscillatory relaxation of cortical MF upon removal of locally-applied external stress. [1] Zhou & Wang, Mol. Biol. Cell **19**:318 (2008); [2] Murthy & Wadsworth, J. Cell Sci. **121**:2350 (2008); [3] Ren et al., Curr. Biol. **19**:1421 (2009); [4] Vale et al., J. Cell Biol. **186**:727 (2009)

10:00AM V39.00011 Biomechanics and dynamics of red blood cells probed by optical tweezers and digital holographic microscopy , NELSON CARDENAS, PATTRICK THOMAS, LINGFENG YU, Nanoscope Technologies LLC, SAMARENDRA MOHANTY — Red blood cells (RBC), with their unique viscoelastic properties, can undergo large deformations during interaction with fluid flow and migration through narrow capillaries. Both local and overall viscoelastic property is important for cellular function and change in these properties indicate diseased condition. Though biomechanics of the cells have been studied using variety of physical techniques (AFM, optically-trapped anchoring beads and microcapilary aspiration) in force regime $>$ 10pN, little is studied at low force regime $<$1pN. Such perturbations are not only hard to exercise on the cell membrane, but quantification of such deformations becomes extremely difficult. By application of low power optical tweezers directly on cell membrane, we could locally perturb discotic RBC along the axial direction, which was monitored dynamically by digital holographic microscopy-a real time, wide-field imaging method having nm axial resolution. The viscoelastic property of the RBC at low force regime was found to be significantly different from that of high-force regime. The results were found to be in good agreement with the simulation results obtained using finite element model of the axially-stretched RBC. The simulations and results of viscoelestic measurements will be presented.

10:12AM V39.00012 Effect of Surface Adhesion on Individual and Collective Migration[1] , WOLFGANG LOSERT, University of Maryland, COLIN MCCANN, University of Maryland and NCI, ERIN RERICHA, University of Maryland, CAROLE PARENT, LCMB, NCI, NIH — Cell-surface adhesion plays a critical role in amoeboid cell motion by supplying the traction allowing a cell to move itself forward. The amoeba Dictyostelium discoideum, a model system for individual and collective cell migration, naturally exhibits both cell-substrate and cell-cell adhesion during the aggregation process. We used both high- and low-magnification time-lapse microscopy to investigate the individual and collective migration of D. discoideum on substrates of varying adhesiveness, as well as on interfaces between surfaces. We find that surface adhesion can affect both individual cell migration as well as the behavior of cell groups. At the population scale, non-ideal surfaces slow down the initiation of aggregation and change the aggregation dynamics. At the scale of single cells, we measure both adhesion ability as well as the area of contact between cells and surface for individual cells and cells that are part of groups. We find that comparable forces are needed to pull cells off all surfaces, indicating that surface adhesion is actively regulated by migrating cells.

[1]Supported by NCI and NSF-PoLS.

10:24AM V39.00013 Importance of spectrin network reorganization in computer simulations of RBC shapes[1] , ULF SCHILLER[2], TONY LADD, Department of Chemical Engineering, University of Florida, Gainesville — The shape of red blood cells (RBCs) has been the subject of intensive investigations in both experiments and theoretical models. Various computational models for RBCs have also been developed. However, a rigorous quantitative comparison of the observed shapes is still lacking. We have developed a flexible model that allows to study the influence of the various contributions to the membrane stress and their relevance for RBC shape. Our model reveals that a pure curvature model does not fully explain the experimentally observed discocyte shapes. We demonstrate that the in-plane stresses of the spectrin network have a crucial effect on the cell shapes and their transitions, and that the dynamic relaxation of the stresses due to spectrin reorganization is important. We present an extended model that incorporates the effects of dynamic spectrin remodeling and study their role on the dynamics of RBC shapes.

[1]Financial support from the Volkswagen Foundation is gratefully acknowledged.
[2]on leave from Institute of Solid State Research, Research Center Juelich, Germany

10:36AM V39.00014 The contribution of cytoskeleton networks to stretch is strain dependent[1] , KENECHUKWU DAVID NNETU, TOBIAS KIEßLING, ROLAND STANGE, JOSEF KÄS, University of Leipzig — The interaction between the cytoskeleton filaments in a cell provides it with mechanical stability and enables it to remodel its shape. The rheological response of cells has been characterized either as viscoelastic or soft-glassy which neglects the molecular origin of cell response. In this work, by using a large amount of cells ($>$10,000 in total) exceeding previous statistics by a decade, we link observed cell response to its molecular origin by showing that actin and microtubule networks maintain the mechanical integrity of cells in a strain dependent manner. While the actin network solely regulated cell deformation at small strain, the microtubule network was responsible for cell relaxation. At large strain, actin and microtubule networks dominated cell response with microtubules having a bipolar effect on cells upon stabilization. This effect could explain the relapse of some cancer after chemotherapy treatment using Taxol thus providing a bridge between soft condense matter physics and systems biology.

[1]This work was supported by the ESF-BuildMoNa and Exprimage (funded by the German Federal Ministry of Education and Research (BMBF)).

10:48AM V39.00015 Magnetic Carbon nanoparticles enabled efficient photothermal alteration of mammalian cells , L. GU, V. VARDARAJAN, A. KANNEGANTI, A. KOYMEN, S.K. MOHANTY, UT Arlington — While cw near-infrared (NIR) laser beams have been finding widespread application in photothermal therapy of cancer and pulsed NIR laser microbeams are recently being used for optoporation of exogeneous impermeable materials into cells. Since, carbon nanomaterials are very good in photothermal conversion, we utilized carbon nanoparticles (CNP) doped with Fe, so that they can be localized in a defined area by two fold selectivity, (i) external magnetic field for retention of the CNP in targeted area and (ii) surface functionalization for binding the targeted cells. Here, we report efficient photothermal therapy as well as poration of cells using magnetic CNPs with very low power continuous wave laser beam. Localization of CNPs on cell membrane under application of magnetic field was confirmed by scanning electron microscopy. At different power levels, cells could be damaged or microinjected with fluorescence protein-encoding plasmids or impermeable dyes. Monte Carlo simulation showed that the dose of NIR laser beam is sufficient to elicit response for magnetic CNP based photothermal treatment at significant depth. The results of our study suggest that magnetic CNP based photothermal alteration is a viable approach to remotely guide treatments offering high efficiency with significantly reduced cytotoxicity.

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V40 DBP: Thesis Award Session: Nucleic Acids – Structure, Function, and the Genome

A122/123

8:00AM V40.00001 2010 Award for Outstanding Doctoral Thesis Research in Biological Physics Talk: How the Genome Folds , EREZ LIEBERMAN-AIDEN, Harvard Society of Fellows — I describe Hi-C, a novel technology for probing the three-dimensional architecture of whole genomes by coupling proximity-based ligation with massively parallel sequencing. Working with collaborators at the Broad Institute and UMass Medical School, we used Hi-C to construct spatial proximity maps of the human genome at a resolution of 1Mb. These maps confirm the presence of chromosome territories and the spatial proximity of small, gene-rich chromosomes. We identified an additional level of genome organization that is characterized by the spatial segregation of open and closed chromatin to form two genome-wide compartments. At the megabase scale, the chromatin conformation is consistent with a fractal globule, a knot-free conformation that enables maximally dense packing while preserving the ability to easily fold and unfold any genomic locus. The fractal globule is distinct from the more commonly used globular equilibrium model. Our results demonstrate the power of Hi-C to map the dynamic conformations of whole genomes.

8:36AM V40.00002 Recognition Tunneling towards Next Generation Single Molecule DNA Sequencing , SHUO HUANG, Arizona State University — A novel approach has been developed to trap and sequence DNA within a molecular junction formed by a pair of functionalized Au electrodes so individual DNA nucleotides could be recognized on small pieces of DNA with single base resolution. The cost of labeling reagents is totally eliminated since different nucleotides are recognized through their intrinsic physical properties. Unexpectedly long residence time of DNA (on the order of a second) in the molecular gap is observed which indicates that a pN force is required to achieve the sequencing speed as fast as 10 bases/Sec. Providing such ionic driving force, a nanopore device incorporated with recognition tunneling reader will provide a revolutionary way for fast, accurate and economic next generation DNA sequencing.

8:48AM V40.00003 Electronic Signatures of all Four DNA Nucleosides in a Tunneling Gap[1] , SHUAI CHANG, Arizona State University — New approaches to DNA sequencing are required to reduce costs and increase the availability of personalized genomics. Using Scanning Tunneling Microscope as a tool, we report measurements of the current signals generated as free nucleosides diffuse into a tunnel junction in which both electrodes are functionalized with a reagent that presents a hydrogen bond donor and acceptor to the nucleosides. This functionalization serves to both limit the range of molecular orientations in the tunnel gap and reduce the contact resistance, increasing the selectivity of the tunneling signal, so that a direct readout may be possible with a few repeated reads.

[1]This work was supported by a grant from the Sequencing Technology Program of the National Human Genome Research Institute (HG004378).

9:00AM V40.00004 Gel electrophoresis of partially denatured DNA: split-ends, bubbles, and squids , DAVID SEAN, GARY W. SLATER, University of Ottawa — Gel electrophoresis separates partially denatured DNA fragments based on chemical sequence. Upon an increase in temperature, AT-rich regions melt into two strands which is thought to be the main contributor to the rapid reduction of the fragment's mobility. The reduction in mobility is often predicted from the average number of denatured bases regardless of their positions. We re-visit the theoretical basis of this approach and determine that the analysis only holds for denatured domains that occur at the ends. Langevin Dynamics simulations are used to study the effect that the placement of the melted regions has on the mobility by discriminating between denatured domains which occur in the middle of the fragment (bubbles) and at the ends (split-ends). It is found that the split-ends dominate the blocking mechanism. In addition, we find a novel conformation (the "squid") which seems to be responsible for the blocking at high fields.

9:12AM V40.00005 Temperature dependence of two distinct DNA overstretching transitions , XINGHUA ZHANG, BioSyM, SMART, HONGXIA FU, Mechanobiology Institute, Singapore, National University of Singapore, PATRICK DOYLE, Department of Chemical Engineering, MIT, JIE YAN, Mechanobiology Institute, Singapore, National University of Singapore; Department of Physics, National University of Singapore — Recent experiments show that two distinct transitions are involved in the DNA overstretching that occurs at around 65 pN: a strand-unpeeling transition leading to strand separation from free DNA ends or nicks, and a B to S transition leading to an overstretched double-stranded DNA called "S-DNA." Here we show that the two transitions have distinct temperature dependence: in the strand-unpeeling transition, the transition force decreases when the temperature increases; while in the B to S transition, the temperature dependence of the transition force is opposite. Our results are in agreement with the notion that the two transitions involve distinct types of double-helix reorganization.

9:24AM V40.00006 An Analytic Theory for Single Molecule Manipulation of DNA[1] , CRISTIANO NISOLI, Theoretical Division and CNLS Los Alamos National Laboratory, Los Alamos NM — We introduce a minimal, analytically solvable model for thermo-mechanical behavior of DNA under tension and torque, and predict critical temperature for denaturation at unwinding and overwinding, phase diagrams for stable b–DNA, and supercoling-elongation curves as functions of applied torque, tension and temperature. Our results are in agreement with experimental data from experiments in single molecule manipulation. We also propose simple thermodynamical formulae for temperature, tension, torque, and supercoiling at criticality.

[1]This work was carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396.

9:36AM V40.00007 Multimerization of DNA Origami Structures in Two Dimensions[1] , DANIEL SCHIFFELS, Ludwig-Maximilians-Universität München, DEBORAH FYGENSON, University of California Santa Barbara, TIM LIEDL, Ludwig-Maximilians-Universität München — DNA nanotechnology, here in particular DNA origami, is based on self-assembly and can be used to construct arbitrary three-dimensional structures with nanometer precision. The dimensions of such DNA origami structures are typically on the order of a hundred nanometers or smaller. To achieve large-scale two-dimensional lattices that could be employed as scaffolds for crystalline arrangement of biomolecules and proteins, individual DNA origami tiles need to be assembled hierarchically. We work on the multimerization of DNA origami structures into extended one- and two- dimensional lattices that can cover areas of several square micrometers. This is achieved by complementary single stranded DNAs (sticky ends) at specific positions on the DNA origami objects that we intend to grow into periodic structures. We study the effect of varying multimerization conditions such as annealing temperatures, length of sticky ends and salt concentration on the quality and size of the resulting lattice.

[1]Financial support by the Elite Network of Bavaria (International Doctorate Program NanoBioTechnology) is gratefully acknowledged.

9:48AM V40.00008 Fluctuation Pressure Assisted Ejection of DNA From Bacteriophage , MICHAEL J. HARRISON, Michigan State University — The role of thermal pressure fluctuations excited within tightly packaged DNA while it is ejected from protein capsid shells is discussed in a model calculation. At equilibrium before ejection we assume the DNA is folded many times into a bundle of parallel segments that forms an equilibrium conformation at minimum free energy, which presses tightly against capsid walls. Using a canonical ensemble at temperature T we calculate internal pressure fluctuations against a slowly moving or static capsid mantle for an elastic continuum model of the folded DNA bundle. It is found that fluctuating pressures on the capsid from thermal excitation of longitudinal acoustic vibrations in the bundle whose wavelengths are exceeded by the bend persistence length may have root-mean-square values that are several tens of atmospheres for typically small phage dimensions. Comparisons are given with measured data on three mutants of lambda phage with different base pair lengths and total genome ejection pressures.

10:00AM V40.00009 Effects of sequence on DNA wrapping around histones[1] , VANESSA ORTIZ, Department of Chemical Engineering, Columbia University — A central question in biophysics is whether the sequence of a DNA strand affects its mechanical properties. In epigenetics, these are thought to influence nucleosome positioning and gene expression. Theoretical and experimental attempts to answer this question have been hindered by an inability to directly resolve DNA structure and dynamics at the base-pair level. In our previous studies we used a detailed model of DNA to measure the effects of sequence on the stability of naked DNA under bending. Sequence was shown to influence DNA's ability to form kinks, which arise when certain motifs slide past others to form non-native contacts. Here, we have now included histone-DNA interactions to see if the results obtained for naked DNA are transferable to the problem of nucleosome positioning. Different DNA sequences interacting with the histone protein complex are studied, and their equilibrium and mechanical properties are compared among themselves and with the naked case.

[1]NLM training grant to the Computation and Informatics in Biology and Medicine Training Program (NLM T15LM007359)

10:12AM V40.00010 A quantitative model of nucleosome dynamics , ROBERT FORTIES, JUSTIN NORTH, SARAH JAVAID, OMAR TABBAA, RICHARD FISHEL, MICHAEL POIRIER, RALF BUNDSCHUH, The Ohio State University — The expression, replication and repair of eukaryotic genomes require the fundamental organizing unit of chromatin, the nucleosome, to be unwrapped and/or disassembled. We have developed a quantitative model of nucleosome dynamics which provides a fundamental understanding of these DNA processes. We calibrated this model using results from high precision single molecule nucleosome unzipping experiments, and then tested its predictions for experiments in which nucleosomes are disassembled by the DNA mismatch recognition complex hMSH2-hMSH6. We found that this calibrated model quantitatively describes hMSH2-hMSH6 induced disassembly rates of nucleosomes with two separate DNA sequences and four distinct histone modification states. In addition, this model provides mechanistic insight into nucleosome disassembly by hMSH2-hMSH6 and the influence of histone modifications on this disassembly reaction. This model's precise agreement with current experiments suggests that it can be applied more generally to provide important mechanistic understanding of the numerous nucleosome alterations that occur during DNA processing.

10:24AM V40.00011 Fitness and structure landscapes for pre-miRNA processing , RALF BUNDSCHUH, Departments of Physics and Biochemistry, The Ohio State University, JULIETTE DE MEAUX, Fachbereich Biologie, Universitaet Muenster, MICHAEL LASSIG, Institut fuer theoretische Physics, Universitaet zu Koeln — The processing from pre-miRNA to mature miRNA in plants involves a mechanism, which depends on an extended stem in the secondary structure of the pre-miRNA. Here, we show how natural selection acts on this secondary structure to produce evolutionary conservation of the processing mechanism together with modularity of the pre-miRNA molecules, making this molecular function independent of others. Our main results are: 1. Selection on miRNA processing can be described by a fitness landscape which depends directly on the secondary structure of the pre-miRNA. 2. This fitness landscape predicts the divergence of the phenotype between orthologous pre-miRNA molecules from different species. 3. Actual pre-miRNA structures are modular: their phenotype is significantly less affected by deleterious mutations in the remainder of the molecule than for random RNA molecules.

10:36AM V40.00012 DNA-damage by free radicals in solution , P.K. BISWAS, Tougaloo College, RAMIN ABOLFATH, U. Texas at Dallas, R. RAJNARAYANAM, SUNY at Buffalo, K. CHO, U. Texas at Dallas, T. BRABEC, Ottawa U., L. PAPIEZ, U. Texas, UTSW — We employ a molecular simulation based on GROMACS-CPMD QM/MM method to study the initial damage to a fragment of DNA-molecule in the solution by ionizing radiation. We illustrate that the diatomic OH-radicals that are primary product of megavoltage ionizing radiation in water-based systems form a network of hydrogen bonds with the nearby water molecules. Our molecular simulation illustrates that the Hydrogen bonds strongly alter the relative orientation of the OH-radicals and DNA molecule. This results to an angular anisotropy in the chemical pathway and a lower efficiency in the hydrogen abstraction mechanisms than previously anticipated for identical system in the vacuum. We illustrate that the thermal fluctuations of the water molecules in the solution strongly compete with the H-abstraction that shows more energitically favorable in solution than in vacuum. As a result the chemical reaction takes place with slower rate in solution than in vacuum.

10:48AM V40.00013 Transport properties of nucleotides in a graphene nanogap for DNA sequencing[1] , J. PRASONGKIT, A. GRIGORIEV, R.H. SCHEICHER, Condensed Matter Theory Group, Dept of Physics and Astronomy, Uppsala University, Sweden, R. AHUJA, Condensed Matter Theory Group, Uppsala University, and Royal Institute of Technology (KTH), Stockholm, Sweden — The application of graphene nanogaps for DNA sequencing has been proposed [H. W. Ch. Postma, Nano Lett. 10, 420 (2010)]. We used density functional theory and the non-equilibrium Green's function method to study the electron transport properties of nucleotides located inside a graphene nanogap. Our setup considered different positions and orientations of the bases with respect to the graphene electrodes, and we analyzed how the transmission spectra depend on such shifts and rotations. Even when taking into account current changes due to base fluctuations, we find that each nucleotide possesses a different characteristic current magnitude, owing to its distinctive electronic properties. Based on our results, it thus seems that the electrical readout from a graphene nanogap could in principle be sufficiently sensitive to distinguish between the four nucleotides, and thus achieve the goal of rapid and economical whole-genome sequencing.

[1]Swedish Research Council (VR, grant no. 621-2009-3628)

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V41 DCP: Focus Session: The Role of Water in Energy Production and Utilization II

A115/117

8:00AM V41.00001 The structure of water/hydroxyl phases at metal interfaces , ANDREW HODGSON, The University of Liverpool — On all but the least reactive metals, the first contact layer with water is a mixture of water and hydroxyl, often formed by spontaneous dissociation [1]. Understanding the composition and stability of these layers is a key step in describing both the wetting and the redox behavior of the surface. Here we discuss the wetting of Cu(110) and the formation of mixed water-hydroxyl layers by reaction with adsorbed O. This surface does not conform to the traditional hexagonal symmetry associated with an ice Ih, and the hydrogen bonding structure must accommodate to the surface symmetry. A number of unusual structures are seen, including 1D chains of interlocking pentagons [2], an intact 2D network with a (7x8) unit cell at higher coverage [3] and several partially dissociated structures, including both 1D and 2D phases [4]. The composition of these structures and hydrogen bonding arrangements will be discussed, highlighting the way changing the composition and relative metal-adsorbate and adsorbate-adsorbate interactions drives the structural rearrangement of these phases.

[1] A. Hodgson and S. Haq, Surf. Sci. Rep., 64(9), 381 (2009).
[2] J. Carrasco et al. Nat. Mat., 8, 427 (2009).
[3] T. Schiros et al., Chem. Phys. Lett., 429, 415 (2006).
[4] M. Forster et al., submitted.

8:36AM V41.00002 Quantum nature of the proton in water-hydroxyl overlayers on metal surfaces , ANGELOS MICHAELIDES, XINZHENG LI, London Centre for Nanotechnology and Department of Chemistry, University College London, MATTHEW PROBERT, Department of Physics, University of York, ALI ALAVI, Department of Chemistry, University of Cambridge — Using *ab initio* path integral molecular dynamics we show that water-hydroxyl overlayers on transition metal surfaces exhibit surprisingly pronounced quantum nuclear effects. The metal substrates serve to reduce the classical proton transfer barriers within the overlayers and, in analogy to ice under high pressure, to shorten the corresponding intermolecular hydrogen bonds. Depending on the substrate and the intermolecular separations it imposes, the traditional distinction between covalent and hydrogen bonds is lost partially (e.g. on Pt(111) and Ru(0001)) or almost entirely (e.g. on Ni(111)). We suggest that these systems provide an excellent platform on which to systematically explore the magnitude of quantum nuclear effects in hydrogen bonds.

8:48AM V41.00003 Water adsorption on oxygen covered Ru(0001) surfaces , SABINE MAIER[1], Lawrence Berkeley National Laboratory, PEPA CABRERA-SANFELIX, Donostia International Physics Center, San Sebastian, Spain, INGEBORG STASS, Lawrence Berkeley National Laboratory, DANIEL SANCHEZ-PORTAL, ANDRES ARNAU, Donostia International Physics Center, San Sebastian, Spain, MIQUEL SALMERON, Lawrence Berkeley National Laboratory — We present a combined scanning tunneling microscopy (STM) and density functional theory (DFT) study of the adsorption of water on a Ru(0001) surface covered with half monolayer of oxygen. The adsorption of water causes a shift of half of the oxygen atoms in the O(2x1) structure from hcp sites to fcc sites, creating a honeycomb structure where water molecules bind strongly to the exposed Ru atoms [1]. The energy cost of reconstructing the oxygen overlayer is more than compensated by the larger adsorption energy of water on the newly exposed Ru atoms. STM images reveal a (4x2) superstructure due to alternating orientations of the water molecules. Heating to 185 K results in the complete desorption of the water layer, leaving behind the oxygen honeycomb structure, which is metastable relative to the original (2x1). This stable structure is not recovered until after heating to temperatures close to 260K.

[1] S. Maier et al. Phys. Rev. B 82, 075421 (2010).

[1]Now at University of Erlangen-Nuremberg, Germany

9:00AM V41.00004 Water monolayers on metals – a new framework[1] , PETER J. FEIBELMAN, Sandia National Laboratories — The first wetting layer on a solid embodies the boundary condition for water transport along its surface, is the template for ice nucleation, and governs aqueous surface chemistry. Today's talk is focused on the wetting of close-packed, precious metal surfaces, which are both relatively easily prepared, and susceptible to study by a host of surface science techniques. For decades, wetting layers on such surfaces have been thought to be "ice-like" – strained into registry with the metal lattice, but otherwise like the layers that stack to form the naturally occurring crystal, ice Ih. Interpretations of STM images of periodic wetting layers on Pt(111) [1], of TPD [2], and of IR absorption spectra [3] contradict the "ice-like" picture, but submit to a common, physics-based and DFT-supported interpretation. It is that several ice-like hexagonal rings of H_2O molecules, per repeated cell, are replaced by pentagons and heptagons, allowing a compact subset of H_2O's, with planes parallel to the metal surface, to approach the metal exceptionally closely and to anchor the wetting layer strongly to it. This motif, amounting to formation of energetically favorable di-interstitial "defects," appears to be general; similar molecular arrangements account for what we know experimentally (and, largely, could not previously explain) of water bonding to Ni, Ru, and Pd close-packed surfaces.

[1] S. Nie, P. J. Feibelman, N.C. Bartelt, and K. Thürmer, Phys. Rev. Lett. **105**, 026102(2010).
[2] P. J. Feibelman, N.C. Bartelt, S. Nie, and K. Thürmer. J. Chem. Phys. **133**, 154703(2010).
[3] P. J. Feibelman, G. A. Kimmel, B. D. Kay, N. Petrik, R. S. Smith and T. Zubkov, unpublished.

[1]Work supported by the DOE Office of Basic Energy Sciences, Division of Materials Science and Engineering, under contract DE-AC04-94AL85000.

9:36AM V41.00005 First-principles simulation of water on graphene using different levels of theory[1] , P. GANESH, P.R.C. KENT, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, TN, DE-EN JIANG, Chemical Sciences Division, Oak Ridge National Laboratory, TN — We show results from molecular-dynamics simulations of water confined between flat graphene sheets using different levels of theory. DFT simulations using PBE exchange-correlation show strong layering near the graphene sheet, with the hydrogens closer to the graphene surface. Correlations die off to bulk values after ∼10Å from the surface. Inclusion of an empirical Grimme-type van der Waals potential has a small effect on the interfacial C-H distance but a seemingly large effect from the second coordination shell onwards from the surface. Existing reactive force-fields for water, e.g. ReaxFF, do not capture the structure of water on graphene accurately and require refitting to more closely reproduce the DFT results. Molecular dynamics results with available self-consistent vDW-DFx kernels and contrasts with existing classical water models will also be presented.

[1]Work supported by the FIRST Cneter, an EFRC funded by U.S. DOE under award ERKCC61.

9:48AM V41.00006 How Water Meets Graphene , HUA ZHOU, PAUL FENTER, Argonne National Laboratory, JAKE MCDONOUGH, VOLKER PRESSER, YURI GOGOTSI, Department of Materials Science and Engineering, Drexel University, MATTHEW WANDER, KEVIN SHUFORD, Department of Chemistry, Drexel University — The interactions of electrolyte fluids with solids control many complex interfacial processes encountered in electrochemical energy storage systems. In this talk, we will demonstrate how to develop a fundamental atomic-scale understanding of interfacial structures at the water-graphene interface, a model fluid-solid interface combination. We have performed systematic measurements of high resolution X-ray reflectivity from epitaxial graphene films in contact with electrolytes including deionized water and aqueous salt solutions. The electron density profiles and structural models from the fully analyzed data reveal the intrinsic interfacial structures. It is noted that the interfacial water structure above the first graphene layer exhibits remarkable differences with those of subsequent graphene layers. The latter one, resembling water on freestanding graphene, is well predicted by parallel computational simulations. Moreover, the pH of aqueous solutions was found to have a subtle influence on the interfacial water structure above the first graphene layer. This may well be an indication of the interfacial structural distortions that might exist in this layer, and which may play an important role in controlling the chemical activity of monolayer epitaxial graphene.

10:00AM V41.00007 The Dynamics of Supercooled Water , FRANCESCO MALLAMACE, Dept of Physics, University of Messina, Italy — We present an overview of recent experiments performed on transport properties of water in the deeply supercooled region, a temperature region of fundamental importance in the science of water. We report data of nuclear magnetic resonance, quasi-elastic neutron scattering, Fourier-transform infrared spectroscopy, and Raman spectroscopy, studying water confined in nano-meter-scale environments (nano-tubes and the protein hydration water) and in bulk solutions. When contained within small pores, water does not crystallise, and can be supercooled well below its homogeneous nucleation temperature Th. On this basis it is possible to carry out a careful analysis of the well known thermodynamical anomalies of water. Studying the temperature and pressure dependencies of water dynamics, we show that the liquid-liquid phase transition (LLPT) hypothesis represents a reliable model for describing liquid water. In this model, water in the liquid state is a mixture of two different local structures, characterised by different densities, namely the low density liquid (LDL) and the high-density liquid (HDL). The LLPT line should terminate at a special transition point: a low-T liquid-liquid critical point. In particular We discuss the following experimental findings on liquid water: (i) a crossover from non-Arrhenius behaviour at high T to Arrhenius behaviour at low T in transport parameters; (ii) a breakdown of the Stokes-Einstein relation; (iii) the existence of a Widom line, which is the locus of points corresponding to maximum correlation length in the p-T phase diagram and which ends in the liquid-liquid critical point; (iv) the direct observation of the LDL phase; (v) a minimum in the density at approximately 70K below the temperature of the density maximum. In our opinion these results represent the experimental proofs of the validity of the LLPT hypothesis.

10:36AM V41.00008 Structural, Dynamic, and Spectroscopic Properties of the SCC-DFTB Water Model , LAURA KINNAMAN, KATHIE NEWMAN, STEVEN CORCELLI, University of Notre Dame — The interactions of water and many interfaces are not understood at a mechanistic level. The accuracy of simulations of the system are limited by the accuracy of the water model used. Classical models such as SPC/E use empirically derived parameters to match their behavior to desired bulk water properties, but cannot participate in reactions that require the making or breaking of bonds. Ab initio quantum mechanical methods such as Car-Parrinello (CP) do allow water to dissociate, but are computational intractable for large systems. A potential middle ground is the self-consistent charge density-functional tight-binding method (SCC-DFTB), which has a smaller associated computational cost, and therefore can access larger systems than CP, while still allowing for the making and breaking of bonds. The DFTB+ implementation of SCC-DFTB allows for 2nd and 3rd order expansions of the density fluctuations in the energy and, in the 3rd order expansion, an optional damping correction factor. For each of these models we compare the structural, dynamic, and spectroscopic properties of bulk SCC-DFTB water to classical SPC/E and experimental results.

10:48AM V41.00009 Interfacial water on TiO_2 anatase (101) and (001) surfaces: First-principles study with TiO_2 slabs dipped in bulk water[1] , YOSHITAKA TATEYAMA, MASATO SUMITA, International Centre for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), CHUNPING HU, Tokyo University of Science — Density functional molecular dynamics simulations using supercells with "bulk" water between the TiO_2 anatase (101) and (001) surfaces were carried out to elucidate the behaviour of water molecules and hydrogen bond networks on the interfaces of representative photocatalysts. It is demonstrated that the adsorption manners (molecular or dissociative) of water molecules on the vacuum surfaces still hold in the presence of "bulk" water on the interfaces. We also showed explicit atomistic structures of strong and weak hydrogen bonds on the TiO_2/water interfaces, which had been proposed experimentally so far. We then suggested a two-layer model for the interfacial water on both surfaces investigated. Our results also give insights into the H_2O or OH adsorption coverage on the interfaces and their hydrophobicity- hydrophilicity, which is important to understand the photocatalytic reaction mechanisms microscopically.

[1]This work wassupported by JST-PRESTO, JST-CREST and KAKENHI.

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V42 DPOLY DBP: Focus Session: Supramolecular Self-Assembly–Controlling Network and Gel Formation II A302/303

8:00AM V42.00001 Control of semi-flexible polymer networks by architecture and dynamic cross-linking , FRED MACKINTOSH, Vrije Universiteit, Amsterdam — The rigidity of elastic networks depends sensitively on their internal connectivity and the nature of interactions between constituents. Particles interacting via central forces become rigid above the isostatic connectivity threshold first identified by Maxwell. Stiff or semi-flexible polymers, such as those that form the cellular cytoskeleton, develop a finite network shear modulus G at a lower threshold, although the degree to which the mechanics of such networks are governed by filament bending resistance remains a subject of considerable debate. Such networks also exhibit rich viscoelastic properties. For cytoskeletal networks, there is increasing evidence that the network response is governed by the compliance and dynamics of the cross-links, many of which are transient in nature. Here we study the effects of both local network architecture and dynamic cross-linking in disordered fibrous networks. Surprisingly, the network mechanics in both 2D and 3D are still governed by the central-force isostatic point, which acts as a zero-temperature critical point. Near this point, we find divergent strain fluctuations and an associated diverging length-scale, as well as an anomalous elastic regime that exhibits fractional power-law dependence of G on both fiber bending stiffness and stretch modulus. Furthermore, dynamic cross-linking gives rise to a broad, power-law viscoelastic regime at low frequency ω in which $G \sim \omega^{1/2}$.

8:36AM V42.00002 Macro- and microphase separation in multifunctional supramolecular polymer networks , ZOLTAN MESTER, University of California Santa Barbara, ARUNA MOHAN, Exxon-Mobil, GLENN FREDRICKSON, University of California Santa Barbara — We develop a field-based model for a binary melt of multifunctional polymers that can reversibly bond to form copolymer networks. The mean-field phase separation behavior of several model networks with heterogeneous bonding is calculated via the random phase approximation (RPA). The extent of bonding between polymers is controlled by specified bond energies. The phase boundary calculated via RPA is the stability limit of the homogeneous disordered phase to coexisting homogeneous macrophases, for low bond strengths, and to microphases, for high bond strengths. An isotropic Lifshitz point separates these two regions along the spindodal boundary. It is demonstrated that higher functionality and higher bond strength suppresses macrophase separation due to greater connectivity between unlike species. Gelation first occurs at a bond strength higher than the Lifshitz point for tri- or higher functional polymer components.

8:48AM V42.00003 Equilibrium and nonequilibrium gelation in TPR protein/linker mixtures[1] , TIANQI SHEN, ROBERT S. HOY, COREY S. O'HERN, Yale University — Using simulations we model gelation in two-component systems consisting of tetratricopeptide repeat (TPR) proteins and peptide cross linkers. These have recently been shown [1] to form strong, mechanically stable gels with remarkable shape recovery - but only within narrow parameter regimes. Within our minimal, coarse grained model, we elucidate the effects of the packing fraction ϕ, temperature T and concentration ratio r of TPR and cross linkers on the gel transition. Two gelation mechanisms are identified. At low ϕ and T, nonequilibrium microphase-separated gels may be formed by rapid temperature quenches. At higher ϕ and T, homogeneous equilibrium gelation occurs. At low r, gelation is suppressed due to depletion of linkers, while at high r gelation is suppressed due to the "coating" of proteins by linkers. The gel transition line in the (r, T) plane has an unusual, asymmetric form. We also briefly compare these results to those for a more realistic "patchy" model which incorporates the directional TPR-linker binding present in the experimental systems.

[1] T. Z. Grove *et. al.*, JACS, **132**, 14024 (2010).

[1]T. S. acknowledges support from NSF grant no. PHY-1019147.

9:00AM V42.00004 Effects of inclusions on the dynamics of viscoelastic media , STEPHEN MIRIGIAN, MURUGAPPAN MUTHUKUMAR, University of Massachusetts — The modification of material properties due to the presence of inclusions in solutions and elastic composites are well known, modifying properties such as viscosity and elastic moduli. We calculate the mobility of such an inclusion in a viscoelastic medium as well as effective dynamic material properties due to the presence of such inclusions at various frequencies.

9:12AM V42.00005 Conformation and mechanical properties of diblock fibers[1] , SUMANTH SWAMINATHAN, Northwestern University, FRANCISCO SOLIS, Northwestern University / Arizona State University, MONICA OLVERA DE LA CRUZ, Northwestern University, OLVERA TEAM — We analyze the conformations of closed diblock fibers comprised of different bending rigidities and spontaneous curvatures. In each fiber, one block is a bare polymer while the other is an adsorbed protein-filament complex. The length fraction of each component and the total fiber length is controlled by tunable chemical potentials. We analytically calculate the shape of these two-component polymers for all values of the material parameters and chemical potentials. Our results yield: a complete analytical description of all possible two-component polymer conformations in two and three dimensions, a phase portrait detailing the parameter spaces in which these shapes occur, and the identification of spontaneous transitions between shapes driven by environmental changes.

[1]By the US Department of Energy, Office of Basic Energy Sciences as part ofthe Non-Equilibrium Energy Research Center (NERC), an Energy Frontier Research Center.

9:24AM V42.00006 The Role of Multiple, Reformable Parallel Bonds on the Self-healing Behavior of Dual Crosslinked Nanogel Materials , ISAAC G. SALIB, GERMAN V. KOLMAKOV, CHET N. GNEGY, Chemical Engineering Department, University of Pittsburgh, KRZYSZTOF MATYJASZEWSKI, Department of Chemistry, Carnegie Mellon University, ANNA C. BALAZS, Chemical Engineering Department, University of Pittsburgh — Using computational modeling, we design novel self-healing materials composed of nanoscopic polymer gel particles, or nanogels. The particles are interconnected via both labile bonds (e.g., disulfide bonds) and stronger, less reactive bonds (e.g, C-C bonds) and therefore the nanogels form a "dual crosslinked" network. The stable bonds provide a rigid backbone while the labile bonds allow the material to undergo a dynamic reconfiguration in response to stress. We adapt the Hierarchical Bell Model (HBM) to describe the labile bonding interactions. The HBM effectively allows us to model cases where the ligands on neighboring nanogels interact through multiple sites. We show that the introduction of a small number of labile bonds that lie in parallel significantly increases the strength of the material relative to samples crosslinked solely by the stable bonds. We also isolate an optimal range of labile interconnections that provide high-strength, tough materials that are capable of self-repair.

9:36AM V42.00007 Forming Reversible Gels with Triblock Polyelectrolytes: a Field-theoretic Study , DEBRA AUDUS, GLENN FREDRICKSON, UC Santa Barbara — Recently, two research groups have formed reversible gels using triblock polyelectrolytes (Lemmers et al. 2010; Hunt et al., in preparation). This gel formation is driven by a phenomenon called complex coacervation, in which two oppositely charged homopolymers in solution phase separate into a polymer rich phase, known as a coacervate, and a solution phase. If instead, the polymers are triblocks with a neutral midblock and charged end blocks, under appropriate conditions they will microphase separate into micelles with cores of coacervated charged groups and coronas of neutral midblocks. These neutral midblocks act as bridges between the micelles, thereby creating a gel. One of the advantages of forming gels in this way is that the coacervate domains, and thus the gel, can be easily tuned by varying parameters such as pH, salt concentration and temperature. In order to understand the microstructures and solution sensitivity of these reversible gels, we have numerically simulated field-theoretic models of triblock polyelectrolyte mixtures in an implicit solvent. Because coacervation is driven by charge correlations, the usual mean-field assumption fails, and it is necessary to study the model beyond the level of SCFT.

9:48AM V42.00008 Supramolecular Arrest and Activation for the Network Formation of Acid Catalyzed Epoxy Polymerization , MATTHEW SPENCER, JAMES CRIVELLO, CHANG Y. RYU, Rensselaer Polytechnic Institute — Epoxy resins are limited currently as they must be externally activated by radiation in combination with a photo acid generator or implemented using the more ubiquitous two-component approach. Two component systems begin to react upon mixing are while UV cured epoxies are limited to situations where light can reach the monomer. We propose a novel one-component system that is externally activated with the application of heat. A considerable room temperature lifetime is attributed to the systems ability to sequester super acids through a system of hydrogen bonding coordination. The model system utilizes an alkyl glycidal ether which is made universal by the addition of crown ethers to non-ether epoxy monomers. Our supramolecular-based approach to retard and trigger the epoxy polymerization is likely to enable more widespread applications in microelectronic packaging.

10:00AM V42.00009 Polymer Phononic Meta-material Networks[1] , CHEONGYANG KOH, EDWIN THOMAS, DMSE, MIT — Phononic Meta-materials (PMM) offer unique opportunities for molding the flow of phonons through artificial structuring of the material at relevant length scales; however, most structures rely on combining mechanically "stiff" and "soft" materials to create the desired phononic properties, usually focusing on resonances to stop phonon flow. Such an approach suffers from lack of scalability, placing fabrication and material compatibility constraints on technological realization. Here, we show that these constraints are unnecessary and that phonon propagation behavior relies on the fundamental requirements of avoided crossings in the frequency dispersion relations. In particular, we demonstrate 1) polymer/air PMMs possessing i) multiple complete spectral gaps (MCSG), ii) negative index bands, iii) both a complete sub-wavelength transverse gap and Bragg-type longitudinal gap and 2) waveguides of pma2 *Frieze* group symmetry that possess MCGS; we verify their dispersion relation using Brillouin light scattering. This opens up the ability to develop novel integrated low-cost all-polymer phononic platforms for information processing via mesoscale polarization manipulation, filtering and superlensing.

[1]This work was supported by grants no.NSF-DMR 0308133 and ISN W91NF-07-D-0004.

10:12AM V42.00010 Formation of Anisotropic Block Copolymer Gels[1] , CHYA YAN LIAW, KENNETH SHULL, KEVIN HENDERSON, DERK JOESTER, Northwestern University — Anisotropic, fibrillar gels are important in a variety of processes. Biomineralization is one example, where the mineralization process often occurs within a matrix of collagen or chitin fibers that trap the mineral precursors and direct the mineralization process. We wish to replicate this type of behavior within block copolymer gels. Particularly, we are interested in employing gels composed of cylindrical micelles, which are anisotropic and closely mimic biological fibers. Micelle geometry is controlled in our system by manipulating the ratio of molecular weights of the two blocks and by controlling the detailed thermal processing history of the copolymer solutions. Small-Angle X-ray Scattering and Dynamic Light Scattering are used to determine the temperature dependence of the gel formation process. Initial experiments are based on a thermally-reversible alcohol-soluble system, that can be subsequently converted to a water soluble system by hydrolysis of a poly(t-butyl methacrylate) block to a poly (methacrylic acid) block.

[1]MRSEC

10:24AM V42.00011 Microstructural Organization of Elastomeric Polyurethanes with Siloxane-Containing Soft Segments , TAEYI CHOI, The Pennsylvania State University, JADWIGA WEKLSER, AJAY PADSALGIKAR, Aortech Biomaterials, JAMES RUNT, The Pennsylvania State University — In the present study, we investigate the microstructure of two series of segmented polyurethanes (PUs) containing siloxane-based soft segments and the same hard segments, the latter synthesized from diphenylmethane diisocyanate and butanediol. The first series is synthesized using a hydroxy-terminated polydimethylsiloxane macrodiol and varying hard segment contents. The second series are derived from an oligomeric diol containing both siloxane and aliphatic carbonate species. Hard domain morphologies were characterized using tapping mode atomic force microscopy and quantitative analysis of hard/soft segment demixing was conducted using small-angle X-ray scattering. The phase transitions of all materials were investigated using DSC and dynamic mechanical analysis, and hydrogen bonding by FTIR spectroscopy.

10:36AM V42.00012 Viscoelastic Properties of Photo-crosslinked Shape Memory Elastomers[1] , JIAHUI LI, CHRISTOPHER LEWIS, DARCY CHEN, MITCHELL ANTHAMATTEN, University of Rochester — Lightly crosslinked polymer networks containing self-complementary hydrogen-bonding side-groups (e.g. ureidopyrimidinones, UPy) have been shown to exhibit unique shape-memory properties. Our synthetic approach, involving photo-crosslinking, enables both the crosslink density and UPy-content to be systematically varied. To better understand how hydrogen bond dynamics impact viscoelastic properties, dynamic mechanical analysis was performed on a series of photo-crosslinked elastomers. The presence of UPy side-groups imparts a broad dynamic transition over a frequency range that depends on the UPy content. The UPy side-group dynamics result in a high level of mechanical damping, and they enable damping characteristics to be tailored. Time temperature superposition (TTS) analysis was performed, and resulting shift factors show Arrhenius behavior. Activation energies were calculated, and elastomers with higher UPy content exhibit higher activation energies.

[1]Research was funded by NSF DMR-0906627.

10:48AM V42.00013 Origins and stability of the polydomain regime in isotropic-genesis nematic elastomers , BING LU, FANGFU YE, University of Illinois, XIANGJUN XING, Shanghai Jiao Tong University, PAUL GOLDBART, University of Illinois — We address the physical properties of nematic elastomers that have been randomly crosslinked in the high-temperature isotropic state. We do this by constructing a replica Landau theory in terms of a coupled pair of order-parameter fields: one for vulcanization, the other for nematic order. We focus on the correlations of the trapped-in nematic fluctuations as a diagnostic of the structure of the elastomer, determining them for a range of temperatures and disorder strengths. Our analysis shows that, in fewer than four spatial dimensions, the quenched randomness associated with the crosslinking prevents the emergence of long-range order, either of the mondomain nematic or of the spatially modulated type. It also shows that, for sufficiently strong disorder and low enough temperatures, the system exhibits unusual short-range oscillatory structure in the local nematic alignment.

Thursday, March 24, 2011 8:00AM - 11:00AM –
Session V43 DPOLY DBP: Focus Session: Translocation Through Nanopores II A306/307

8:00AM V43.00001 The Statistics of DNA Capture and Re-Capture by Solid-State Nanopores[1] , MIRNA MIHOVILOVIC, ERIN TEICH, NICK HAGERTY, JASON CHAN, DEREK STEIN, Brown University — We studied repeated electrophoretic translocations of the same DNA molecule through ∼10 nm nanopores using the voltage-reversal re-capture technique. Correlations were observed in the folding conformations of molecules re-captured within the Zimm relaxation time of the polymer. A trend was observed, whereby more compact conformations of DNA evolved over time. Consecutive event charge deficit measurements were narrowly distributed about a well defined mean, suggesting that the analysis of multiple translocations through a pore can be used to improve estimates of the length of long polymers.

[1]This work was supported by Intel Corporation and NSF through grant CBET-0846505.

8:12AM V43.00002 DNA translocation through a solid-state nanopore coated with a self-assembled monolayer , BINQUAN LUAN, GUSTAVO STOLOVITZKY, GLENN MARTYNA, IBM RESEARCH TEAM — The translocation of DNA through a solid-state nanopore can be dramatically affected by surface properties of a pore, such as charge density, roughness and hydrophobicity, since the pore surface serves as a boundary for the hydrodynamic flow accompanying with DNA motion. Recent experiment demonstrated the coating of a self-assembled monolayer (SAM) on the surface of a nanopore, allowing an active control on the surface property. Using all-atom molecular dynamics simulation, we investigated the tribological effect on DNA translocation through a solid-state nanopore coated with a SAM. When DNA is confined to the center of a pore, i.e. no direct interaction between DNA and pore surface, charge density and roughness of a pore surface can affect electroosmotic and hydrodynamic flows inside a nanopore, respectively. When allowing direct interaction between DNA and a SAM, adhesive interaction via hydrogen bonds can substantially increase friction force on DNA during translocation but repulsive interaction permits a fast translocation of DNA. We found two types of motion of DNA, stick-slip and steady-sliding, that are qualitatively explained using a Langevin-like model.

8:24AM V43.00003 Nanopore DNA translocation studies of tri-oligomer DNA with two hybridization segments[1] , VENKAT BALAGURUSAMY, PAUL WEINGER, XINSHENG LING, Brown University — We have earlier detected 12-base hybridizations in trimer DNA complexes formed by three single-stranded DNA oligomers hybridized at their ends sequentially, using nanopores of ∼ 10 nm diameter [1]. These complexes are connected to a polystyrene bead at one end to slow down their translocation. Here, we report translocation experiments at different voltages with nanopores ∼ 5 nm diameter. The measured time lapses between the passage of consecutive double-strand DNA segments in a trimer complex allow us to study the translocation dynamics. The measured mean-first-passage time between two consecutive hybridization segments is found to be consistent with theoretical estimates based on the Fokker-Planck equation.

[1] V.S.K.Balagurusamy, P.Weinger and X.S.Ling, *Nanotechnology* 21, 335102 (2010).

[1]This work was supported by a R21 grant from the NIH-NHGRI.

8:36AM V43.00004 Dehydration and Ionic Conductance Quantization in Synthetic Nanopores[1]

, JAMES WILSON, University of California San Diego, MICHAEL ZWOLAK, MASSIMILIANO DI VENTRA — Synthetic nanopores and nanochannels create new opportunities - beyond biological ion channels - to study ionic transport at the nanoscale. One process that occurs at this scale is dehydration. Ions in water do not move freely, but are instead surrounded by tightly bound water molecules held by the charge-dipole interaction. These water molecules are organized into hydration layers. For the ion to move through a nanopore of sufficiently small radius, these hydration layers must be shed as there is not enough space within the pore to accommodate them. We use molecular dynamics simulations to develop a model of dehydration based on the energy cost associated with removing water molecules. We predict that the ionic current would show sudden drops as the pore radius is reduced due to the exclusion of the hydration layers. We also examine the effect of both the sign and magnitude of the ion charge, demonstrating that divalent ions will more clearly exhibit the effect of dehydration on the ionic current.

[1] M. Zwolak, J. Wilson, and M. Di Ventra, J. Phys.: Condens. Matter 22, 454126 (2010); See also M. Zwolak and M. Di Ventra, Phys. Rev. Lett. 103, 128102 (2009)

[1]Work supported in part by NIH.

8:48AM V43.00005 Nanowire-nanopore transistor sensor for DNA detection during translocation

, PING XIE, Harvard University, QIHUA XIONG, Nanyang Technological University Singapore, YING FANG, National Center for Nanoscience and Technology China, QUAN QING, CHARLES LIEBER, Harvard University — Nanopore sequencing, as a promising low cost, high throughput sequencing technique, has been proposed more than a decade ago. Due to the incompatibility between small ionic current signal and fast translocation speed and the technical difficulties on large scale integration of nanopore for direct ionic current sequencing, alternative methods rely on integrated DNA sensors have been proposed, such as using capacitive coupling or tunnelling current etc. But none of them have been experimentally demonstrated yet. Here we show that for the first time an amplified sensor signal has been experimentally recorded from a nanowire-nanopore field effect transistor sensor during DNA translocation. Independent multi-channel recording was also demonstrated for the first time. Our results suggest that the signal is from highly localized potential change caused by DNA translocation in none-balanced buffer condition. Given this method may produce larger signal for smaller nanopores, we hope our experiment can be a starting point for a new generation of nanopore sequencing devices with larger signal, higher bandwidth and large-scale multiplexing capability and finally realize the ultimate goal of low cost high throughput sequencing.

9:00AM V43.00006 How to improve the sensitivity in transverse electronic measurements of DNA for nucleobase distinction?

, YUHUI HE, MING LIU, Institute of Microelectronics, Chinese Academy of Sciences, Beijing, China, ANTON GRIGORIEV, RALPH H. SCHEICHER, Cond. Mat. Theory Group, Dept of Physics and Astronomy, Uppsala University, Sweden, RAJEEV AHUJA, CMT Group at Uppsala; Dept of Mat. Sci. and Eng., Royal Inst. of Tech. (KTH), Stockholm, Sweden — In an attempt to realize third-generation whole-genome sequencing technologies, nanopores have been at the center of the research focus. Key issues with this approach involve how to slow down the translocation speed of DNA and how to achieve single-base resolution. We have previously proposed [arXiv:0708.4011; J. Phys. Chem. C 112, 3456 (2008)] the use of functionalized nanopore-embedded gold electrodes to address both these issues. More recently, we demonstrated [Appl. Phys. Lett. 97, 043701 (2010)] through molecular dynamics and electron transport simulations that the transverse differential conductance of a translocating DNA may allow for distinction between the four bases and can withstand electrical noise caused by DNA structure fluctuations. Our findings demonstrate several advantages of the transverse conductance approach, which may lead to realistic applications in rapid genome sequencing.

9:12AM V43.00007 Novel effects of chain flexibility, external force, and background stochasticity on polymer translocation[1]

, WOKYUNG SUNG, POSTECH — The polymer translocation through membranes and the polymer crossing over activation barriers in general, are ubiquitous in cell biology and biotechnological applications. Because they are interconnected flexible systems, polymers in translocation incur entropic barriers but can thermally surmount them with unusual sensitivity to background biases. In the presence of non-equilibrium noises characteristic of living environments, the translocation can speed up much when resonant activation occurs. As a related issue, I will also discuss the problem of polymer surmounting a potential barrier, where the chain flexibility enhances the crossing. Furthermore, when the chain flexibility leads to conformational changes, the crossing rate can be even more dramatically increased. This conformational flexibility and variability enhance the stochastic resonance, where the chain crossing dynamics at an optimal temperature and chain length is maximally coherent and resonant to a minute periodic force. Utilizing the self-organizing behaviors mentioned above, we may learn about bio-molecular machinery of living as well as clever means of manipulating it.

[1] W. Sung and P. J. Park, Phys. Rev. Lett. **77**, 783 (1996)
[2] J. J. Kasianowicz, E. Branton and D. W. Deamer, Proc. Natl. Acad. Sci. USA **89**,13370(1996)
[3] P. J. Park and W. Sung, J. Chem. Phys. **111**, 5239 (1999)
[4] M. Asfaw and W. Sung, Euro. Phys. Lett. **90**, 30008 (2010)

[1]Korea Research Foundation

9:48AM V43.00008 Simulations of Single DNA Nucleotide Transport Through Nanoslits[1]

, BRIAN NOVAK, KAI XIA, DOREL MOLDOVAN, DIMITRIS NIKITOPOULOS, Louisiana State University, Mechanical Engineering, STEVEN SOPER, Louisiana State University, Chemistry and Mechanical Engineering — Transport of single molecules in nano-scale geometries might be used to identify them via their flight times. The motion of nucleotides in aqueous NaCl solution flowing through atomically smooth nanoslits composed of disordered carbon atoms was studied using nonequilibrium molecular dynamics simulations. The fluid was driven by gravity-like forces or the nucleotide was moved electrophoretically. Velocities were on the order of 1 m/s or 3 m/s, respectively. The relatively hydrophobic base parts of the nucleotides adsorbed to the walls multiple times while moving along the slit. The bases tended to adsorb/desorb with the sugar end of the base contacting the surface last/first. The distance required for separation of the flight time distributions (required channel length) was 8.8 μm for the gravity case. In the electrophoretic case with this surface, the nucleotides moved nearly as fast while adsorbed as while desorbed which made the separation more difficult than in the gravity case.

[1]Work supported in part by NSF-EPSCoR Grant # EPS-1003897 (LA-SiGMA) and by LONI.

10:00AM V43.00009 Heat Treatment to Shrink Solid-State Nanopores[1]

, JOSEPH BILLO, WASEEM ASGHAR, SAMIR M. IQBAL, Department of Electrical Engineering, Nanotechnology Research and Teaching Facility, University of Texas at Arlington — Solid-state nanopores have a promising application in the area of selective sensing of DNA. Therefore, it is imperative to have a simple and repeatable method for nano-fabrication of pores. This paper focuses on solid-state nanopore fabrication in a silicon-dioxide membrane with heat treatment. A 375 μm thick pre-oxidized silicon wafer with approximately 1 μm oxide is used. Photolithography followed by BHF etching, with well-cured photo-resist covering the back-side to preserve its oxide layer, was performed on the wafer in order to open square windows in the front-side oxide layer. Using the front-side oxide layer as a mask and the back-side oxide layer as an etch-stop, the silicon substrate underwent anisotropic etching to create SiO_2 membranes. The wafer was then cut into small squares approximately 1 cm on a side with each containing one membrane. A focused ion beam was used to open an initial pore in each membrane. Finally, a method for causing SiO_2 membranes to diffuse was used to shrink the pores to the desired diameter.

[1]This work was supported by the Metroplex Research Consortium for Electronic Devices and Materials, Dallas, TX.

10:12AM V43.00010 The Nanofluidic Field-Effect in Electrically Actuated Nanopores[1] , ZHIJUN JIANG, DEREK STEIN, Physics Dept., Brown University — We employed high-resolution milling techniques to create solid-state nanopores with integrated electrodes for exerting field-effect control over the transport of ions and single DNA molecules in solution. An embedded, annular gate electrode was used to voltage gate the ionic conductance through a nanopore. An absence of leakage currents confirms the electrostatic origin of this effect. The measurements also reveal strong dependencies on the pH and on the ionic strength of the fluid. These results reflect the crucial difference between the modulation of charge at a solid-liquid interface where surface chemistry plays an important role, versus at a chemically inert semiconductor interface. An electrochemical model of electrofluidic gating that captures the gate-field-induced shift in the chemical equilibrium of the ionizable surface groups describes our measurements quantitatively. We seek to electrostatically control the translocation of DNA through such gated nanopores, and thereby mimic the single-molecule regulatory capabilities of biological transmembrane channels.

[1]This work was supported by the NSF under grant DMR-0805176.

10:24AM V43.00011 FIB direct fabrication of sub-10 nm synthetic nanopores , JACQUES GIERAK, ALI MADOURI, ERIC BOURHIS, JEAN-YVES MARZIN, LPN-CNRS, GHANI OUKHALED, LAURENT BACRI, BENJAMIN CRESSIOT, JUAN PELTA, MPI-LAMBE, RALF JEDE, LARS BRUCHHAUS, Raith, LOÏC AUVRAY, MSC, LPN TEAM, MPI-LAMBE TEAM, RAITH TEAM, MSC TEAM — Nanopores in thin solid state membranes are used as single molecule electronic detectors or sensors. The membrane acts as a dividing wall in an electrolytic cell and draws charged molecules attracted by an electric field through the pore. Among the very few patterning techniques applicable to nanopores, one promising approach is to use a FIB system, which can produce small holes directly at specified locations with customized organization and shape into dielectric membranes. We detail an innovative FIB-based approach and the methodologies developed for sub-10 nm nanopore realization. Our method allows direct fabrication of nanometer-sized pores in relatively large quantities with excellent reproducibility. This approach offers the possibility to further process or to functionalize each pore on the same scale keeping the required nm-scaled positioning and patterning accuracies, for i.e. adding detection marks or local membrane thinning at nanopore site. Then we describe solutions for conditioning surface properties and for integrating such single nanopore devices for translocation experiments. Results involving DNA, proteins, polymers, colloids are presented.

10:36AM V43.00012 Incremental Mean First Passage Analysis of Unbiased Polymer Translocation[1] , GARY W. SLATER, HENDRICK W. DE HAAN, University of Ottawa — To provide a measure of how translocation progresses, we have recently developed a method of mapping the process as a series of mean first passage processes of increasing displacement. Starting with a simplified, "quasi-static" model of translocation, exact numerical and analytic calculations using this Incremental Mean First Passage Time (IMFPT) approach yield insight into the robustness of the scaling of the translocation time τ with polymer length N given by $\tau \sim N^2$ as predicted in early theoretical studies of translocation. This approach reveals fundamental differences in the dynamics between absorbing and reflective boundary conditions when only one monomer is in the pore - both experimentally relevant scenarios. IMFPT is also applied to Langevin Dynamics simulations of a full polymer to test the impact of including features neglected in the simplified model. While the scaling for much of the process is now $\tau \sim N^{2.2}$ due to internal degrees of freedom, the exponent as measured by only the net translocation time is shown to depend greatly on the details of the simulation setup as a result of non-equilibrium effects.

[1]Funded by NSERC.

10:48AM V43.00013 Nanoscale fluid transportation through individual carbon nanotubes[1] , JIN HE, DI CAO, PEI PANG, TAO LUO, STUART LINDSAY, the Biodesign Institute, Arizona State University, PREDRAG KRISTIC, Oak Ridge National Laboratory, COLIN NUCKOLLS, Chemistry Department, Columbia Universtiy — There are great interest in both simulation and experiment of fluid flow on the nanoscale. Carbon nanotubes, with their extremely small inner diameter (usually below 2 nm) and atomic smooth inner surface, are ideal materials for studying nanoconfinement and ion and molecule nanoscale translocation. The excellent electrical properties of CNTs can also be integrated to achieve nanoelectrofluidic device. This presentation describes our recent progress in studying fluid transport through individual carbon nanotubes, including simultaneously ionic and electronic measurements during water, ion and molecule translocation.

[1]This work was supported by the DNA Sequencing Technology Program of the National Human Genome Research Institute (1RC2HG005625-01, 1R21HG004770-01)

Thursday, March 24, 2011 8:00AM - 11:00AM –

Session V44 DMP DPOLY: Focus Session: Organic Electronics and Photonics – Small molecule semiconductors and molecular electronics A309

8:00AM V44.00001 The Electronic Structure of a Local Charge-Transfer-Induced Spin Transition Molecular Adsorbate , XIN ZHANG, Nebraska Center for Materials and Nanoscience, Department of Physics and Astronomy, University of Nebraska-Lincoln, NING WU, ZHENGZHENG ZHANG, JEAN-FRANÇOIS LÉTARD, FRANÇOIS GUILLAUME, Université Bordeaux I, France, BERNARD DOUDIN, Université Louis Pasteur Strasbourg, FRANCE, PETER DOWBEN, University of Nebraska-Lincoln, UNIVERSITY OF NEBRASKA-LINCOLN COLLABORATION, UNIVERSITÉ BORDEAUX I COLLABORATION, UNIVERSITÉ LOUIS PASTEUR STRASBOURG COLLABORATION — The spin crossover phenomena has been identified in the [Fe(H_2B(pz)$_2$) bpy] where pz=(1-pyrazolyl)borate [Fe(H_2B(pz)$_2$) bpy], and but there is currently a lack of knowledge of the physical nature of this phenomena and the electronic structure of this organometallic compound has not been well characterized. We have investigated the interface electronic characteristics of molecular thin films of the metal-organic [Fe(H_2B(pz)$_2$) bpy] by ultraviolet photoelectron spectroscopy (UPS) and inverse photoemission (IPES). X-ray absorption spectroscopy (XAS) and Infrared spectroscopy (IR spectroscopy) were also used to study [Fe(H_2B(pz)$_2$) bpy]. The IPES results coincide with XAS, and the model calculations. The molecular vibrational modes have been identified from a comparison of the IR spectroscopy with model calculations.

8:12AM V44.00002 Raman scattering studies of organic semiconducting charge-transfer compounds , LAURIE MCNEIL, University of North Carolina at Chapel Hill, CHRISTIAN KLOC, Nanyang Technological University (Singapore) — Organic semiconductors offer the possibility of devices with greater mechanical flexibility and lower production costs compared to existing materials. Reports of carrier mobilities in monomolecular organic semiconductors in the 10-50 cm^2/V-s range and success in fabricating electronic devices from organic materials has increased the interest in their properties for electronic applications. However, the range of properties displayed by the monomolecular crystals is rather narrow. Charge-transfer compounds composed of two different organic molecules in which one acts as a donor and the other as an acceptor may represent the next generation of organic semiconductors. Control of their properties by modification of the molecules or changes in stoichiometry and crystalline structure makes them particularly attractive for a wide range of applications provided that the relationship between the structure and constituents of the compounds and their physical properties can be elucidated. Raman scattering studies of single crystals of two representative charge-transfer compounds, perylene-TCNQ and anthracene-TCNQ, will be presented. Theoretical calculations suggest that these materials have the potential for ambipolar charge transport, and so intermolecular interactions in these compounds are of particular interest.

8:24AM V44.00003 Observation of optically forbidden states in $PC_{60}BM$ due to interfacial distortion , HEMANT SHAH, BRUCE ALPHENAAR, University of Louisville — PCBM is a fullerene derivative used extensively in organic solar cells. $PC_{60}BM$ shows strong absorbance at wavelengths below 400 nm. A series of sub-gap transitions exist, but are symmetry forbidden in C_{60}, and only weakly observed in the $PC_{60}BM$ absorbance. Recent theoretical calculations predict that the symmetry rules for C_{60} can be lifted by the proximity of a metallic substrate due to perturbation of the electronic spatial distribution. Here we describe capacitive photocurrent measurements of $PC_{60}BM$ in which the optically forbidden features are strongly observed. In agreement with the theoretical predictions, this is thought to be due to the influence of a high conductivity ITO layer in contact with the $PC_{60}BM$. The influence of the ITO is tested by introducing a thin insulator (Al_2O_3) of varying thickness between the $PC_{60}BM$ and the ITO. The photocurrent due to the symmetry forbidden states drops strongly compared to the above gap photocurrent with increasing separation. Implications of these results on the polythiophene/fullerene blends will also be discussed. DOE-3048103802-08-073, NSF- DMR-0906961

8:36AM V44.00004 Free exciton emission and vibrations in pentacene monolayers[1] , RUI HE, Columbia University — Pentacene is a benchmark organic semiconductor material because of its potential applications in electronic and optoelectronic devices. Recently we demonstrated that optical and vibrational characterizations of pentacene films can be carried out down to the sub-monolayer limit. These milestones were achieved in highly uniform pentacene films that were grown on a compliant polymeric substrate. Films with thickness ranging from sub- monolayer to tens of monolayers were studied at low temperatures. The intensity of the free exciton (FE) luminescence band increases quadratically with the number of layers N when N is small. This quadratic dependence is explained as arising from the linear dependence of the intensity of absorption and the probability of emission on the number of layers N. Large enhancements of Raman scattering intensities at the FE resonance enable the first observations of low-lying lattice modes in the monolayers. The measured low- lying modes (in the 20 to 100cm^{-1} range) display characteristic changes when going from a single monolayer to two layers. The Raman intensities by high frequency intra-molecular vibrations display resonance enhancement double-peaks when incident or scattered photon energies overlap the FE optical emission. The double resonances are about the same strength which suggests that Franck-Condon overlap integrals for the respective vibronic transitions have the same magnitude. The interference between scattering amplitudes in the Raman resonance reveals quantum coherence of the symmetry-split states (Davydov doublet) of the lowest intrinsic singlet exciton. These results demonstrate novel venues for ultra-thin film characterization and studies of fundamental physics in organic semiconductor structures.

[1]In collaboration with Nancy G. Tassi (Dupont), Graciela B. Blanchet (Nanoterra, Cambridge, MA), and Aron Pinczuk (Columbia University)

9:12AM V44.00005 The interaction of charge carriers with lattice phonons in oligoacene crystals , VEACESLAV COROPCEANU, YUAN LI, YUANPING YI, ROBERT BROWN, JEAN-LUC BREDAS, Center for Organic Photonics and Electronics and School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332-0400, USA — We use density functional theory calculations to investigate the non-local electron-phonon interactions between charge carriers and lattice phonons (i.e., the modulation of transfer integrals by vibrations) in oligoacene crystals as a function of molecular size from naphthalene through pentacene. The results point to a significant coupling to both translational and librational intermolecular phonon modes as well as to intra-molecular vibrational modes. The impact of the interplay among these mechanisms on charge transport is investigated by treating the lattice dynamics classically. The impact of quadratic electron-phonon interaction on charge transport is studied as well.

9:24AM V44.00006 Spectroscopy of organic semiconductors from first principles , SAHAR SHARIFZADEH, Molecular Foundry, LBL, ARIEL BILLER, LEEOR KRONIK, Weizmann Institute of Science, JEFFERY NEATON, Molecular Foundry, LBNL — Advances in organic optoelectronic materials rely on an accurate understanding their spectroscopy, motivating the development of predictive theoretical methods that accurately describe the excited states of organic semiconductors. In this work, we use density functional theory and many-body perturbation theory (GW/BSE) to compute the electronic and optical properties of two well-studied organic semiconductors, pentacene and PTCDA. We carefully compare our calculations of the bulk density of states with available photoemission spectra, accounting for the role of finite temperature and surface effects in experiment, and examining the influence of our main approximations – e.g. the GW starting point and the application of the generalized plasmon-pole model – on the predicted electronic structure. Moreover, our predictions for the nature of the exciton and its binding energy are discussed and compared against optical absorption data. We acknowledge DOE, NSF, and BASF for financial support and NERSC for computational resources.

9:36AM V44.00007 Angle resolved photoemission study of rubrene single crystal , YONGLI GAO, HUANJUN DING, IRFAN IRFAN, University of Rochester, COLIN REESE REESE, Stanford University, ANTTI MAKINEN, Naval Research Laboratory, ZHENAN BAO, Stanford University — We report the direct experimental observation of the band structure of a bulk organic single crystal. The electronic structure of rubrene single crystal grown by physical vapor transport method was studied with angle-resolved photoemission spectroscopy. Highly reproducible dispersive features were observed with nice symmetry about the Brillouin zone center and boundaries, representing the band structure measured for a bulk organic single crystal. The high quality of the surface was confirmed with scanning tunneling microscopy. The energy dispersion of the highest occupied molecular orbitals derived bands showed strong anisotropic behavior in the a-b plane of the unit cell. The measured band structure, however, differs unexpectedly from theoretical calculations in terms of the amount of the dispersion and the separation of the bands.

9:48AM V44.00008 Charge localization and inhibition of self-assembly in tetraphenyl porphyrin on Cu(111) , GEOFFREY ROJAS, XUMIN CHEN, DONNA KUNKEL, JIE XIAO[1], PETER A. DOWBEN, AXEL ENDERS, University of Nebraska-Lincoln, ENDERS RESEARCH TEAM, DOWBEN RESEARCH TEAM — A study of the nature of the electronic structure and inter-molecular interaction of the adsorbed tetraphenyl porphyrin (H_2TPP)/Cu(111) system using scanning tunneling spectroscopy (STS) and inverse photoemission spectroscopy (IPES) is presented. By studying STS and IPES spectra as a function of increasing coverage, significant upshifts in the local shockley surface state near the adsorbate as a well interfacial HOMO-LUMO gap state are observed in monolayer-thick films. This, combined with observations of changes in the local workfunction and distortions of the Cu(111) surface within 1 Å of the molecules, indicates strong molecule-interface electronic interaction and stronger bonding. Such strong electron transfers and resulting charge dipoles are the origin of observed inter-molecular Coulomb repulsion, thereby preventing self-assembly of first-monolayer H_2TPP/Cu(111) systems, while allowing for self-assembly of second-monolayer and higher, where no such surface states are observed.

[1]Now at the University of Erlangen-Nuremberg

10:00AM V44.00009 Scanning Tunneling Spectroscopy measurements of the Electronic Structure of C60 films on the Cu(100) surface[1] , D.R. DAUGHTON, J.A. GUPTA, The Ohio State University, Department of Physics — Successful implementation of organometallic electronic and photoelectronic device architectures requires understanding and engineering of molecule-electrode interfaces. Here we investigate the electronic structure of a monolayer film of C60 on a Cu(100) surface with low temperature (5 K) scanning tunneling microscopy (STM) and spectroscopy. C60 adopts four unique orientations on the Cu(100) surface, and shifts in the molecular orbital resonances for the four geometries indicate different degrees of electronic molecule-surface hybridization. At higher bias, Stark-shifted image state resonances are shown to spatially vary across the molecular film. Modulation of the image state energies are attributed to shifts in the interfacial dipole that derive from the interplay of interfacial charge transfer, surface reconstruction, and orientational ordering of the molecular film. These observations suggest the need for nanoscale interface characterization for optimizing the performance of molecular electronic devices.

[1]Funding by the Arnold and Mabel Beckman Foundation.

10:12AM V44.00010 Highly Conducting Contacts for Single Molecule Transport Measured by STM-Break Junction[1] , JONATHAN R. WIDAWSKY, ZHAN-LING CHENG, RACHID SKOUTA, SEVERIN T. SCHNEEBELI, HECTOR VAZQUEZ, MARK S. HYBERTSEN, RONALD BRESLOW, LATHA VENKATARAMAN, Columbia University and CFN, Brookhaven National Laboratory — We present a novel method to directly link single alkane chains to gold electrodes using trimethyl tin ($SnMe_3$) linkers. We characterize electron transport through single molecule junctions using the STM-based break-junction technique, where a gold point contact is repeatedly formed and broken in a solution of the $SnMe_3$-alkanes while conductance is measured. Based on analysis of more than 10,000 individual junctions, we find that we create single molecule junctions which are $\sim$100 times more conducting than those with alkanes terminated with any other linker previously studied. The contact resistance, determined by extrapolating to zero carbons, is 4kΩ, two orders of magnitude lower than analogous values found using amine linkers. Strong evidence supports the hypothesis that *in situ* cleaving of the $SnMe_3$ end groups facilitates the formation of a direct bond between the carbon backbone and gold leads, thereby enhancing conductance. We corroborate this result by comparing the conductance of junctions formed from SnMe3- and Ph_3PAu-terminated benzenes.

[1]Funded Primarily by NSEC Prog. of NSF under Grant CHE-0641523

10:24AM V44.00011 34 nm Charge Transport through DNA[1] , JASON SLINKER, The University of Texas at Dallas, NATALIE MUREN, SARA RENFREW, JACQUELINE BARTON, California Institute of Technology — Long-range charge transport through DNA has broad-reaching implications due to its inherent biological recognition capabilities and unmatched capacity to be patterned into precise, nanoscale shapes. We have observed charge transport through 34 nm DNA monolayers (100 base pairs) using DNA-mediated electrochemistry. Cyclic voltammetry of multiplexed gold electrodes modified with 100mer DNAs reveal sizable peaks from distally-bound Nile Blue redox probes for well matched duplexes but highly attenuated redox peaks from 100mer monolayers containing a single base pair mismatch, demonstrating that the charge transfer is DNA-mediated. The 100mers on the gold surface are efficiently cleaved by the restriction enzyme RsaI. The 100mers in the DNA film thus adopt conformations that are readily accessible to protein binding and restriction. The ability to assemble well-characterized DNA films with these 100mers permits the demonstration of charge transport over distances surpassing most reports of molecular wires.

[1]Supported by funding from the NIH/NIBIB.

10:36AM V44.00012 Electrical properties of metal-molecule-silicon structures with varying molecular backbones, dipoles, and atomic tethers , CURT A. RICHTER, NADINE GERGEL-HACKETT, MARIONA COLL, CHRISTINA A. HACKER, Semiconductor Electronics Division, NIST — We present the results of an extensive experimental investigation of metal-monolayer-silicon junctions. By varying the molecular dipole, the molecular backbone, the Si-molecule linkage, and the Si-doping, we indentified critical features that determine the electrical transport and injection properties of the junctions. Two basic structures were used. One is an enclosed planar structure in which an organic monolayer is directly assembled on silicon and contacted with evaporated silver. The other was made via Flip Chip Lamination, a novel approach that relies on the formation of monolayers on a gold surface first, which enables the study of a wider range of molecular layers on silicon of very high-quality. Two charge transport regimes dominate: (1) a Schottky barrier limited regime where the molecular dipole results in silicon band bending at the junction interface, and (2) a tunneling regime where the molecular dipole creates a small local electric field that screens the electrical transport. Transition Voltage spectroscopy was used to identify electrical differences between π-conjugated and alkyl backbones attributed to the extended π-delocalization and variations due to the chemical nature of Si-atom linkage.

10:48AM V44.00013 Engineering controlled Au/GaAs junctions with partial molecular monolayers , C. MARGINEAN, J.P. PELZ, The Ohio State University, H. HAICK, D. CAHEN, Weizmann Institute — Advances in molecular electronics offer the possibility to use molecular-based components to enhance integrated circuits and other electronic devices. Therefore, the studies of the electronic transport properties of junctions containing molecular layers are of great interest. The local hot-electron transmittance at buried metal-dicarboxylic acid-semiconductor [1] interfaces was directly investigated with nanometer spatial resolution and meV- level energy resolution using BEEM by spatially mapping hot-electrons that were injected into the top metal thin film and passed through the diode [2]. That study found that the dominant electronic transport mechanism for some dicarboxylic ligands was though pinholes rather than direct tunneling through the molecular film, and that the effective Schottky barrier height (SBH) at the pinholes was increased by a negative electric dipole moment in the surrounding molecular film [2]. We present the results of finite element electrostatic calculations of Au/discontinuous-molecular film/GaAs structures with both positive and negative dipole films, and show that the expected decrease (or increase) of the effective SBH is consistent with BEEM measurements of these types of samples. Work supported by NSF Grant No. DMR-0805237. [1] H. Haick et al., Adv. Mater. 16, 2145 (2004). [2] H. Haick, et. al., Phys. Stat. Sol. (A) 2031, 3438 (2006).

Thursday, March 24, 2011 8:00AM - 10:48AM –

Session V45 DAMOP: Rotation and Artificial Gauge Fields: Vortices and Quantum Hall Physics

A310

8:00AM V45.00001 Acoustic Hawking radiation in dynamically expanding Bose-Einstein condensate , TAKAO MORINARI, Yukawa Institute for Theoretical Physics, Kyoto University — Black holes are not just an absorver but emit radiation. Verification of this phenomenon, called Hawking radiation, for real black holes is almost hopeless because the characteristic temperature is much lower than the cosmic microwave background radiation. There are attempts to verify Hawking radiation physics using acoustic black holes. In this paper, I will present a numerical simulation result for a dynamically expanding Bose-Einstein condensate of cold atoms. The result shows that the radiation spectrum obeys the Planck distribution function with the temperature on the order of 0.1nK and the particle creation occurs near the horizon. I will discuss the result from the view point of the phase coherence of Bose-Einstein condensate.

8:12AM V45.00002 Interferometry with Synthetic Gauge Fields[1] , BRANDON ANDERSON, JACOB TAYLOR, VICTOR GALITSKI, University of Maryland and Joint Quantum Institute — We propose a compact atom interferometry scheme for measuring weak, time-dependent accelerations. Our proposal uses an ensemble of dilute trapped bosons with two internal states that couple to a synthetic gauge field with opposite charges. The trapped gauge field couples spin to momentum to allow time dependent accelerations to be continuously imparted on the internal states. We generalize this system to reduce noise and estimate the sensitivity of such a system to be $S \sim 10^{-7} \frac{\mathrm{m/s^2}}{\sqrt{\mathrm{Hz}}}$.

[1]US-ARO and JQI

8:24AM V45.00003 Pulling Fluxes Away from Particles in Quantum Hall States of Atomic Gases[1] , WEIRAN LI, TIN-LUN HO, The Ohio State University — Quantum Hall states are often described as states with magnetic fluxes attached to the particles. In the case of rapidly rotating atomic gases, we show that by deforming the trapping potential of a rotating cluster, one can in fact pull the fluxes away from the particles in their quantum Hall state, as a consequence of the balance between rotational energy and interaction energy. This phenomenon can be revealed clearly from the density profile of the clusters after releasing the atoms from the trap, as well as from photoassociation experiments which measure the short range correlations.

[1]Work supported by Grants from DARPA and ARO through the OLE Program

8:36AM V45.00004 Lattice Quantum Hall Effect , LAYLA HORMOZI, Joint Quantum Institute, NIST and University of Maryland, GUNNAR MOLLER, University of Cambridge, STEVEN SIMON, University of Oxford — We study the groundstate of a two-dimensional system of interacting ultra-cold atoms (bosons and fermions), trapped in the periodic potential of an optical lattice, under the influence of a strong synthetic magnetic field. In the absence of inter-particle interactions, the energy spectrum is depicted by the Hofstadter butterfly — a fractal structure seemingly very different from the Landau levels in the continuum. However, when the number of flux quanta per lattice cell is close to a rational fraction, the energy splittings in the Hofstadter butterfly resemble Landau levels. Inspired by this similarity we establish a mapping between the wavefunctions of the non-interacting system in the lattice near rational fractions and the corresponding wavefunctions in the continuum. Using these single-particle wavefunctions we calculate pseudopotential coefficients for the interacting system. These effective interaction potentials can then be used to construct trial wavefunctions for the groundstate of the interacting system on a lattice. For the case of bosons with contact interaction, in addition to the interaction obtained by Palmer et al. [1], we find anomalous terms in the pseudopotential coefficients resembling the umklapp process.
[1] R. N. Palmer, A. Klein and D. Jaksch, Phys. Rev. A 78, 013609 (2008).

8:48AM V45.00005 Fractionalization via Z_2 Gauge Fields at a Cold Atom Quantum Hall Transition , YAFIS BARLAS, KUN YANG, National High Magnetic Field Laboratory — We study a single species of fermionic atoms in an "effective" magnetic field at total filling factor $\nu_f = 1$, interacting through a p-wave Feshbach resonance, and show that the system undergoes a quantum phase transition from a $\nu_f = 1$ fermionic integer Quantum Hall state to $\nu_b = 1/4$ bosonic fractional Hall state as a function of detuning. The transition is in the $(2+1)$D-Ising universality class. We formulate a dual theory in terms of quasiparticles interacting with a Z_2 gauge field, and show that charge fractionalization follows from this topological quantum phase transition. The resultant effective theory contains the lattice Z_2 gauge theory action along with a "Hopf" term which encodes the quasiparticle statistics. The transition occurs in the Z_2 sector and is a confinement-deconfinement transition for the quasiparticles.

9:00AM V45.00006 Bogoliubov theory of interacting bosons on a lattice in a synthetic magnetic field , STEPHEN POWELL, RYAN BARNETT, Condensed Matter Theory Center and Joint Quantum Institute, University of Maryland, RAJDEEP SENSARMA, Condensed Matter Theory Center, University of Maryland, SANKAR DAS SARMA, Condensed Matter Theory Center and Joint Quantum Institute, University of Maryland — We present a theoretical study of the effect of a magnetic field on a bosonic superfluid in a tight-binding lattice, motivated by advances in the synthesis of gauge potentials for ultracold atoms. An analysis based on the magnetic symmetry group shows that the superfluid has simultaneous spatial order, and that this depends on commensuration between the magnetic field and lattice. We predict clear signatures of many-body effects in time-of-flight images, and use a Bogoliubov expansion to calculate quasiparticle spectra that may be measured using Bragg spectroscopy. This work has been supported by JQI-NSF-PFC, ARO-DARPA-OLE, and Atomtronics-ARO-MURI.

9:12AM V45.00007 How does a synthetic non-Abelian gauge field influence the bound states of two spin-$1/2$ fermions?[1] , JAYANTHA VYASANAKERE, VIJAY SHENOY, Indian Institute of Science, Bangalore — We study the bound states of two spin-$1/2$ fermions interacting via a contact attraction (characterized by the scattering length) in the singlet channel in $3D$ space in presence of a uniform non-Abelian gauge field. The configuration of the gauge field that generates a Rashba type spin-orbit interaction is described by three coupling parameters $(\lambda_x, \lambda_y, \lambda_z)$. For a generic gauge field configuration, the critical scattering length required for the formation of a bound state is *negative*, i.e., shifts to the "BCS side" of the resonance. Interestingly, we find that there are special high-symmetry configurations (e.g., $\lambda_x = \lambda_y = \lambda_z$) for which there is a two body bound state for *any* scattering length however small and negative. Our results show that the BCS-BEC crossover is drastically affected by the presence of a non-Abelian gauge field. We discuss possible experimental signatures of our findings both at high and low temperatures.

[1]Work supported by DST, India through Ramanujan grant

9:24AM V45.00008 Dynamic vortex unbinding following a quantum quench in bosonic mixtures , LUDWIG MATHEY, Joint Quantum Institute, KENNETH GUENTER, JEAN DALIBARD, Laboratoire Kastler Brossel, ENS, ANATOLI POLKOVNIKOV, Boston University, CHARLES CLARK, Joint Quantum Institute — We study the many-body dynamics of a mixture of two hyperfine states of bosonic atoms in 2D, following a pi/2-pulse. Using both a numerical implementation of the Truncated Wigner approximation and an analytical approach, we find that a dynamic phase transition can be triggered, in which the system relaxes from a superfluid to a disordered state via vortex unbinding. This process can be dynamically suppressed, which creates a long-lived metastable supercritical state. We discuss the realization and detection of these effects.

9:36AM V45.00009 Macroscopic superposition states of cold bosons in an asymmetric double well with Orbital Degrees of freedom[1] , MIGUEL-ANGEL GARCIA-MARCH, LINCOLN D. CARR, Colorado School of Mines — We study the dynamics of ultracold bosons in three-dimensional double wells when they are allowed either to condense in single-particle ground states or to occupy excited states. On the one hand, the introduction of second level single-particle states opens a range of new dynamical regimes. On the other, since the second level eigenstates can carry angular momentum, NOON-like macroscopic superposition (MS) states of atoms with non-zero angular momentum can be obtained. This leads to the study of the dynamics of atoms carrying vorticity while tunneling between wells. We obtain new tunneling processes, like vortex hopping and vortex-antivortex pair superposition along with the sloshing of atoms between both wells. The resulting vortex MS states are much more robust against decoherence than the usual NOON states, as all atoms in the vortex core region must be resolved, not just a single atom.

[1]L.D.C acknowledges support from the National Science Foundation under Grant PHY-0547845 as part of the NSF CAREER program. M.A.G.M acknowledges support by the Fulbright Commission, MEC, and FECYT.

9:48AM V45.00010 Optical Lattice Hamiltonians for Relativistic Quantum Electrodynamics , ELIOT KAPIT, ERICH MUELLER, Cornell University — We show how interpenetrating optical lattices containing Bose-Fermi mixtures can be constructed to emulate the thermodynamics of 2+1d quantum electrodynamics (QED3). We present a model of neutral atoms on planar lattices whose low energy effective action reduces to that of photons coupled to Dirac fermions. We overview the properties of QED3 and discuss how two of its most interesting features, chiral symmetry breaking and Chern-Simons physics, could be observed experimentally in our cold atom system.

10:00AM V45.00011 Vortex Dynamics and Hall Conductivity of Hard Core Bosons , ASSA AUERBACH, Technion - Israel Institute of Technology, NETANEL LINDNER, California Institute of Technolgoy, DANIEL AROVAS, University of California at San Diego — Magneto-transport of hard core bosons (HCB) is studied using an XXZ quantum spin model representation, appropriately gauged on the torus to allow for an external magnetic field. We find strong lattice effects near half filling. An effective quantum mechanical description of the vortex degrees of freedom is derived. Using semiclassical and numerical analysis we compute the vortex hopping energy, which at half filling is close to magnitude of the boson hopping energy. The critical quantum melting density of the vortex lattice is estimated at 6.5x10-5 vortices per unit cell. The Hall conductance is computed from the Chern numbers of the low energy eigenstates. At zero temperature, it reverses sign abruptly at half filling. At precisely half filling, all eigenstates are doubly degenerate for any odd number of flux quanta. We prove the exact degeneracies on the torus by constructing an SU(2) algebra of point-group symmetries, associated with the center of vorticity. This result is interpreted as if each vortex carries an internal spin-half degree of freedom ('vspin'), which can manifest itself as a charge density modulation in its core. Our findings suggest interesting experimental implications for vortex motion of cold atoms in optical lattices, and magnet-transport of short coherence length superconductors.

10:12AM V45.00012 Birefringent break up of Dirac fermions in a square optical lattice[1] , NAZANIN KOMEILIZADEH, KAMRAN KAVEH, PETER M. SMITH, MALCOLM P. KENNETT, Simon Fraser University — We introduce a model of spinless fermions on a square lattice in a spatially periodic magnetic field. This model has Dirac points in its spectrum when there is an average flux of half a flux quantum per plaquette. The dispersion in the vicinity of these Dirac points has the unusual feature that the double degeneracy of Dirac cones is broken. This corresponds to a situation in which the low energy excitations have two different "speeds of light." This is a consequence of broken chiral symmetry in the model, which occurs in the kinetic energy term, and hence leaves the spectrum gapless in the vicinity of the Dirac points. This chiral symmetry breaking is fundamentally different from spontaneous chiral symmetry breaking that leads to mass generation in field theoretic models. We investigate the effects of several perturbations on the spectrum such as staggered potentials, nearest neighbor interactions, and domain wall topological defects. We provide a physical setting in which this model might be realized, namely for fermions in an optical lattice in an artificial magnetic field.

[1]Supported by NSERC.

10:24AM V45.00013 Generation and Characterization of Free Electron Vortices , BENJAMIN MCMORRAN, AMIT AGRAWAL, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, IAN ANDERSON, Surface and Microanalysis Science Division, National Institute of Standards and Technology, GREGG GALLATIN, HENRI LEZEC, JABEZ MCCLELLAND, JOHN UNGURIS, Center for Nanoscale Science and Technology, National Institute of Standards and Technology — Free electron vortex beams – composed of electron wavefunctions imprinted with a helical phase – are remarkable for their unique topology, quantized orbital angular momentum, and magnetic moment. We recently produced free electron vortex beams in a transmission electron microscope (TEM) using nanofabricated diffraction holograms. We used this technique to generate well-defined free electron vortices in various orbital states, demonstrating beams with up to 100 $\hbar$ of orbital angular momentum per electron.The helical phase of the electrons was measured directly using interferometric techniques. The orbital magnetic moment of the electron vortex scales with the topological charge of the vortex, and leads to interesting behavior in magnetic fields. As one example of several immediate applications for the electron vortex beam, we discuss how these beams can provide elementally sensitive magnetic imaging capabilities in a TEM by using the transfer of quantized orbital angular momentum to induce preferred atomic excitations in a sample.

10:36AM V45.00014 Vortex structures in ultra-rapidly rotating two-component Bose-Einstein condensates[1] , C.-H. HSUEH, National Taiwan Normal University, I.-G. LIU, S.-C. GOU, National Changhua University of Education, W.C. WU, National Taiwan Normal University — We investigate the vortex structures in rotating two-component Bose-Einstein condensates with a rotating frequency larger than the harmonic trapping frequency. Representative cases for the three phases, miscible, symmetric phase-separated, and asymmetric phase-separated, are studied. It is shown that the three different phases are manifested in the vortex structures to which at the cannular region around the center, vortices of each component form an annular structure and interlace with those of the other component. To determine the vortex structure in an authentic equilibrium state, the result obtained via imaginary-time propagating method is used as the initial state of the stochastic Gross-Pitaevskii equation and one keeps it propagating until the density profile saturates.

[1]We acknowledge financial support from the NSC, Taiwan.

Thursday, March 24, 2011 11:15AM - 1:39PM –

Session W1 DCMP: Superconducting Qubits: Advances in Single-Shot QND Readout Ballroom A1

11:15AM W1.00001 DC-SQUID Quantum Non-Demolition Readout of Superconducting Flux Qubits , KEES HARMANS, Kavli Institute, Delft University of Technology — Extracting state information from a quantum system is a central theme in quantum mechanics. As the process of state extraction by a detector implies system-detector entanglement, reverse action from the detector onto the quantum object can not be avoided. Consequently, detectors that minimise this back action are crucial. For superconducting flux qubits [1] commonly a DC-SQUID detector is used, either in an AC dispersive scheme or in a switching mode. The latter can be by AC bifurcation or by direct DC switching. The DC approach combines simplicity in use with complexity in dynamical behaviour. This complexity results from the fast Josephson phase dynamics and the significant generation of quasi-particles in the dissipative detector ON-state. This gave rise to the long-standing belief that it can not act as a "good" detector. This includes it to fail as a Quantum Non-Demolition (QND) detector, i.e. the preservation of the state of the quantum object after a state readout. In a recent experiment for relatively weak qubit-SQUID interaction strength [2] we investigated the detection properties of such a DC-switching SQUID, finding a remarkably good QND fidelity. This was achieved by shunting the SQUID by a low-value resistor, thus strongly suppressing the generation of quasi-particles. Also the detector ON-time was minimised to a few tens of ns using a nearby cryogenic amplifier. The QND-ness was obtained from measuring the correlation between two successive readouts, and found to reach 75% QND fidelity. The weak qubit-detector interaction leads to a limited readout contrast. We will discuss the results as well as its consequences, including the potential for combining high contrast and good QND fidelity.

[1] J.E. Mooij et. al., Science **285**, 1036 (1999)
[2] T. Picot et. al., Phys. Rev. Lett. **105**, 040506 (2010)

11:51AM W1.00002 Novel approaches to high fidelity qubit state measurement in circuit quantum electrodynamics , ERAN GINOSSAR, Yale University — Qubit state measurement ('readout') in solid state systems is an open problem, which is currently the subject of intensive experimental and theoretical research. Achieving high fidelity in a single-shot measurement is an interesting quantum control problem, as well as an important component for the successful implementation of quantum information protocols. For superconducting qubits we can distinguish between linear dispersive and nonlinear methods, the latter relying on the bistability of a nonlinear resonator. In the context of circuit quantum electrodynamics, the transmon qubit is strongly coupled to a linear resonator and described by a generalized Jaynes-Cummings model (JCM) with external drive and dissipation. Recent novel approaches to achieve high-fidelity readout in the dispersive regime rely on the intrinsic nonlinearity of the JCM and its ultimate linearity in the high excitation regime. In the degenerate regime we rely on the photon blockade and precise transient dynamics of the system. This regime presents a theoretical challenge and the driven damped JCM model exhibits a dynamical phase transition. Another proposed approach extends the Josephson Bifurcation Amplifier and employs the dynamical effects of frequency chirping of the drive on the coupled qubit-resonator system. We will discuss the physics of these different regimes and describe the readout schemes which have been demonstrated by recent experiments and quantum simulations, as well as the role of quantum fluctuations and optimal control.

12:27PM W1.00003 Observation of quantum jumps in a superconducting quantum bit[1] , R. VIJAY, Quantum Nanoelectronics Laboratory, University of California, Berkeley CA 94720 — Superconducting qubit technology has made great advances since the first demonstration of coherent oscillations more than 10 years ago. Coherence times have improved by several orders of magnitude and significant progress has been made in qubit state readout fidelity. However, a fast, high-fidelity, quantum non-demolition measurement scheme which is essential to implement quantum error correction has so far been missing. We demonstrate such a scheme for the first time where we continuously measure the state of a superconducting quantum bit using a fast, ultralow-noise parametric amplifier. This arrangement allows us to observe quantum jumps between the qubit states in real time. The key development enabling this experiment is the use of a low quality factor (Q), nonlinear resonator to implement a phase-sensitive parametric amplifier operating near the quantum limit. The nonlinear resonator was constructed using a two junction SQUID shunted with an on-chip capacitor. The SQUID allowed us to tune the operating band of the amplifier and the low Q provided us with a bandwidth greater than 10 MHz, sufficient to observe jumps in the qubit state in real time. I will briefly describe the operation of the parametric amplifier and discuss how it was used to measure the state of a transmon qubit in the circuit QED architecture. I will discuss measurement fidelity and the statistics of the quantum jumps. I will conclude by discussing the implications of this development for quantum information processing and further improvements to the measurement technique.

[1]We acknowledge support from AFOSR and the Hertz Foundation

1:03PM W1.00004 Probing the quantum fluctuations of a nonlinear resonator with a superconducting qubit , PATRICE BERTET, CEA Saclay — Coupling a superconducting quantum bit to a superconducting resonator offers the opportunity to investigate the interaction between light and an atom in regimes hardly accessible otherwise [1]. Making the resonator nonlinear has enabled important recent progress in the readout of qubits. Indeed, when pumped by a microwave field of well-chosen amplitude and frequency, nonlinear resonators (NRs) provide parametric amplification close to the quantum limit. In other drive conditions, the intra-cavity field can take two stable values between which the resonator can switch stochastically. Both regimes have been shown to yield a high-fidelity qubit readout [2,3]. Qubits can also be used to obtain interesting insight into the physics of NRs. In this work we use a transmon qubit [4] coupled to such a pumped NR as a probe of its quantum fluctuations. The qubit-NR coupling is manifested by the appearance around the qubit spectral line of two sidebands that we interpret as processes in which the driven resonator fluctuations are effectively cooled down or heated with the assistance of the qubit. The ratio of the sidebands amplitudes gives thus a direct experimental access to the pumped NR effective temperature which is found to be in quantitative agreement with the theory, bringing a clear support to the quantum description of a driven nonlinear resonator [5].

[1] A. Wallraf, D. I. Schuster, A. Blais, L. Frunzio, R.-S. Huang, J. Majer, S. Kumar, S. M. Girvin and R. J. Schoelkopf, Nature 431 162 (2004).
[2] R. Vijay, D.H. Slichter, I. Siddiqi, arxiv:cond-mat/1009.2969.
[3] F. Mallet, F.R. Ong, A. Palacios-Laloy, F. NGuyen, P. Bertet, D. Vion, and D. Esteve, Nature Physics 5, 791-795 (2009).
[4] J. Koch, T.M. Yu, J.M. Gambetta, A.A. Houck, D.I Schuster, J. Majer, A. Blais, M.H. Devoret, S.M. Girvin, and R.J. Schoelkopf, Phys. Rev. A 76, 042319 (2007).
[5] M. Marthaler and M.I. Dykman, PRA 73, 042108 (2006).

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W2 DCMP: CVD Graphene: Synthesis, Properties and Applications Ballroom A2

11:15AM W2.00001 Chemical Vapor Deposition of Large-size Monolayer Graphene and Properties[1] , RODNEY RUOFF, The University of Texas at Austin — Graphene is of interest in part due to its electronic and thermal transport, mechanical properties including high stiffness and the possibility of high strength and toughness, high specific surface area, and that it can act as an atom thick layer, barrier, or membrane. Our top-down micromechanical exfoliation approaches conceived of in 1998 [1, 2] yielded multilayer graphene. Two main areas of our research are: (i) CVD growth of large area graphene films on metal substrates, characterization and properties of such films, and (ii) The generation, study, and use of colloids containing graphene-based platelets. We present our work on CVD growth of graphene on metal substrates, including the first achievement of large area growth of monolayer graphene [3], studies on understanding growth [related references: 3-6]. Properties such as TCE [7], thermal conductivity [8], and mechanical properties [related reference: 9], will be presented. An excellent review of graphene is [10]. A history of experimental work on graphene (from its discovery in 1969 until now) will be available on our web site: http://bucky-central.me.utexas.edu/ prior to the meeting. Ruoff group publications: http://bucky-central.me.utexas.edu/publications.htm.

[1] Tailoring graphite with the goal of achieving single sheets, Nanotechnology 10, 269-272 (1999).
[2] APL 75, 193-195 (1999).
[3] Large-area synthesis of high-quality and uniform graphene films on copper foils, Science 324, 1312-1314 (2009).
[4] Evolution of Graphene Growth on Ni and Cu by Carbon Isotope Labeling, Nano Letters 9, 4268 (2009).
[5] Synthesis, Characterization, and Properties of Large-Area Graphene Films, ECS Transactions 19, 41-52 (2009).
[6] Graphene Films with Large Domain Size by a Two-Step Chemical Vapor Deposition Process, Nano Letters, (2010).
[7] Transfer of large-area graphene films for high-performance transparent conductive electrodes, Nano Letters, 9, 4359-4363 (2009).
[8] Thermal Transport in Suspended and Supported Monolayer Graphene Grown by Chemical Vapor Deposition, Nano Letters, 10, 1645-1651 (2010).
[9] Mechanical Properties of Monolayer Graphene Oxide, ACS Nano, (2010).
[10] Graphene and Graphene Oxide: Synthesis, Properties, and Applications, Advanced Materials, 22, 3906-3924 (2010).

[1]Support of our work by DARPA, ONR, SWAN NRI, NSF, ARO, and AEC is appreciated.

11:51AM W2.00002 Roll-to-roll production of 30-inch graphene films for transparent electrodes[1] , BYUNG HEE HONG, Sungkyunkwan University — The outstanding electrical1, mechanical and chemical properties of graphene make it attractive for applications in flexible electronics. However, efforts to make transparent conducting films from graphene have been hampered by the lack of efficient methods for the synthesis, transfer and doping of graphene at the scale and quality required for applications. Here, we report the roll-to-roll production and wet-chemical doping of predominantly monolayer 30-inch graphene films grown by chemical vapour deposition onto flexible copper substrates. The films have sheet resistances as low as ∼125 Ohm/sq with 97.4% optical transmittance, and exhibit the half-integer quantum Hall effect, indicating their high quality. We further use layer-by-layer stacking to fabricate a doped four-layer film and measure its sheet resistance at values as low as ∼30 Ohm/sq at ∼90% transparency, which is superior to commercial transparent electrodes such as indium tin oxides. Graphene electrodes were incorporated into a fully functional touch-screen panel device capable of withstanding high strain.

[1]Work done in collaboration with Sukang Bae, Hyeongkeun Kim, Youngbin Lee, and Jong-Hyun Ahn, Sungkyunkwan University.

12:27PM W2.00003 Structural and electronic properties of graphene grown by chemical vapor deposition (CVD) , YONG CHEN, Purdue University — Graphene grown by chemical vapor deposition (CVD) has brought many exciting opportunities for both fundamental studies and practical applications. In this talk, I will present our studies of the structural and electronic properties of graphene synthesized by ambient CVD based growth on polycrystalline Ni and Cu foils. Our earlier work on graphene layers and large scale graphitic thin films grown on Ni and transferred to insulators [1,2] show that such films can have excellent electronic properties, despite their structural non-uniformity. We also characterized the wrinkles in such films, yielding insights on their growth and buckling processes [3]. On Cu foils, we have synthesized wafer-scale graphene films consisting of predominantly monolayer graphene [4]. We have studied the electronic transport properties [4], including field effect, "half-integer" quantum Hall effect (electronic hall-mark of graphene) and weak localization (probing carrier scattering) in such synthetic graphene transferred to SiO2/Si substrates and characterized its structural properties by Raman mapping, transmission electron microscopy (TEM) and scanning tunneling microscopy (STM). We have also studied thermal transport in CVD graphene using both electrical and Raman measurements [5]. Finally, one of the outstanding issues in large scale CVD graphene, which can be monolayer but generally polycrystalline, is the role of grain boundaries. I will present our recent studies of single crystal graphene grains (hexagonally-shaped with edges macroscopically aligned close to zigzag directions) grown on Cu, and how individual grain boundaries affect the electronic transport properties [6]. Work in collaboration with Q. Yu, H. Cao, L. Jauregui, J. Tian, N. Guisinger, R. Colby and E.A.Stach.

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1:03PM W2.00004 Atomistic view in the initial stages of growth of epitaxial graphene on metal substrates[1] , ZHENYU ZHANG, Oak Ridge National Laboratory / U of Tennessee — For both fundamental studies and potential development of graphene electronics, it is pressing to search for reliable methods for mass production of quality graphene. Epitaxial growth of graphene on catalytic metal substrates combined with post-growth transfer has become a promising route towards this goal [1,2]. However, to better control the quality and yield of graphene, a comprehensive understanding of the growth kinetics is essential. In particular, how the carbon atoms adsorbed on the metal surface (or dissolved into the metal) meet to nucleate into stable carbon islands will greatly influence both the growth rate and quality of larger carbon entities such as graphene sheets. In this talk, we first show that the delicate competition between carbon-carbon bonding and carbon-metal bonding dictates the initial nucleation sites of graphene on metal surfaces [3]. These results are discussed in connection with the experimental findings that on Ir(111) and Ru(0001) substrates graphene nucleates from the step edges [4,5]. We also predict that on Cu(111) nucleation should take place everywhere on a terrace [3]. Next we study larger carbon clusters on Cu(111) and explicitly compare the stability of linear and compact structures. We find that the linear carbon "nanoarches" are more stable than compact islands consisting of up to 13 carbon atoms, and these nanoarched structures may serve as the missing bridge between carbon dimers and larger graphene nanodomes. Based on these improved understanding of the atomistic rate processes involved, we propose a few kinetic pathways that may lead to better growth control of bilayer graphene and graphene nanoribbons as elemental building blocks for developing graphene electronics.

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1:39PM W2.00005 Graphene synthesis, characterization, and processing: an atomic-scale investigation , NATHAN GUISINGER, Argonne National Laboratory — Graphene is nature's ideal two-dimensional conductor that is comprised of a single sheet of hexagonally packed carbon atoms. Since the first electrical measurements made on graphene, researchers have been trying to exploit the unique properties of this material for a variety of applications that span numerous scientific and engineering disciplines. In order fully realize the potential of graphene, large scale synthesis of high quality graphene and the ability to control the electronic properties of this material on a nanometer length-scale remain key challenges. This talk will focus on atomic-scale characterization of graphene synthesis on various materials (SiC, Cu(111), Cu foil, etc) via scanning tunneling microscopy. These fundamental studies explore growth dynamics, film quality, and the role of defects. The chemical modification of graphene following exposure to atomic hydrogen will be discussed, while additional emphasis will be made on graphene's unique structural (not electronic) properties.

Thursday, March 24, 2011 11:15AM - 2:15PM –
Session W3 DCMP DMP: Advances in ZnO Physics and Applications Ballroom A3

11:15AM W3.00001 Hybrid functional studies of defects and impurities in ZnO[1] , JOHN LYONS, University of California, Santa Barbara — Zinc oxide is regarded as a highly promising material for light-emitting diodes and lasers. Its features include a direct band gap of 3.4 eV, a large exciton binding energy of 60 meV, and the availability of high-quality single-crystal substrates. Despite the rapid development, fundamental issues regarding p-type doping remain unresolved. The most significant barrier to realizing ZnO-based optoelectronic devices is the difficulty in producing reliable and reproducible p-type material. Among the possible acceptor impurities, N has been considered the most promising because it has an atomic size close to that of O. In addition, N has been conclusively shown to act as a shallow acceptor in other II-V semiconductors, such as ZnSe. In spite of many published reports on p-type conductivity in N-doped ZnO, reproducibility and stability are still major issues, and devices based on $p-n$ homojunctions have remained elusive. In this work, we study the properties of the nitrogen acceptor using advanced density functional techniques. Our first principles calculations are based on hybrid functionals, which include a portion of exact exchange and correct the band gap of semiconductors, allowing us to accurately predict defect and impurity transition levels. Contrary to the conventional wisdom, we find the N acceptor has an exceedingly high ionization energy of 1.3 eV above the valence band, meaning that N cannot lead to hole conductivity in ZnO [1]. We have also analyzed the optical transitions (absorption and luminescence) and charge distribution associated with the N impurity, which offer characteristic signatures that can be compared to experimental results.

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11:51AM W3.00002 Limits of Conductivity in ZnO Thin Films: Experiment and Theory , DAVID C. LOOK, Wright State University — Transparent conductive oxides (TCOs) have major (multi-$B) roles in applications such as flat-panel displays, solar cells, and architectural glass. The present workhorse TCO is indium-tin-oxide (ITO), but the recent huge demand for ITO has made In very expensive; moreover, it is toxic. The most commonly suggested replacement for ITO is ZnO, doped with Al, Ga, or In, and indeed the ISI lists 628 papers on Group-III-doped ZnO in 2009. However, to our knowledge, none of these papers has included calculations of donor N_D and acceptor N_A concentrations, the fundamental components of conductivity in semiconductors. We have developed a simple model for the calculation of N_D and N_A from temperature-dependent measurements of carrier concentration n, mobility μ, and film thickness d. With the inclusion of phonon scattering in the model, excellent fits of n and μ are obtained from 15 – 300 K. Experimentally, we have shown that highly conductive ZnO films can be grown by pulsed laser deposition in a pure Ar ambient, rather than the usual O_2. In a 278-μm-thick film, we have achieved a room-temperature resistivity $\rho = 1.96 \times 10^{-4}$ Ω-cm, carrier concentration n = 1.14 x 10^{21} cm^{-3}, and mobility μ = 28.0 cm^2/V-s. From our model, we calculate $N_D = 1.60 \times 10^{21}$ and $N_A = 4.95 \times 10^{20}$ cm^{-3}; however, the model also predicts that a significant reduction of N_A would give $\mu = 42.5$ cm^2/V-s and $\rho = 7.01 \times 10^{-5}$ Ω-cm, a world record. Such a reduction in N_A may be possible by in-diffusion of Zn after growth, since there is evidence that one of the major acceptor species in these films is the Zn-vacancy/Ga_{Zn} complex. We can also decrease the resistivity by annealing in forming gas, and have recently attained $\rho = 1.46 \times 10^{-4}$ Ω-cm, n = 1.01 x 10^{21} cm^{-3}, and $\mu = 42.2$ cm^2/V-s, giving $N_D = 1.13 \times 10^{21}$ and $N_A = 1.09 \times 10^{20}$ cm^{-3}. In very thin films, quantum effects must be considered.

12:27PM W3.00003 The Electronic Properties of Native Point Defects at ZnO Surfaces and Interfaces[1] , LEONARD BRILLSON, The Ohio State University — Despite nearly sixty years of research, several fundamental issues surrounding ZnO remain unresolved. Among the key roadblocks to ZnO optoelectronics have been the difficulty of p-type doping and the role of compensating native defects. Oxygen vacancies (V_O), Zn interstitials (Zn_I), and residual impurities such as H, Al, Ga, and In are reported to be donors in ZnO, while Zn vacancies (V_{Zn}) are considered to be acceptors. Electrically active complexes of V_O, Zn_I, and V_{Zn} can also exist. Although their impact on free carrier compensation and recombination is recognized, the physical nature of the donors and acceptors dominating carrier densities in ZnO and their effects on carrier injection at contacts is unresolved. The impact of these electronic states on ZnO carriers at the nanoscale is only now being explored. We can now address these issues using a combination of depth-resolved and scanned probe techniques. Taken together, we clearly identify the optical transitions and energies of V_{Zn} and V_{Zn} clusters, effects of annealing on their spatial distributions in ion-implanted ZnO, and how V_{Zn} and V_{Zn} clusters modify the near- and sub-surface carrier densities. Indeed, these native point defects can directly impact the activation of extrinsic dopants. We have now discovered that nanostructures form spontaneously on ZnO polar surfaces and create sub-surface V_{Zn} locally because of Zn diffusion that feeds the nanostructure growth. Overall, this work reveals the interplay between ZnO electronic defects, polarity, and surface nanostructure.

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1:03PM W3.00004 Realization of high performance random laser diodes[1] , S.F. YU, Hong Kong Polytechnic University — For the past four decades, extensive studies have been concentrated on the understanding of the physics of random lasing phenomena in scattering media with optical gain. Although lasing modes can be excited from the mirrorless scattering media, the characteristics of high scattering loss, multiple-direction emission, as well as multiple-mode oscillation prohibited them to be used as practical laser cavities. Furthermore, due to the difficulty of achieving high optical gain under electrical excitation, electrical excitation of random lasing action was seldom reported. Hence, mirrorless random cavities have never been used to realize lasers for practical applications – CD, DVD, pico-projector, etc. Nowadays, studies of random lasing are still limited to the scientific research. Recently, the difficulty of achieving 'battery driven' random laser diodes has been overcome by using nano-structured ZnO as the random medium and the careful design of heterojunctions. This lead to the first demonstration of room-temperature electrically pumped random lasing action under continuity wave and pulsed operation. In this presentation, we proposed to realize an array of quasi-one dimensional ZnO random laser diodes. We can show that if the laser array can be manipulated in a way such that every individual random laser can be coupled laterally to and locked with a particular phase relationship to its adjacent neighbor, the laser array can obtain coherent addition of random modes. Hence, output power can be multiplied and one lasing mode will only be supported due to the repulsion characteristics of random modes.

[1]This work was supported by HK PolyU grant no. 1-ZV6X.

1:39PM W3.00005 Nanogenerators and Piezotronics , ZHONG LIN WANG, Georgia Institute of Technology — Developing wireless nanodevices and nanosystems is of critical importance for sensing, medical science, environmental/infrastructure monitoring, defense technology and even personal electronics. It is highly desirable for wireless devices to be self-powered without using battery. This is a new initiative in today's energy research for mico/nano-systems in searching for sustainable self-sufficient power sources [1]. We have invented an innovative approach for converting nano-scale mechanical energy into electric energy by piezoelectric zinc oxide nanowire arrays [2]. As today, a gentle straining can output 1-3 V from an integrated nanogenerator, using which a self-powered nanosensor has been demonstrated. A commercial LED has been lid up [3-5]. Due to the polarization of ions in a crystal that has non-central symmetry, a piezoelectric potential *(piezopotential)* is created in the crystal by applying a stress. The effect of piezopotential to the transport behavior of charge carriers is significant due to their multiple functionalities of piezoelectricity, semiconductor and photon excitation. Electronics fabricated by using inner-crystal piezopotential as a "gate" voltage to tune/control the charge transport behavior is named *piezotronics [6,7].Piezo-phototronic effect* is a result of three-way coupling among piezoelectricity, photonic excitation and semiconductor transport, which allows tuning and controlling of electro-optical processes by strain induced piezopotential [8].

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Thursday, March 24, 2011 11:15AM - 2:15PM –
Session W4 DCMP GSNP: Glassy Dynamics and Jamming Ballroom A4

11:15AM W4.00001 Growing length-scales at the glass and jamming transition , GIULIO BIROLI, IPhT CEA Saclay — Growing timescales are usually associated to growing length-scales. The glass transition is no exception. Recent experimental, numerical and theoretical results unveiled that the slowing down of the dynamics is accompanied by growing dynamic and static correlation lengths.
The aim of this talk is to present an overview of what has been recently understood about growing length-scales at the glass transition and their role in glassy dynamics. I will also discuss the main open questions and the predictions of different theoretical approaches.

11:51AM W4.00002 Structural rearrangements that govern flow in colloidal glasses , PETER SCHALL, University of Amsterdam — We use colloidal glasses to obtain insight into the flow of amorphous materials. In three dimensions and real time, we track the individual colloidal particles in a flowing glass, and we visualize structural rearrangements that occur during flow. The individual particle trajectories are used to identify regions of non-affine deformation, in which shear concentrates. Under slow shear, we observe thermally activated 'shear transformation zones' embedded in an otherwise elastic amorphous material. Connections between these zones result in flow, which is homogeneous on macroscopic length scales. We calculate correlation functions for the fluctuations of non-affine displacements, and find a remarkable scaling, indicating that the flow of glasses is highly correlated in space. By reconstructing the entire three-dimensional strain distribution, we demonstrate that these system-spanning correlations arise from the elastic interactions between shear transformations.

12:27PM W4.00003 Order in amorphous solids , JORGE KURCHAN, PMMH-ESPCI — A solid is a system which has density modulations that are not erased by thermal motion, even on long timescales. The typical example is a crystal. Particles with soft, inter-penetrable cores may form such a solid. The remarkable fact that one can build a hard building with soft bricks can only be explained by the cooperation between an infinite number of particles. If soft particles may form a true, glassy solid phase, then we are forced to accept that an infinite coherence length must also exist for them. And yet, when we look at glass configurations, they appear definitely disordered, liquid-like. This is the mystery of glasses, which motivates the quest for a hidden order. I shall describe a coherence length that is accessible experimentally, and should diverge in an ideal glass state.

1:03PM W4.00004 Low frequency vibrational modes and particle rearrangements in colloidal glasses[1] , KE CHEN, University of Pennsylvania — We investigate the correlation between low frequency vibrational modes and fragile regions in two dimensional binary colloidal glasses, consisting of thermosensitive microgel particles. The sample packing fraction is tuned by small changes in temperature. The particles remain in their equilibrium positions in jammed states, and rearrangements are observed during temperature changes when packing fraction is changing. Using the particle displacement covariance matrix, we extract the intrinsic vibrational modes of the "shadow" colloidal network (i.e., with same geometric configuration and interactions but absent damping). Spatial correlations are observed between low frequency quasi-localized modes and rearranging clusters. The low frequency modes are found to contribute much more to particle rearrangement than high frequency modes. The number of rearranging clusters, as well as the size of particle rearrangements, increases as the system approaches jamming transition.

[1]This work is supported by NSF DMR-0804881, MRSEC DMR-0520020, NASA NNX08AO0G.

1:39PM W4.00005 Space-time phase transitions in models of glasses , JUAN P. GARRAHAN, University of Nottingham — Glass forming systems have a much richer dynamical phase structure than their thermodynamics would suggest. I will show how to explore this by means of large-deviation methods. In particular, I will demonstrate the existence of space-time phase transitions in kinetically constrained models of glasses. Similar space-time transitions seem to be present in atomistic models of supercooled liquids. In contrast to equilibrium phase transitions, which occur in configuration space, these transitions occurs in trajectory space, and are controlled by variables that drive the system out of equilibrium. Glass formers appear to live at, or close to, first-order coexistence between two distinct dynamical phases: an active and equilibrium phase, and an inactive and non-equilibrium one. This space-time coexistence helps explain observed fluctuation effects such as dynamic heterogeneity and transport decoupling. The connection of the glass transition to a true order-disorder dynamical transition offers the possibility of a unified picture of glassy phenomena.

Thursday, March 24, 2011 11:15AM - 2:15PM –
Session W5 FIAP FEd: Educating Physicists for Industrial Careers Ballroom C1

11:15AM W5.00001 SPIN-UP and Preparing Undergraduate Physics Majors for Careers in Industry[1] , RUTH HOWES, Ball State University — Seven years ago, the Strategic Programs for Innovations in Undergraduate Physics (SPIN-UP) Report produced by the National Task Force on Undergraduate Physics identified several key characteristics of thriving undergraduate physics departments including steps these departments had taken to prepare students better for careers in industry. Today statistical data from AIP shows that almost 40% of students graduating with a degree in physics seek employment as soon as they graduate. Successful undergraduate physics programs have taken steps to adapt their rigorous physics programs to ensure that graduating seniors have the skills they need to enter the industrial workplace as well as to go on to graduate school in physics. Typical strategies noted during a series of SPIN-UP workshops funded by a grant from NSF to APS, AAPT, and AIP include flexible curricula, early introduction of undergraduates to research techniques, revised laboratory experiences that provide students with skills they need to move directly into jobs, and increased emphasis on "soft" skills such as communication and team work. Despite significant success, undergraduate programs face continuing challenges in preparing students to work in industry, most significantly the fact that there is no job called "physicist" at the undergraduate level.

[1]supported by grant NSF DUE-0741560

11:51AM W5.00002 From Grad School to the Glass Industry: One Perspective , PAUL MEDWICK, PPG Industries, Inc. — This presentation will reflect one physicist's thoughts regarding a research and development career in the glass industry.

12:27PM W5.00003 Applying Physics: Opportunities in Semiconductor Technology Companies , GREG REDINBO, Varian Semiconductor — While many physicists practice in university settings, physics skills can also be applied outside the traditional academic track. Identifying these opportunities requires a clear understanding of how your physics training can be used in an industrial setting, understanding what challenges technology companies face, and identifying how your problem solving skills can be broadly applied in technology companies. In this talk I will highlight the common features of such companies, discuss what specific skills are useful for an industrial physicist, and explain roles (possibly unfamiliar) that may be available to you.

1:03PM W5.00004 How a Physicist Can Add Value In the Oil and Gas Industry , MARTIN POITZSCH, Schlumberger-Doll Research — The talk will focus on some specific examples of innovative and fit-for-purpose physics applied to solve real-world oil and gas exploration and production problems. In addition, links will be made to some of the skills and areas of practical experience acquired in physics education and research that can prove invaluable for success in such an industrial setting with a rather distinct and unique culture and a highly-collaborative working style. The oil and gas industry is one of the largest and most geographically and organizationally diverse areas of business activity on earth; and as a 'mature industry,' it is also characterized by a bewildering mix of technologies dating from the 19th century to the 21st. Oil well construction represents one of the largest volume markets for steel tubulars, Portland cement, and high-quality sand. On the other hand, 3D seismic data processing, shaped-charge perforating, and nuclear well logging have consistently driven forward the state of the art in their respective areas of applied science, as much or more so than defense or other industries. Moreover, a surprising number of physicists have made their careers in the oil industry. To be successful at introducing new technology requires understanding which problems most need to be solved. The most exotic or improbable technologies can take off in this industry if they honestly offer the best solution to a real problem that is costing millions of dollars in risk or inefficiency. On the other hand, any cheaper or simpler solution that performs as well would prevail, no matter how inelegant! The speaker started out in atomic spectroscopy (Harvard), post-doc'ed in laser cooling and trapping of ions for high-accuracy time and frequency metrology (NIST), and then jumped directly into Drilling Engineering with Schlumberger Corp. in Houston. Since then, his career has moved through applied electromagnetics, geological imaging, nuclear magnetic resonance logging, some R and D portfolio management, and more recently, management of applied physics research for evaluating reservoir rocks and fluids and enhancing the productivity of reservoirs.

1:39PM W5.00005 Internet Courses for Career Path Redirections , DAVID ATTWOOD, University of California, Berkeley — The Internet provides a cost-efficient means to reach out to larger audiences, not only to graduate students soon to enter the work force, but also to practicing scientists and engineers who wish to update their own knowledge base and perhaps consider new career directions. In this presentation we describe experience with several graduate courses at the University of California, Berkeley, that were broadcast live over the internet and posted first as Google videos and later at www.youtube.com. Full graduate class lectures, typically 28 per class, together with all presentation materials available for download, plus homeworks (and solutions upon request) are found at www.coe.berkeley.edu/AST/srms and www.coe.berkeley.edu/AST/sxr2009. The video lectures are also available at www.youtube.com by clicking on "videos" and then searching "david attwood". Based on e-mail queries and personal feedback it is clear that the lectures are widely viewed, both as training lectures in industry and as classes at various universities worldwide.

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W6 DAMOP: Alkaline Earth Atoms and SU(N) Magnetism Ballroom C2

11:15AM W6.00001 Two-orbital SU(N) magnetism with ultracold alkaline-earth atoms , ALEXEY GORSHKOV, California Institute of Technology — Fermionic alkaline-earth atoms have unique properties that make them attractive candidates for the realization of atomic clocks and degenerate quantum gases. At the same time, they are attracting considerable theoretical attention in the context of quantum information processing. In this talk, we demonstrate that when such atoms are loaded in optical lattices, they can be used as quantum simulators of unique many-body phenomena. In particular, we show that the decoupling of the nuclear spin from the electronic angular momentum can be used to implement many-body systems with an unprecedented degree of symmetry, characterized by the SU(N) group with N as large as 10. Moreover, the interplay of the nuclear spin with the electronic degree of freedom provided by a stable optically excited state should enable the study of physics governed by the spin-orbital interaction. Such systems may provide valuable insights into the physics of strongly correlated transition-metal oxides, heavy-fermion materials and spin-liquid phases. [Reference: Nature Phys. 6, 289 (2010)]

11:51AM W6.00002 Double-degenerate Bose-Fermi mixture of strontium , FLORIAN SCHRECK, IQOQI, OEAW — We report on the attainment of a double-degenerate Bose-Fermi mixture of strontium. A sample of fermionic ^{87}Sr atoms is spin-polarized and sympathetically cooled by interisotope collisions with the bosonic isotope ^{84}Sr. A degeneracy with $T/T_F = 0.30(5)$ is reached for a ^{87}Sr Fermi sea of 2×10^4 atoms together with an almost pure ^{84}Sr BEC of 10^5 atoms. The rich electronic structure and the large nuclear spin of ^{87}Sr make it a promising candidate for quantum simulation of SU(N) magnetism and quantum information processing.

12:27PM W6.00003 Degenerate Fermi Gas of Strontium-87[1] , THOMAS KILLIAN, Rice University — Degenerate Fermi gases of alkaline earth metal atoms such as strontium and ytterbium open new possibilities in the study of many-body physics because of the existence of isotopes with large nuclear spin I (e.g. I=9/2 in strontium-87). With the closed-shell electronic ground state in these atoms, the nuclear spin is decoupled from other degrees of freedom. Interactions between atoms are spin-independent, leading to a large SU(N=2I+1) symmetry of the Hamiltonian. This results in a large degeneracy of the ground state, which has been predicted to result in novel spin liquid and valence bond states. Strong attractive interactions would favor formation of N-particle singlets, in analogy to the formation of baryons in quantum chromodynamics. (For a short overview, see C. Wu, *Physics* **3**, 92 (2010).) We will describe the experimental realization of a degenerate Fermi gas of strontium-87 and characterization of an optical Feshbach resonance in this system that would be needed to manipulate the atom-atom interactions.

[1]This work was supported by the National Science Foundation and the Welch Foundation

1:03PM W6.00004 Realization of an SU(6) invariant Fermi system , YOSHIRO TAKAHASHI, Kyoto University — We report the realization of a novel Fermi system with an enlarged spin symmetry of SU(6) in a cold atomic gas of ytterbium ^{173}Yb with nuclear spin I=5/2, which will open up a new opportunity for exotic many-body physics . While the achievement of quantum degeneracy of ^{173}Yb with 6 spin components was already reported three years ago, an important technique of the separate imaging of the nuclear spin components was not developed. Recently we have made this possible by exploiting an optical Stern-Gerlach effect using a spatially inhomogeneous laser beam. The metallic state to Mott insulator transition for SU(6) Fermi gas is also investigated by loading ^{173}Yb atoms into a 3D optical lattice. We find some results suggesting the formation of SU(6) Mott state at low lattice temperatures expected for SU(N) systems. The similar adiabatic cooling effect is also observed in the Bose-Fermi mixture of spinless boson of ^{174}Yb and the SU(6) Fermi system of ^{173}Yb. In addition, an all-optical sympathetic evaporative cooling method is applied to the two fermionic isotopes of ytterbium ^{171}Yb with the nuclear spin I=1/2 and ^{173}Yb, and we successfully cool the mixture below the Fermi temperatures. The same scattering lengths for different spin components make this mixture featured with the novel SU(2) x SU(6) symmetry. The mixture is loaded into a 3D optical lattice to implement the SU(2) x SU(6) Hubbard model. In particular, we find interaction-induced suppression of Bloch oscillations for the mixture in the 3D lattice.

1:39PM W6.00005 Exotic magnetism and new states of matter with alkaline earth atoms[1] , MICHAEL HERMELE, Department of Physics, University of Colorado at Boulder — A crucial basic property of antiferromagnetic insulators with SU(2) symmetry is that adjacent spins can (and tend to) combine to form singlets, or valence bonds. The classical analog of this fact is that adjacent spins prefer to be antiparallel. These two facts underly much of our thinking about ground states of quantum antiferromagnets. Ultracold alkaline earth atoms can be used to realize magnetic insulators with SU(N) symmetry, where a minimum of N spins is required to form a singlet, and where N can be as large as 10. These systems belong to a largely unexplored class of quantum magnets. In this talk, I will discuss some of the remarkable new states of matter that are strong candidates to arise in these systems, including chiral spin liquids with fractional and non-Abelian statistics. I will also briefly discuss the issue of temperature, and point out an advantage of high-spin alkaline earths as compared to spin-1/2 magnetic systems.

[1]This work is supported by the U.S. Department of Energy, under grant no. DE-SC0003910

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W8 GMAG DAMOP: Bose-Einstein Condensation of Magnons and Related Phenomena

Ballroom C4

11:15AM W8.00001 Spin Dimers: from BEC to Luttinger liquids[1] , THIERRY GIAMARCHI, University of Geneva — Localized spin systems, and in particular dimer systems, provide a fantastic laboratory to study the interplay between quantum effects and the interaction between excitations. Magnetic field and temperature allow an excellent control on the density of excitations and various very efficient probes such as neutrons and NMR are available. They can thus be used as "quantum simulators" to tackle with great success questions that one would normally search in itinerant interacting quantum systems. In particular they have provided excellent realizations of Bose-Einstein condensates [1,2]. This allowed not only to probe the properties of interacting bosons in a variety of dimensions but also to study in a controlled way additional effects such as disorder. If the dimensionality is reduced they also allow to test in a quantitative way Luttinger liquid physics [3,4,5]. I will discuss these various cases, and show that we have now good theoretical tools [6] to make quantitative comparisons with the experiments. Finally, how to go from this low dimensional case where the spins behave essentially as fermions, to the higher dimensional case where they behave as (essentially free) bosons, is a very challenging, and experimentally relevant issue.

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[1]This work was supported in part by the Swiss SNF under MaNEP and division II.

11:51AM W8.00002 Luttinger–liquid and BEC physics in spin ladders[1] , CHRISTIAN RUEGG, Paul Scherrer Institute — Spin ladder materials serve as model systems in which the fundamental phases, exotic order, and elementary excitations of low-dimensional quantum magnets can be studied experimentally and compared quantitatively to predictions by theory. We have utilised the optimal energy scale of the exchange interactions and excellent low dimensionality of the metal–organic spin ladder material $(C_5H_{12}N)_2CuBr_4$ to study spin Luttinger–liquid (LL) and magnon Bose–Einstein Condensate (BEC) physics realized at low temperatures and in high magnetic fields in this magnetic insulator. Furthermore, the inherent chemical flexibility and the structural tunability of such metal–organic compounds enable studies of the effects of bond randomness and of non–magnetic and magnetic dopants on the spin LL and magnon BEC. Bose glass phases form and the localized impurities dominate the physics near the intrinsic quantum critical points of the ladder. Measurements of the elementary excitations, phase diagrams, and thermodynamic and magnetic properties of the LL and BEC have also been extended recently to $BiCu_2PO_6$ in which these phenomena are combined intriguingly with frustration of the magnetic exchange interactions.

[1]Research supported by the Royal Society, EPSRC and the Swiss National Science Foundation.

12:27PM W8.00003 Bose-Einstein Condensation and Asymmetry induced by Quantum Fluctuations in $NiCl_2$-4SC$(NH_2)_2$[1] , VIVIEN ZAPF, National High Magnetic Field Lab, Los Alamos National Lab — I will review Bose-Einstein condensation (BEC) in quantum magnets, in particular the compound $NiCl_2$-4SC$(NH_2)_2$. This compound exhibits field-induced XY antiferromagnetism of the S = 1 Ni system for magnetic fields along the tetragonal c-axis between H_{c1} = 2.1 and H_{c2} = 12.6 T, and the axial symmetry of the spin environment allows us to understand the quantum phase transitions at H_{c1} and H_{c2} in terms of BEC of the spin system. Here the tuning parameter for the BEC transition is the magnetic field and not the temperature. It turns out that mass of the bosons that condense can be strongly suppressed by quantum fluctuations, resulting in a remarkable asymmetry between the properties at H_{c1} and H_{c2}. Here I will present magnetization, thermal conductivity and specific heat data to probe BEC and in particular the effect of quantum fluctuations on the boson mass.

[1]We acknowledge the National Science Foundation, US Dept of Energy and the state of Florida, as well as the LANL LDRD program and the Brazillian agency CNPq.

1:03PM W8.00004 Spin Superfluidity and Magnone BEC in He-3[1] , YURY BUNKOV, Institut Neel, Grenoble — The spin superfluidity – superfluidity in the magnetic subsystem of a condensed matter – is manifested as the spontaneous phase-coherent precession of spins first discovered in 1984 in ^{3}He-B. This superfluid current of spins – spin supercurrent – is one more representative of superfluid currents known or discussed in other systems, such as the superfluid current of mass and atoms in superfluid ^{4}He; superfluid current of electric charge in superconductors; superfluid current of hypercharge in Standard Model of particle physics; superfluid baryonic current and current of chiral charge in quark matter; etc. Spin superfluidity can be described in terms of the Bose condensation of spin waves – magnons. We discuss different states of magnon superfluidity with different types of spin-orbit coupling: in bulk ^{3}He-B; magnetically traped "Q-balls" at very low temperatures; in ^{3}He-A and ^{3}He-B immerged in deformed aerogel; etc. Some effects in normal ^{3}He can also be treated as a magnetic BEC of fermi liquid. A very similar phenomena can be observed also in a magnetic systems with dinamical frequensy shift, like $MnC0_3$. We will discuss the main experimental signatures of magnons superfluidity: (i) spin supercurrent, which transports the magnetization on a macroscopic distance more than 1 cm long; (ii) spin current Josephson effect which shows interference between two condensates; (iii) spin current vortex – a topological defect which is an analog of a quantized vortex in superfluids, of an Abrikosov vortex in superconductors, and cosmic strings in relativistic theories; (iv) Goldstone modes related to the broken $U(1)$ symmetry – phonons in the spin-superfluid magnon gas; etc. For recent review see Yu. M. Bunkov and G. E. Volovik J. Phys. Cond. Matter. **22**, 164210 (2010)

[1]This work is partly supported by the Ministry of Education and Science of the Russian Federation (contract N 02.740.11.5217).

1:39PM W8.00005 Bose-Einstein condensation of magnons at room temperature , SERGEY DEMOKRITOV, Institute for Applied Physics, University of Mnster — This abstract not available.

Thursday, March 24, 2011 11:15AM - 2:15PM –
Session W9 DFD: Self Assembly II followed by Vesicles and Micelles II D220

11:15AM W9.00001 Self-assembly of two-dimensional systems with off-center core-corona architecture , DANIEL SALGADO, CARLOS MENDOZA, Instituto de Investigaciones en Materiales, UNAM — Physical systems with core-corona architecture, such as dendritic polymers or hyper-branched star polymers which are characterized by two repulsive length scales, related to the hard and soft repulsions, respectively, show the spontaneous formation of stripe phases. Here we study, by using Monte Carlo simulations, how robust is the stripe formation process upon a shift in the center of the core with respect to the corona in a two-dimensional system of colloidal particles. We find that for sufficiently large shifts, the strip phases are replaced by a sort of plastic (or glassy) colloidal crystal consisting of a regular lattice of coronas inside of which disordered aggregates of cores coexist. The model investigated in this work could be useful for the design of colloidal plastic crystals.

11:27AM W9.00002 Limit of validity of Ostwald's rule of stages in a model of solution crystallization[1] , LESTER HEDGES, STEPHEN WHITELAM, Molecular Foundry, Lawrence Berkeley National Laboratory — Many systems take "nonclassical" crystallization pathways, forming ordered solids via intermediates that do not share the architecture of the stable material. We possess only rules-of-thumb to explain such dynamics. Chief among them is Ostwald's rule of stages, which states that the phase that first emerges is the one closest in free energy to the parent phase. Although widely applicable, the rule breaks down in many experiments and computer simulations. It is therefore clear that the rule is without firm theoretical foundation, but it is not clear when it should apply. To this end we test Ostwald's rule of stages in a lattice model of solution crystallization. We find that rule holds in certain regions of parameter space and breaks down in others. We argue that its breakdown can be predicted using simple arguments. In addition, we find that crystallization pathways depend qualitatively on both the thermodynamic landscape prescribed by inter-particle interactions and on the relative rates of particle rotations and translations.

[1]Supported by the Center for Nanoscale Control of Geologic CO2, a U.S. D.O.E. Energy Frontier Research Center, Contract No. DE-AC02-05CH11231.

11:39AM W9.00003 Mesophase behavior and rheology of polyhedral particles[1] , UMANG AGARWAL, FERNANDO ESCOBEDO, School of Chemical and Biomolecular Engineering, Cornell University — Translational and orientational excluded volume fields can guide assembly of particles with anisotropic shape to diverse morphologies. A roadmap elucidating correlations between phase behavior and particle shape may help devising efficient strategies for self-assembly of desired nanocrystal superlattices. To explore these complex correlations we performed detailed Monte Carlo simulations of six convex multi-faceted shapes belonging to the diverse class of space-filling polyhedrons. Simulations predict formation of various novel liquid-crystalline and plastic-crystalline phases at intermediate volume fractions. By correlating these findings with particle anisotropy and order of rotational symmetry, simple guidelines for predicting phase behavior of polyhedral particles are proposed. Moreover, detailed analysis of the structures of mesophases reveals importance of dynamical order in defining these phases and preliminary information about kinetics of these transitions is also obtained. Finally, to elucidate the effect of particle shape anisotropy on rheology, preliminary results will be reported from non equilibrium molecular dynamics simulations of the isotropic and cubatic(LC) phase of cuboidal particles.

[1]This work was supported by a Department of Energy Basic Energy Science Grant ER46517

11:51AM W9.00004 Triblock Janus Spheres , QIAN CHEN, SUNG CHUL BAE, STEVE GRANICK, University of Illinois at Urbana Champaign — We show that spheres that attract one another on two polar regions but repel at the middle band ("triblock Janus") assemble into nontrivial reticulated networks. We have constructed such spheres and have visualized their aqueous assembly dynamics on the single-particle level. The building blocks are simple micron-sized colloidal spheres whose interactions (electrostatic repulsion in the middle, hydrophobic attraction at the poles) are likewise simple, but their self-assembly into this open structure contrasts with previously-known close-packed periodic arrangements of spheres. This strategy of "convergent" self-assembly from facilely fabricated colloidal building blocks encodes the target supracolloidal architecture not in localized attractive spots but rather in large redundantly attractive regions of the building blocks. The idea extends to designing other supracolloidal networks.

12:03PM W9.00005 Novel structure formation of dipolar Janus particles (JP) in electrolytes: A molecular dynamic (MD) simulation study , MAHDY MALEKZADEH, BAMIN KHOMAMI, Materials Research and Innovative Laboratory (MRAIL), Department of Chemical and Biomolecular Engineering, University of Tennessee, Knoxville — There have been tremendous number of experimental studies and number of simulations in recent years trying to elucidate the underlying principals which determine structure formation of colloidal systems of JP. However most of simulations utilize relatively simple models and lack inclusion of long range columbic interactions. In this work MD simulations have been performed to understand effects of surface charge density and volume fraction (0.01-0.17) on structure formation and radial pair distribution function (RDF) of JPs of 6 nm in diameter with opposite charges on each hemisphere. Inclusion of long range columbic interaction via Ewald summation leads to formation of novel structures such as rings, chains and layered large spheres (about hundreds of nanometers) in accord to experimental observations. Moreover based on possibility of defect formation during synthesis, defects were introduced into each JP by slightly altering the uniform charge distribution on each hemisphere. Our results show in presence of small amount of defects ($<$10%) no significant changes occur in RDF, however increasing defect sites up to around 20% will significantly changes structure formation and combination of aforementioned structures concur to SFM and SEM images.

12:15PM W9.00006 Glassy Dynamics in the Rotator Phase of Two-Dimensional Janus Crystals , JING YAN, SHAN JIANG, JONATHAN WHITMER, STEPHEN ANTHONY, ERIK LUIJTEN, Department of Materials Science and Engineering and Department of Engineering Sciences and Applied Mathematics, Northwestern University, STEVE GRANICK, Departments of Materials Science and Engineering, Physics, and Chemistry — Janus particles, spheres with two different sides, represent the simplest building blocks whose interparticle interaction is orientation dependent. When confined on regular lattices, they epitomize basic physical problems from the arrangement of spins in magnetic materials, to rotating molecules in plastic crystals. Here we study both in experiment and in simulation, the heterogeneous dynamics in a two-dimensional crystal of amphiphilic Janus spheres. Single particle tracking reveals that orientation along can generate phenomenology resembling conventional translational supecooled liquids and glasses. Characteristic cage break events, which requires anti- correlated rotation of particles sitting on neighboring lattices, were indentified and characterized in detail. Recent experiments aiming at selectively perturbing the system using external field, such as magnetic field, will also be discussed.

12:27PM W9.00007 Chiral Control of Interfacial Tension , MARK ZAKHARY, THOMAS GIBAUD, EDWARD BARRY, ROBERT MEYER, ZVONIMIR DOGIC, Brandeis University — The interfacial tension between molecular species in self-assembling systems plays a crucial role in determining the physical properties of the mesoscopic assemblages. The predominant method for controlling interfacial tension is the addition of surfactant molecules, which preferentially adsorb onto the interface and modify the interactions between the two phases. In this talk, using a model colloidal membrane composed of chiral, rod-like *fd* viruses, I will present a new method for controlling interfacial tension which does not require additional surfactant components, but instead utilizes the intrinsic chirality of the constituent rods. I will demonstrate that chirality can be used to continuously tune the interfacial tension of a membrane and to drive a dramatic phase transition from two-dimensional membranes to one-dimensional twisted ribbons. Using a wide variety of microscopic techniques, this transition is characterized over all relevant length-scales, ranging from nanometers to microns.

12:39PM W9.00008 ABSTRACT WITHDRAWN –

12:51PM W9.00009 Dynamics of a compound vesicle in shear flow , SHRAVAN VEERAPANENI, NYU, YUAN-NAN YOUNG, NJIT, PETIA VLAHOVSKA, Brown University, JERZY BLAWZDZIEWICZ, Texas Tech University — The dynamics of compound vesicle (a lipid bilayer membrane enclosing a fluid with a suspended particle) in shear flow is investigated using both numerical simulations and theoretical analysis. We find that the non-linear coupling (via hydrodynamic interaction) between the inclusion motion and the confining membrane deformation gives rise to new features in the vesicle dynamics. Transition from tank–treading to tumbling can occur even in the absence of any viscosity mismatch. An initially non-concentric inclusion induces transient vesicle waltzing. A swinging-like vesicle motion is observed if the enclosed particle is an ellipsoid. The rheology of a suspension of compound vesicles is also strongly affected by the inclusion confinement. Our results highlight the complex effects of internal cellular structures on cell dynamics in external flow.

1:03PM W9.00010 Exploring Structure, Shape, and Dynamics of Elastin-like Polypeptide Nanoparticles , KIRIL A. STRELETZKY, Cleveland State University, KAITLIN VANDEMARK, ALI GHOORCHIAN, NOLAN HOLLAND, Cleveland State University — Environmentally responsive nanoparticles synthesized from elastin-like polypeptides (ELP) present a promising system for applications as biosensors, drug delivery vehicles, and viscosity modifiers. These nanoparticles undergo a transition from a soluble state at room temperature to micellar aggregates above the transition. The size, shape, and dynamics of micelles above the transition as well as effects of the solvent salt concentration and pH on the transition are important to understand from a fundamental science point of view as well as for potential applications. The system has been characterized with high resolution multiangle Dynamic and Static Light Scattering Spectroscopies. It was confirmed that the system undergoes a transition from mixture of ELP extended trimers and their non-spherical formations to a solution of micelles. It was discovered that micellar size and structure are very sensitive to solution's pH. The micelles were generally found to exhibit properties of the hyperbranched spheres below pH of 10 and above pH of 10.3 with their shape becoming significantly elongated in the pH window of 10 to 10.3. It was also found that the size of micelles strongly depends on salt concentration displaying at least two size regimes (20-45nm at 0-20mM and 100-150nm at 25-40mM) with different salt concentration dependences.

1:15PM W9.00011 The Lipid domain Phase diagram in a Dipalmitoyl-PC/Docosahaexnoic Acid-PE/Cholesterol System[1] , CHAI LOR, LINDA HIRST[2], University of California, Merced — Lipid domains in bilayer membrane and polyunsaturated fatty acids (PUFAs) are thought to play an important role in cellular activities. In particular, lipids containing docosahaexnoic acid are an interesting class of PUFAs due to their health benefits. In this project, we perform oxidation measurements of DHA-PE to determine the rate of oxidation in combination with antioxidants. A ternary diagram of DPPC/DHA-PE/cholesterol is mapped out to identify phase separation phenomena using atomic force microscope (AFM). Fluorescence microscopy is also used to image lipid domains in a flat bilayer with fluorescent labels. As expected, we observe the phase, shape, and size of lipid domains changes with varying composition. Moreover, we find that the roughness of the domains changes possibly due to overpacking of cholesterol in domains. This model study provides further understanding of the role of cholesterol in the bilayer membrane leading towards a better understanding of cell membranes.

[1]NSF award # DMR 0852791, "CAREER: Self-Assembly of Polyunsaturated Lipids and Cholesterol In The Cell Membrane."
[2]Ph.D

1:27PM W9.00012 Interfacial Microrheology with a Magnetic Needle Viscometer and Two-Particle Correlated Motion , JAMES SEBEL, KENNETH W. DESMOND, ERIC R. WEEKS, Emory University — We measure the viscoelastic moduli of thin films using two different methods. First, we use a magnetic needle viscometer. Our apparatus employs Helmholtz coils to control the position and orientation of the needle in the film. By driving the needle we can produce a response in the film which allows us to probe the bulk viscoelastic properties of the film. Second, we use two particle microrheology to probe the local properties of the film. Tracking the correlated motion between two particles as they undergo Brownian motion probes the local viscoelastic properties of any heterogeneous domains. Examining the correlations between pairs of particles with large separations helps us infer information about the bulk properties. Coupling this technique with the magnetic needle viscometer provides information on the effect local viscoelastic properties have on the bulk properties.

1:39PM W9.00013 Ion-Specific Induced Charges at Aqueous Soft Interfaces[1] , WENJIE WANG, ALEX TRAVESSET, DAVID VAKNIN, Ames Laboratory, and Department of Physics, Iowa State University, Ames, Iowa 50011 — Surface-sensitive X-ray scattering and spectroscopic techniques are employed to monitor ion binding specifically to Langmuir monolayers of densely packed carboxyl or phosphate groups. By systematically varying pH of Fe^{3+}, Fe^{2+} and La^{3+} solutions, we show that the critical surface pressure at the tilted (L2) to untilted (LS) transition is ionic specific and pH dependent. While the maximum density of surface bound La^{3+} per carboxylic group is ~ 0.3, the amount necessary to neutralize the fully charged surface, for Fe^{3+} it is nearly 0.6. Furthermore, the binding of Fe^{3+} is accompanied with a significant accumulation of Cl^- co-ions implying interfacial charge inversion. Similar experiments with charged phosphate groups at the interface show that the bindings of Fe^{2+} and La^{3+} are electrostatically driven. Our results have implications on biomineralization processes and ionic functions at cell membranes.

[1]Supported by the Office of BES, U.S. Department of Energy Cont. No. DE-AC02-07CH11358.

1:51PM W9.00014 Structural characterization of a multiple stacked supported bilayer system , CURT DECARO, JUSTIN BERRY, LAURENCE LURIO, Northern Illinois University, YICONG MA, GANG CHEN, SUNIL SINHA, University of California San Diego, LOBAT TAYEBI, ATUL PARIKH, University of California Davis — Supported Lipid Bilayers are a popular model system for cell membranes since their defined orientation allow characterization with probes such as AFM, x-ray and neutron scattering. A significant concern, however, is that strong interactions with the substrate can suppress dynamics within the bilayer. One method that has been successful at overcoming this limitation is to cushion the supported bilayer on a softer material. In the present work, we have stacked up to five successive bilayers of DPPE on top of each other, in effect using the lower bilayers as cushions. X-ray reflectivity shows that each stack preserves the orientation of the first, and that each bilayer exhibits full coverage of the one below. The roughness of each bilayer is found to increases with distance from the substrate as would be expected if thermal fluctuations are increasing with distance from the substrate. We also find that upon heating from the gel to the fluid state that an unbinding transition is observed.

2:03PM W9.00015 Shape and Size of highly concentrated micelles in CTAB/NaSal solutions by small angle neutron scattering (SANS) , HU CAO, HELMULT KAISER, NARAYAN DAS, PAUL SOKOL, Center for the Exploration of Energy and Matter, Indiana University, Bloomington, IN 47408, JOSEPH GLADDEN, Dept. of Physics and Astronomy, University of Mississippi, University, MS 38677 — Highly concentrated micelles CTAB/NaSal with a fixed salt/surfactant ratio of 0.6 have been studied by small angle neutron scattering (SANS) as a function of temperature and concentrations. A modeling analysis with a combination of ellipsoid, Gaussian size distribution and Hard Sphere Model (HSM) on SANS data suggests that these micelle solutions have an ellipsoidal structure, which is independent on the concentrations and temperature. However, the micelle size decreases monotonically as increasing the temperature or concentration. Besides, it was found that the number density of particles increases as increasing the temperature, while the total volume keeps unchanged. These observations indicate that large micelles at low temperature begin to break to form small ones as increasing the temperature and these broken surfactant molecules aggregate again under the effect of strongly binding counterions to form more micelles.

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W10 DCMP: Adsorption, Wetting, and Complex Interfaces D221

11:15AM W10.00001 Surface Tension Anisotropy of Lennard-Jones Systems , EMRE ESENTURK, University of Pittsburgh — Anisotropy in the surface tension plays a significant role in the evolution of interfaces and in determining the equilibrium shapes of materials (dendritic growth, motion of grain boundaries). We present a discrete version of integral Phase Field Model with non-local potential for the crystal-melt interfaces of Lennard-Jones Systems. The model provides a methodology to understand the process of transfer of microscopic anisotropy to macroscopic scale. We calculate the surface tension and the anisotropy of the crystal-melt interface in the [100] and [110] directions and compare our results with recent simulations.

11:27AM W10.00002 Adsorption of Methane and Propane on a LJ Wall and on Molybdenum Surface: A Simulation Study , ALI ABU NADA, Southern Illinois University at Carbondale, GARY LEUTY, MESFIN TSIGE, University of Akron — Atomic-scale MD simulations were used to study multilayer adsorption as a function of temperature for two different alkanes (CH_4 and C_3H_8) on a fixed Lennard-Jones wall and on the (001) surface of molybdenum. In sets of simulations on the molybdenum surface, the substrate atoms were made to interact via a Lennard-Jones potential in one study and via an embedded-atom model (EAM) potential in the next. The results show that CH_4 and C_3H_8 on the flat wall possess a highly ordered packing arrangement exhibiting a higher degree of order than films adsorbed on the molybdenum substrate. Additionally, the number of ordered layers seen in the case of adsorption of CH_4 was noted to be greater than the number of ordered layers in the case of adsorption of C_3H_8. In each case, the first layer appears frozen, implying there is no translational motion for the molecules in this layer, and we can confidently surmise that the first adsorbed layer exists in the solid phase far above the bulk melting temperature.

11:39AM W10.00003 Evaporation kinetics of CO_2 laser heated fused silica[1] , SELIM ELHADJ, M.J. MATTHEWS, S.T. YANG, D. COOKE, J.S. STOLKEN, M.D. FEIT, LLNL — Laser-based machining strategies of optical surfaces remain mostly empirical, yet, systematic and controlled studies that relate gas chemistry and surface temperature to evaporation kinetics are limited, especially at extreme temperatures (>2800K) reached during laser irradiation. We present experimental results of CO_2 laser heating of silica in oxidizing and non-oxidizing environments, along with analysis of surface shape from which a near-equilibrium evaporation model is derived. Based on this model, temperature dependent enthalpies of evaporation are determined and compared to published results. This model reproduces experimental laser-etch rates, while still accounting for laser, mass transport, and gas chemistry parameters. Although heat and mass transport processes are complex and tightly coupled, general conditions for which such an approach can be used to guide laser-based evaporation will be presented.

[1]Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration under Contract DE-AC52-07NA27344.

11:51AM W10.00004 ABSTRACT WITHDRAWN –

12:03PM W10.00005 Simulation study on structure of water in aqueous solutions confined between graphene electrodes under very high applied electric field[1] , GARY LEUTY, MESFIN TSIGE, The University of Akron, SAIKAT TALAPATRA, Southern Illinois University at Carbondale — Arising from questions regarding electric double-layer capacitors utilizing graphene electrodes and aqueous electrolyte (KOH solution), atomistic MD simulations of electrolyte confined between graphene electrodes were performed to understand the behavior of electrolyte as a function of electric field strength and solution concentration, from pure water to 6M KOH. It was noted that the strength of the electric field had a demonstrable effect on the structure of pure water between the electrodes (as has previously been seen in highly confined multilayer water systems), creating regularly spaced channels and densely packed sheets of highly ordered molecules. We also saw a clear effect due to the presence of electrolyte ions and their separation from the water due to the action of the field; different field strengths appear to greatly alter the distribution of ions, which in turn affects the structure and ordering of the water. Time dependence in the strength of the electric field was also studied to determine what effect, if any, it has on induced structure.

[1]Authors gratefully acknowledge support from the ACS Petroleum Research Fund and the National Science Foundation

12:15PM W10.00006 Thermodynamics and kinetics of wetting transition of an oily fluid on surfaces with nanoscale roughness: A molecular dynamics study , ELIZABETH SAVOY[1], FERNANDO ESCOBEDO, Cornell University — Surface wettability has garnered significant interest in recent years, as design and manufacture of nanoscale features allows fabrication of highly non-wetting surfaces. Such behavior is more difficult to achieve for low surface-tension fluids such as oils, and requires novel approaches. One approach is to create roughness features that provide an energy barrier to the fluid's transition from the composite to fully wetted state. We use molecular dynamics of small droplets in combination with various simulation techniques, such as umbrella sampling and forward flux sampling, to probe the energy landscape associated with the wetting transition and compute transition rates and their dependence on key topological parameters such as feature height. We find that the drop does not transition with a flat liquid-vapor interface when it penetrates and wets the subsurface features (as is often assumed in continuum treatments) and that the hysteresis in the wetting and dewetting transitions is associated with differences in the evolution of that interface.

[1]Corning Incorporated

12:27PM W10.00007 Understanding and designing of steam-phobic surfaces[1] , ILA BADGE, SUNNY SETHI, ALI DHINOJWALA, The University of Akron — The wetting behavior of a surface under steam condensation depends on its intrinsic wettability and micron or nanoscale surface roughness. A typical superhydrophobic surface may not be suitable as a steam-phobic surface due to nucleation and growth of water inside the valleys and thus, failure to form air-liquid- solid composite interface. Here, we present the results of steam condensation on chemically modified nano-structured carbon nanotube carpets. The combination of surface chemistry and surface roughness provides a mechanism to retain superhydrophobicity of the nanotube surfaces under steam condensation. Ability of withstand steam temperature and pressure also implies improved hydrostatic stability of the surface.

[1]National Science Foundation

12:39PM W10.00008 Effects of host relaxation on gas uptake in porous media , MILTON COLE, Pennsylvania State University, ANNIE GROSMAN, University of Paris VI, SUSANA HERNANDEZ, University of Buenos Aires, ANGELA LUEKING, Penn State University — We have recently predicted [1] an *imbibition transition* as a prototype of a general phenomenon-substrate relaxation due to adsorption. That transition is exemplified by a graphene sheet's lifting off of a surface in order to intercalate gas. Other relevant phenomena include the expansion of nanotube bundles or MOFs to accommodate imbibed gases. In our new work, we first analyze the relaxation problem, in general, and then address infinite cylindrical and slit pore geometries, for which simplifications occur because there is just one finite dimension. Research supported by DOE.

[1] K. E. Noa, A. D. Lueking and M. W. Cole, *Imbibition transition: gas intercalation between graphene and silica*, submitted to J. Low Temp. Phys.

12:51PM W10.00009 Surface metal-oxygen bond length on hydrated rutile(110) and cassiterite(110) surface - A measure of the local environment , NITIN KUMAR, Department of Physics, Penn State University, PAUL KENT, Center for Nanophase Materials Sciences and Chemical Sciences Division, Oak Ridge National Laboratory, ANDREI BANDURA, St. Petersburg State University, DAVID WESOLOWSKI, Chemical Sciences Division, Oak Ridge National Laboratory, JAMES KUBICKI, Department of Geosciences, Penn State University, JORGE SOFO, Department of Physics, Penn State University — We study the dynamics of water on the surface of rutile (110) and cassiterite (110) using ab-initio molecular dynamics simulation. The water molecule covalently attach with the fivefold coordinated metal atoms on the surface. It can remain in a molecular form or it can dissociate to form hydroxyls on the surface. The distance between the metal and the oxygen depends on the protonation state of the latter. Moreover, we find that the local environment is not only limited to the number of covalently bonded hydrogen but it also depends on number of hydrogen bonds and the species participating in it. In general, the metal oxygen distance shows much larger fluctuations in rutile compared with cassiterite. The half width half maximum (HWHM) of the metal oxygen distance histogram, for the terminal oxygen, is 0.27 Angstrom for rutile and 0.16 Angstrom for cassiterite. Also, for bridging oxygen HWHM is 0.18 and 0.12 Angstrom for rutile and cassiterite, respectively.

1:03PM W10.00010 Water-Thin-Film Adsorption on Alpha-Quartz (0001) Surface[1] , YUN-WEN CHEN, YAN WANG, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida — We investigated thin water films adsorbed on quartz (0001) surfaces using first-principles density functional theory calculations. Interfacial structure and energetics were studied through a layer-by-layer deposition. From monolayer to multilayer, the low energy state configurations and adsorption sites show a transition due to formation of a highly stable bilayer membranelike structure. The water adsorption energy on a quartz surface coated by this membrane is of typical hydrogen bond strength for both dry and fully hydroxylated surfaces. The interactions between the surface and the water films are short-ranged due to shielding of the bilayer.

[1]This work is supported by the NSF under Grant No. DMR-0804407.

1:15PM W10.00011 Mn Adsorption on MgO/Ag(100): DFT and DFT+U Calculations , HOSSEIN HASHEMI, Martin-Luther-Universität Halle-Wittenberg, Friedemann-Bach-Platz 6, D-06099 Halle, Germany, BARBARA JONES, IBM Almaden Research Center, San Jose, CA 95120-6099, USA — The adsorption properties of a Mn adatom on MgO ultrathin films deposited on a Ag(100) substrate are determined from first principles DFT calculations and compared with the corresponding adsorption characteristics from DFT+U calculations. First, we investigate the properties of a pure Ag (100) surface and a MgO/Ag(100) system. The structural relaxation, work function and surface energy for the Ag(100) surface, as a function of thickness dependence, is discussed. Next, we discuss the addition of a Mn adatom. Regular (U=0) DFT calculations show that the most stable site for Mn adsorption on MgO/Ag(100) is the bridge site, followed closely by the Oxygen site, and a very unlikely position, the Mg site. We have also investigated the role of strong electron correlations in the substrate on the chemisorption properties of a Mn adatom. DFT+U calculations predict the Oxygen site to be the most stable site, instead of the bridge site, in contrast to U=0 DFT calculations. The energies, geometry, and magnetic properties of the Mn adatom are all influenced by adding a Coulomb energy. Altogether our results show that the on-site Coulomb repulsion in the Mn d band plays an important role in the description of adsorption on MgO/Ag(100).

1:27PM W10.00012 Stabilizing Graphitic Thin Films of Wurtzite Materials by Epitaxial Strain[1] , DANGXIN WU, FENG LIU, University of Utah — Recent theoretical and experimental work showed that (0001) ultrathin films of wurtzite materials transform into a stable graphite-like structure if their thickness is reduced to only a few atomic layers. Using first-principles calculations of both freestanding and substrate-supported thin films, we predict that the thickness range of stable graphitic films can be greatly extended by epitaxial tensile strain but reduced by compressive strain. The band gap of the resulting graphitic films can be tuned by strain and film thickness either above or below that of the bulk wurtzite phase. Our prediction suggests a plausible physical mechanism to be explored by future experiments for strain engineering of graphitic films from wurtzite materials with a wide range of potential applications.

[1]This work is supported by DOE-BES.

1:39PM W10.00013 Simulating phase formation during exothermic reactions in Al/Ni and Al/Zr multilayered foils[1] , RONG-GUANG XU, Department of Physics and Astronomy, Johns Hopkins University, MICHAEL L. FALK, Department of Materials and Engineering, Department of Mechanical Engineering and Department of Physics and Astronomy, Johns Hopkins University, HONG-WEI SHENG, Department of Computational and Data Sciences, George Mason University, JOHNS HOPKINS UNIVERSITY TEAM, GEORGE MASON UNIVERSITY COLLABORATION — Reactive multilayered foils are composed of thousands of alternating micro- to nano- scale layers of elements which have a large negative enthalpy of mixing. When a small pulse of energy (such as an electric spark or a thermal pulse) is provided, highly exothermic, self-propagating chemical reactions can be triggered. Both theoretical models and experimental data indicate that even a relatively small amount of premixing can have a dramatic effect on the heats and velocities of the propagating reaction front. We have implemented molecular dynamics simulation to study the phase transformation sequence during multilayered reactions and to elucidate how premixing can affect the sequence of phase formation during such reactions.

[1]Research supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-09ER46648

1:51PM W10.00014 Chemical Reactivity at the Ti/CuO Interface[1] , A. CHOURASIA, J. EDMONDSON, Texas A&M Univ.-Commerce — The chemical reactivity between titanium and copper oxide at the Ti/CuO interface has been investigated using x-ray photoelectron spectroscopy. About 15 nm thick copper film was deposited on silicon substrates by the e-beam method. Such samples were oxidized in an oxygen environment in a quartz tube furnace at 400 °C. The formation of CuO was checked by the XPS spectral data. Thin films of titanium were then deposited on these CuO samples. The titanium 2p, oxygen 1s and copper 2p regions were investigated by XPS. The magnesium anode (energy = 1253.6 eV) has been used for this purpose. The spectral data show chemical reactivity at the Ti/CuO interface. The samples were annealed afterwards in air at 400 °C. The spectral data were recorded at different take-off angles. Comparison of the data with the pre-annealed samples shows diffusion of Cu through the titanium overlayer alongwith the formation of CuO.

[1]Supported by Organized Research, TAMU-Commerce

2:03PM W10.00015 Composite TiO2-Carbon nano films with enhanced photocatalytic activity[1] , DINKO CHAKAROV, RAJA SELLAPPAN, Chalmers University of Technology — Composite TiO2-carbon thin films prepared by physical vapor deposition techniques on fused silica substrates show enhanced photocatalytic activity, as compared to pure TiO2 films of similar thickness, towards decomposition of methanol to CO2 and water. Raman and XRD measurements confirm that annealed TiO2 films exhibit anatase structure while the carbon layer becomes graphitic. Characteristic for the composite films is an enhanced optical absorption in the visible range. The presence of the carbon film causes a shift of the TiO2 absorption edge and modifies its grain size to be smaller. The observed enhancement is attributed to synergy effects at the carbon-TiO2 interface, resulting in smaller crystallite size and anisotropic charge carrier transport, which in turn reduces their recombination probability.

[1]Supported by N-INNER through the Solar Hydrogen project (P30938-1 Solväte).

Thursday, March 24, 2011 11:15AM - 2:03PM –

Session W11 FIAP: Electronic Structure: Thermodynamics and Optical Properties D222

11:15AM W11.00001 Comparison of Experimental and Theoretical Vibrational Spectra for Pentacene Derivatives , GREGORY MASLAK, MARK STEWART, LILLIE GHOBRIAL, WES LAURION, Dept. of Physics, SUNY Oswego, JINYUE JIANG, LI TAN, Dept. of Engineering Mechanics, UNL, CAROLINA C. ILIE, Dept. of Physics, SUNY Oswego — The practical use of pentacene in the area of organic field-effect transistors is limited by its sensitivity to oxygen and poor solubility in organic solvents. To overcome these disadvantages, new organic semiconductors as 2,3,9,10-tetrakis(3,5-di-t-butylphenylethynyl)-6,13- bis (trimethylsilylethynyl) pentacene are synthesized. The new pentacene derivatives may be useful for electronic devices such as organic field-effect transistors or organic light-emitting diodes. Here we compare the calculated vibrational spectra to the experimental data in order to characterize the new derivative. The methods and similarities between the theoretical calculations and the experimental data are discussed.

11:27AM W11.00002 Optical characterization of p-doped InP epitaxial layers in mid and far infrared region[1] , R.C. JAYASINGHE, Y.F. LAO, A.G.U. PERERA, Georgia State University, M. HAMMAR, Royal Institute of Technology, Kista, Sweden, C.F. CAO, Chinese Academy of Sciences, Shanghai, China, H. WU, Zhejiang University, Hangzhou, China — The optical properties of p-doped Indium Phosphide (InP) epitaxial thin films with 1, 3, and 24 $\times$ 10^{18} cm^{-3} carrier concentrations were investigated by infrared reflection, transmission, and absorption measurements in 5 - 40 μm wavelength range. The absorption spectra were modeled by complex dielectric function using the classical Lorentz–Drude model. The phonon absorption in InP was modeled using eight Lorentzian oscillators. This method gives a straightforward approach for modeling the experimental absorption spectra when compared to the two-phonon absorption spectroscopy technique. The calculated spectra are in a good agreement with experimental spectra. The effects of doping on fitting parameters are also investigated.

[1]This work was supported in part by the US Army Research Office under Grant No. W911NF-08-1-0448 monitored by Dr. William Clark and Georgia Research Alliance under grant GRAUP

11:39AM W11.00003 Photoluminescence intensity oscillations with magnetic field in InGaAs quantum wells[1] , LARS SCHWEIDENBACK, ANDREAS RUSS, TARIQ ALI, JOSEPH MURPHY, ALEXANDER CARTWRIGHT, ATHOS PETROU, SUNY Buffalo, ALEXANDER GOVOROV, Ohio University, CONNIE LI, AUBREY HANBICKI, BEREND JONKER, Naval Research Laboratory, GEORGE KIOSEOGLOU, University of Crete — We have observed magnetic field oscillations in the photoluminescence (PL) intensity from InGaAs quantum wells (QWs) with indium compositions of 5% and 15% with laser excitation close to the bandgap for temperatures < 20 K. For all samples the intensity maxima occur at 2.2 and 4.5 tesla when the magnetic field is applied perpendicular to the QW plane. Experiments in which the sample normal (z-axis) is tilted with respect to the applied magnetic field B show that the PL intensity maxima positions depend on the magnetic field component B_z. Time-resolved PL comparison with GaAs QWs yields much longer recombination times for the InGaAs QWs. Furthermore, cross sectional scanning tunneling microscopy studies indicate the formation of Indium rich InGaAs clusters in the InGaAs QWs. We interpret the observed oscillations in terms of the Aharonov-Bohm effect and quasi-indirect excitons with ring-like trajectories of carriers. The oscillation period corresponds to orbits with radius equal to 24 nm.

[1]Work at SUNY was supported by ONR and NSF

11:51AM W11.00004 Optical two-dimensional Fourier transform spectroscopy of single GaAs quantum wells , YURI D. GLINKA, ZHENG SUN, XIAOQIN LI, Physics department, University of Texas-Austin, TX 78712 USA, ALLAN BRACKER, Naval Research Lab, Washington, DC 20375 USA — Optical two-dimensional Fourier transform spectroscopy is applied to study the coherent coupling between light-hole and heavy-hole excitons in single GaAs quantum wells instead of those consisted of ten or four periods of GaAs separated by $Al_{0.3}Ga_{0.7}As$ barriers measured previously. The effect of the confinement energy as well as Coulomb and disorder correlation lengths on coherent coupling dynamics is discussed. The financial support from ARO, NSF, and Welch foundation is gratefully acknowledged.

12:03PM W11.00005 Origin of the Terahertz Absorption Peak in Single-Walled Carbon Nanotubes , QI ZHANG, LEI REN, H. GOJUKI, E.H. HAROZ, T. ARIKAWA, J. KONO, ECE Dept., Rice University, C.L. PINT, R.H. HAUGE, Chemistry Dept., Rice University, A.K. WOJCIK, A.A. BELYANIN, Dept. of Physics, Texas A&M Univ., ECE DEPT., RICE UNIVERSITY TEAM, CHEMISTRY DEPT., RICE UNIVERSITY COLLABORATION, DEPT. OF PHYSICS, TEXAS A&M UNIV. COLLABORATION — Single-walled carbon nanotubes (SWNTs) are promising for high-frequency electronics and terahertz (THz) applications, as well as for fundamental studies of finite-frequency dynamics of one-dimensional electronics. Previous studies of dynamic conductivities of various types of SWNTs have revealed a pronounced and broad absorption peak around 4 THz, whose origin has been a matter of controversy. Both the effects of curvature-induced band gaps and plasmonic absorption due to finite lengths have been proposed to be important, but a consensus has not emerged. We have studied 4THz peak in highly aligned and length-controlled SWNT films and metallically-enriched SWNT films through FTIR and THz time-domain spectroscopy. We provide evidence that this peak is observable only when the THz polarization is parallel to the nanotubes and only in metallic tubes. We will discuss the origin of this absorption peak in light of these new findings.

12:15PM W11.00006 UV light emission from ZnO nanostructures in SiO_2 synthesized by ion implantation and thermal annealing , BIMAL PANDEY, AKHILESH SINGH, PRAKASH POUDEL, ARUP NEOGI, DUNCAN WEATHERS, University of North Texas — Zinc Oxide (ZnO) nanostructures were synthesized by the implantation of low energy (35 keV) ZnO molecular ions into thermally grown SiO_2 at a fluence of 5×10^{16} ions/cm^2. Implanted samples were annealed in an oxygen environment to allow the growth of ZnO precipitates. X-ray photoelectron spectroscopy (XPS), Fourier transform spectroscopy (FTIR) and energy dispersive x-ray spectroscopy (EDS), confirm the formation of ZnO. High resolution transmission electron microscopy (HRTEM) shows the formation of nanostructures having diameters ranging from 2 nm to 5 nm in the SiO_2. Photoluminescence (PL) measurements show excitonic and band-edge emission in the ultraviolet region at temperatures ranging from 4 K - 300 K. Time-resolved PL measurements performed at 4K showed an electron-hole recombination lifetime on the order of a few hundred picoseconds.

12:27PM W11.00007 Ab initio calculation of indirect light absorption by free carriers in transparent conducting oxides[1] , HARTWIN PEELAERS, EMMANOUIL KIOUPAKIS, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106-5050 — Phonon-assisted absorption of light by free carriers is an important optical process in many materials and a challenging problem for computational condensed-matter physics. As transparent conducting oxides play an important role as contacts to light emitters and photovoltaic devices, it is important to consider not only the optical absorption across the band gap, but also the absorption by free carriers due to indirect processes mediated by phonons and defects. Here we calculate these losses using a full ab initio methodology as opposed to a phenomenological Drude model containing empirical parameters. These calculations involve the electron-phonon coupling matrix elements, which are dominated by the longitudinal optical phonon modes. We also compare with the Fröhlich model, which describes the electron-phonon matrix elements in the long-wavelength limit.

[1]This work was supported by DOE, the UCSB SSLEC, and the BAEF.

12:39PM W11.00008 Optical absorption of light carrying orbital angular momentum by semiconductors: free-particle quantum kinetics , P.I. TAMBORENEA, G.F. QUINTEIRO, Departamento de Física and IFIBA, Universidad de Buenos Aires, Argentina — We develop a free-carrier theory of the optical absorption of light carrying orbital angular momentum (twisted light) by bulk and quasi-two-dimensional semiconductors. We obtain the optical transition matrix elements for Bessel-mode twisted light and use them to calculate the wave function of photo-excited electrons to first-order in the vector potential of the laser [1]. We then pose the problem of the quantum kinetics of interband transitions in terms of the Heisenberg equations of motion of the electron populations, and interband and intraband coherences [2]. We solve the equations of motion in the low-excitation regime, and obtain analytical expressions for the coherences and populations; with these, we calculate the orbital angular momentum transferred from the light to the electrons and the paramagnetic and diamagnetic electric current densities.

[1] G. F. Quinteiro and P. I. Tamborenea, EPL **85**, 47001 (2009).
[2] G. F. Quinteiro and P. I. Tamborenea, Phys. Rev. B **82**, 125207 (2010).

12:51PM W11.00009 Optical harmonics generation in semiconductor quantum dots: A tunable terahertz source , YAN XIE, Beijing Computational Science Research Center, WEIDONG CHU, SUQING DUAN, WEI ZHANG, Institute of Applied Physics and Computational Mathematics — The high-order harmonic generation (HHG) study have been extended to semiconductor quantum dots (QDs) and coupled QDs (CQDs), the so-called "artificial atoms and molecules." One motivation of the study of the HHG in QDs is to find an efficient way of terahertz wave generation due to their controllable energy spectra and wave functions. With the help of Floquet theory, we show that the HHG in quantum dot structures can be changed from only odd orders to both odd and even orders by controlling the coupling parameters. The selection rules of the odd-even HHG in a noninversion-symmetric multilevel system are determined by the parity of emitted photon numbers during allowable virtual steps. On the other hand, by mapping the optical problem to a transport problem, we find that the terahertz generation efficiency is determined by the bandwidth of the quasienergy spectrum. Our studies are useful for engineering tunable terahertz sources based on semiconductor quantum dots.

1:03PM W11.00010 Ultrafast Quantum Control in Semiconductor Nanostructures using Twisted Light , GUILLERMO QUINTEIRO, PABLO TAMBORENEA, Univ de Buenos Aires, JAMAL BERAKDAR, Martin Luther Univ — We investigate possible uses of twisted light (TL) —or light carrying orbital angular momentum (OAM)— as a tool to control semiconductor-based nanostructures. Two systems are considered, namely quantum dots (QD) and quantum rings (QR). For both structures we employ a simplified two-band model in the effective-mass approximation, having a conduction and a heavy-hole valence bands. In the case of disk-shaped QDs, we predict that the TL would allow to induce optical transitions which are normally regarded to be forbidden. The OAM l and other parameters of the TL beam can be used to precisely control the final state of the electron. In the case of QRs, we study induced electric currents. We analyze the evolution of the system in terms of Heisenberg equations of motion. We find an analytical solution that resembles the standard Optical Bloch Equations. Using this solution, we find the evolution of the z-component of OAM and the electric current circulating the ring. Our results indicate that the electric current could be as large as μA, in the time-scale of pico-seconds. For an appropriate radius of the ring, the photo-induced magnetic field would be large enough to switch within picoseconds the magnetic moment of particles placed within the ring.

1:15PM W11.00011 Far-infrared absorption of PbSe nanorods , BYUNG-RYOOL HYUN, ADAM BARTNIK, Cornell University, WEON-KYU KOH, University of Pennsylvania, NIKOLAY AGLADZE, JUN YANG, AL SIEVERS, Cornell University, CHRISTOPHER MURRAY, University of Pennsylvania, FRANK WISE, Cornell University, OPTICS COLLABORATION, SYNTHESIS COLLABORATION, SPECTROSCOPY COLLABORATION — The far-infrared absorption spectra of PbSe nanodots and nanorods are measured as a function of aspect ratio, and show the expected splitting of the single Frohlich sphere mode in nanocrystals into two modes parallel and perpendicular to the nanorod axis. We analyze this splitting by modeling the dependence of the nanocrystal's local field factor on its shape. Excellent agreements is found with the features measured in experiment. We predict that this shape-dependent local field factor will cause a two-order of magnitude increase of the third-order susceptibility of long nanorods in the near-infrared.

1:27PM W11.00012 Bright spot pattern generation in GaAs/AlGaAs multiple quantum wells[1] , ANGELO MASCARENHAS, BRIAN FLUEGEL, National Renewable Energy Laboratory, D.W. SNOKE, Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania 15260, USA — Exciton photoluminescence pattern generation is investigated in multiple quantum wells. High-contrast outer rings and localized bright spots are generated using efficient field-assisted upconversion of laser light whose photon energy lies below the energy of the luminescing quantum well transition. Time-resolved images of the bright spot reveal that the ring transients are driven by carrier diffusion both from the laser excitation spot as well as from the bright spot. These dynamics are not explained simply by two-dimensional rate equations for generation and diffusion. The behavior must be understood as a result of three-dimensional transport in the vertically extended samples.

[1]We acknowledge the financial support of the Department of Energy, Office of Science, Basic Energy Sciences.

1:39PM W11.00013 Nonlinear optical properties of polychlorotriphenylmethyl radicals: a computational study , CLAUDIA CARDOSO, BRUCE FORBES MILNE, FERNANDO NOGUEIRA, Centro de Física Computacional, Faculdade de Ciências e Tecnologia, Universidade de Coimbra — The special interest in molecular design for the development of novel second-order nonlinear optical (SONLO) materials is driven by their potential applications in new optoelectronic technologies. Various strategies are currently employed to enhance the molecular SONLO activity, and studies revealed that species having open-shell electronic states exhibit larger β values than analogous closed-shell systems. Their open-shell electronic structure leads to accessible low-lying charge transfer electronic states which enhance the β values with respect to their closed-shell counterparts. We present the results of a Density Functional Theory calculations of a series of substituted polychlorinated triphenylmethyl radicals. This family of radicals has been measured by Ratera et al using Hyper-Rayleigh Scattering and showed to have enhanced β values. The present study compares results obtained within LDA and several hybrid functionals, namely long-range corrected functionals. The effect of solvents was also considered through the use of the polarizable continuum model.

1:51PM W11.00014 Binding energies of indirect excitons in double quantum well systems , ALEX ROSSOKHATY, Russian Academy of Sciences, Chernogolovka, STEFAN SCHMULT, WERNER DIETSCHE, KLAUS VON KLITZING, Max-Planck-Institute for Solid State Research, Stuttgart, IGOR KUKUSHKIN, Russian Academy of Sciences, Chernogolovka — A prerequisite towards Bose-Einstein condensation is a cold and dense system of bosons. Indirect excitons in double GaAs/AlGaAs quantum wells (DQWs) are believed to be suitable candidates. Indirect excitons are formed in asymmetric DQW structures by mass filtering, a method which does not require external electric fields. The exciton density and the electron-hole balance can be tuned optically. Binding energies are measured by a resonant microwave absorption technique. Our results show that screening of the indirect excitons becomes already relevant at densities as low as $5{\times}10^9 \mathrm{cm}^{-2}$ and results in their destruction.

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W12 FIAP: Electronic Transport in Novel Materials and Nanostructures D223/224

11:15AM W12.00001 ABSTRACT WITHDRAWN –

11:27AM W12.00002 Random Telegraph Noise in Silicon Nanowire BioFETs , NITIN RAJAN, Yale University, DAVID ROUTENBERG, Scripps Research Institute, JIN CHEN, Stanford University, MARK REED, Yale University — Noise spectroscopy is important for nanostructures because it represents a highly sensitive and non-destructive means of studying surface states/defects. In this study we characterize the low frequency noise of top-down fabricated silicon nanowire FETs with exposed channels at low temperature. For some devices, we observe a change in the noise spectra as temperature is lowered, from 1/f to Lorentzian. This indicates the presence of random telegraph signals (RTS) due to an interface trap which we confirm from the time-domain measurements. By making measurements at different temperatures, we can probe into the dynamic properties of the trap. In this way, the activation energies for the emission and capture of electrons are determined. The nature and position of the trap is deduced from the gate voltage dependence of the emission and capture time constants. We also observe an increase in the relative RTS noise amplitude as temperature is decreased and report on very large (>100%) relative noise amplitudes for measurements carried out at low temperature.

11:39AM W12.00003 Distinct microwave photoresistivity peak in a high-mobility quantum Hall system[1] , A.T. HATKE, M.A. ZUDOV, University of Minnesota, L.N. PFEIFFER, K.W. WEST, Princeton University — We report on a distinct resistivity peak in a microwave-irradiated high-mobility two-dimensional electron system at low temperatures. This peak appears in the regime of well separated Landau levels near the second harmonic of the cyclotron resonance and is in addition to microwave-induced resistance oscillations. This talk will focus on the generic characteristics of this peak, such as its dependence on microwave power and temperature.

[1]This work is supported by DOE DE-SC0002567 and NSF DMR-0548014.

11:51AM W12.00004 Theory of nonlinear transport in separated Landau levels of two-dimensional electron systems[1] , M. KHODAS, University of Iowa, H.-S. CHIANG, A.T. HATKE, M.A. ZUDOV, University of Minnesota, L.N. PFEIFFER, K.W. WEST, Princeton University — Recent experiments have shown that the differential magnetoresistivity of a high mobility two-dimensional electron system (2DES) is strongly suppressed under applied dc bias. This phenomenon is most pronounced when the Landau level width becomes smaller than the cyclotron energy. Using the quantum kinetics approach we calculate the characteristic current responsible for the suppression and compare the results to the experimental data obtained on a high mobility 2DES at low temperatures.

[1]This work is supported by NSF DMR-0548014 and DOE DE-SC0002567.

12:03PM W12.00005 ABSTRACT WITHDRAWN –

12:15PM W12.00006 ABSTRACT WITHDRAWN –

12:27PM W12.00007 Terahertz Spectroscopy of Semiconductor Materials and Nanostructures , WILLIAM BAUGHMAN, SHAWN DAVID WILBERT, LEE BUTLER, NICK HARRIS, GANG SHEN, NABIL DAWAHRE, JOSEPH BREWER, PATRICK KUNG, SEONGSIN MARGARET KIM, The University of Alabama — Terahertz (THz) time-domain spectroscopy is an attractive method to obtain the electronic transport properties in a variety of semiconductor materials and nanostructures. Unlike traditional techniques, THz spectroscopy does not require the realization of electrical contacts or even direct contact to the material probed. Here, we report the use of THz time-domain spectroscopy to determine the dielectric constant of a variety of semiconductor materials in the THz spectral range, and extract the refractive index, absorption coefficient and electrical conductivity. We also present a comparison of the results obtained from other techniques, including four-point probe resistivity measurements.

12:39PM W12.00008 Statistics of excitations in the electron glass model , MATTEO PALASSINI, University of Barcelona — We study the statistics of elementary excitations in the classical electron glass model of localized electrons interacting via the unscreened Coulomb interaction in the presence of disorder. We reconsider the long-standing puzzle of the exponential suppression of the single-particle density of states near the Fermi level, by measuring accurately the density of states of charged and electron-hole pair excitations via finite temperature Monte Carlo simulation and zero-temperature relaxation. We also investigate the statistics of large charge rearrangements after a perturbation of the system, which may shed some light on the slow relaxation and glassy phenomena recently observed in a variety of Anderson insulators. In collaboration with Martin Goethe.

12:51PM W12.00009 Kondo Effect in a mesoscopic system[1] , SEUNGJOO NAH, MICHAEL PUSTILNIK, Georgia Institute of Technology — At low temperatures, transport and thermodynamic properties of Coulomb blockade systems are characterized by the energy scale T_K (the Kondo temperature). We show that the Kondo temperature is subject to strong mesoscopic fluctuations. In a quantum dot system with many single-particle energy levels, the Kondo temperature acquires a log-normal distribution.

[1]This work was supported by the NSF (DMR-4106B23).

1:03PM W12.00010 Two-Dimensional Electrostatic Lattices for Excitons , MIKAS REMEIKA, LEONID BUTOV, University of California, San Diego — We report on a method for the realization of two-dimensional electrostatic lattices for excitons in quantum well structures. The lattice structure is set by an electrode pattern and the amplitude of the lattice potential is controlled by applied voltages. We demonstrate square, hexagonal, and honeycomb lattices created by this method.

1:15PM W12.00011 Non-Markovian effects in the quantum noise of interacting nanostructures , CLIVE EMARY, TU Berlin, DAVID MARCOS, RAMON AGUADO, ICMM, TOBIAS BRANDES, TU Berlin — We present a theory of finite-frequency noise in non-equilibrium conductors, and in particular, interacting nanostructures. We employ a quantum master equation approach and treat correlations between the system and the reservoirs in a nonMarkovian fashion. These correlations are pivotal in properly describing current fluctuations in situations where the measuring frequency is larger than both the applied voltage and the temperature. We explicitly show the importance of nonMarkovian effects in different contexts, including the finite-frequency current noise through a double quantum dot charge qubit and the short-time counting statistics of quantum dots.

1:27PM W12.00012 Nonlinear Insulator in Complex Oxides , ZHIQI LIU, T. VENKATESAN, A. ARIANDO, NANOCORE, NUS TEAM, NTU COLLABORATION — For complex oxides, the very concept of an insulator must be re-examined as they behave differently from conventional insulators such as SiO_2 due to the presence of multiple defect levels within bandgap. As the semiconductor industry is moving to such oxides for high-k materials, we need to truly understand the insulating properties of them under various electrical excitations. We report a class of material which we coin as nonlinear insulators that exhibit reversible electric-field-induced metal-insulator transitions (MIT). We show this behaviour for an insulating $LaAlO_3$thin film with a large bandgap of $\sim$5.6 eV in a metal/$LaAlO_3$/Nb-$SrTiO_3$ heterostructure. The reversible MIT is attributed to the formation of a quasi-conduction band (QCB) in the defect states of $LaAlO_3$ that forms a continuum state with the conduction band of the Nb-$SrTiO_3$. An opposing voltage is required to deplete the charges from the QCB. The implications of these nonlinear insulators are far-reaching. For example, the use of multi-component oxides as insulators in devices (e.g., high-k dielectrics in silicon CMOS devices) must be exercised with caution.

1:39PM W12.00013 Tailoring the Crystal Structure of Individual Silicon Nanowires by Polarized Laser Annealing , CHIA-CHI CHANG, Department of Physics, University of Southern California, HAITIAN CHEN, CHUN-CHUNG CHEN, CHONGWU ZHOU, STEPHEN CRONIN, Department of Electrical Engineering, University of Southern California — We study the effect of polarized laser annealing on the crystalline structure of individual amorphous and nano-crystalline silicon nanowires (Si NWs) using Raman spectroscopy. The crystalline fraction of annealed NWs increases dramatically from 0 to 0.93 with increasing incident laser power. We observe Raman line shape narrowing and frequency hardening upon laser annealing due to the increase in crystal grain size. The Raman anti-Stokes:Stokes intensity ratio is used to determine the local heating temperature caused by the intense focused laser spot, which shows a strong polarization dependence on both single crystal bulk Si and nano-crystalline Si NWs. This method provides a new approach to control the crystal structure rather than by simply adjusting the laser power. Furthermore, strain induced linewidth broadening and frequency softening was also observed in bent nano-crystalline Si NWs, and the deformation stress can be released via laser annealing.

1:51PM W12.00014 A novel method for measuring electrical conductance in thin solid films that is insensitive to contact effects , TAMAR MENTZEL, MOUNGI BAWENDI, MARC KASTNER, Massachusetts Institute of Technology — The synthesis of novel materials has been a primary driver in the emerging fields of organic-based electronics and nanoelectronics. One major obstacle to the research and development of novel materials is the ability to electrically characterize the material without introducing a significant contact resistance or damaging the material. In organic materials, the contact material has been found to alter the morphology of and to penetrate into the organic molecules, to form Schottky barriers, and to be thermally and mechanically unstable. Throughout nanoelectronics, unstable contacts and large contact resistances arise because of the reduced contact area as devices shrink in size. I will present a novel method for measuring electrical conductance in thin solid films that is insensitive to contact effects. In place of standard current measurements, a nanoscale metal-oxide-semiconductor field-effect transistor (MOSFET) is used to sense charge diffusion in a thin film of amorphous germanium. The contact resistance between the amorphous germanium and a pair of gold electrodes can be modulated *in situ* without affecting the conductance measurement. Moreover, our technique enables the measurement of conductance as low as 10^{-19} S with application of only 1 V to the film. This method can be used to electrically characterize any thin film which is sensitive to contact effects or where the resistance is too high to measure with conventional methods.

2:03PM W12.00015 Spectrometry of electron pumping by surface acoustic waves , M.J. BENESH, M. KATAOKA[1], C.J.B. FORD, C.H.W. BARNES, J.P. GRIFFITHS, G.A.C. JONES, I. FARRER, D.A. RITCHIE, University of Cambridge — Surface acoustic waves (SAWs) generate an electrostatic potential wave when applied to a GaAs/AlGaAs heterostructure. Electrons may be captured in a SAW minimum, creating a dynamic quantum dot (QD). SAW-defined QDs may be useful for certain quantum computing schemes, since, for example, they provide reliable single-electron transport and reduce the need for fast gate switching. Surface gates above a 2D electron gas (2DEG) are used to define a quasi-1D channel (Q1DC) at a potential far above the Fermi level. A SAW pulse captures electrons from the 2DEG and pumps a number of them controllably through the Q1DC. As a SAW minimum rises up the potential slope at the channel entrance, the QD is squeezed and some electrons are ejected back into the 2DEG with energies above the Fermi level. In our experiment, we probe the range of energies at which the electrons are emitted using a narrow potential barrier as an energy spectrometer. We can also measure electrons that have been pumped through the channel. We compare these results with a model for the SAW capture/pumping process.

[1]Now at NPL Teddington.

Thursday, March 24, 2011 11:15AM - 1:51PM –

Session W13 GSNP DBP: Applications of Statistical and Nonlinear Physics in the Life Sciences

D225/226

11:15AM W13.00001 Mean-field theory of four species in cyclic competition[1] , C.H. DURNEY, S.O. CASE, M. PLEIMLING, R.K.P. ZIA, Virginia Tech — We consider a simple model of cyclic competition of M species: When a pair of individuals from species k and $k+1$ interact, the latter transforms into the former. Even with no spatial structure, such systems often display interesting and counterintuitive behavior. With possible applications in both biological systems (e.g., Min proteins, E. Coli, lizards) and game theory (e.g., rock-paper-scissors), the $M = 3$ case has attracted considerable recent attention. We study a $M = 4$ system (with no spatial structure) and find major differences, e.g., (1) the presence of macroscopically many absorbing states, (2) coexistence of species, and (3) violation of the "law" of survival of the weakest - a central theme in the $M = 3$ case. Like the game of Bridge, the system typically ends with "partner pairs." After describing the full stochastic model and its master equation, we present the mean-field approximation. Several exact, analytic predictions will be shown. Their limitations and implications for the stochastic system will also be discussed.

[1]Supported in part by NSF-DMR-0705152, 0904999, 1005417.

11:27AM W13.00002 Stochastic evolution of four species in cyclic competition: exact and simulation results[1] , S.O. CASE, C.H. DURNEY, M. PLEIMLING, R.K.P. ZIA, Virginia Tech — We study a stochastic system with N individuals, consisting of four species competing cyclically: $A + B \longrightarrow A + A$, $\cdots$, $D + A \longrightarrow D + D$. Randomly choosing a pair and letting them react, N is conserved but the fractions of each species evolve non-trivially. At late times, the system ends in a static, absorbing state – typically, coexisting species AC or BD. The master equation is shown and solved exactly for $N = 4$, providing a little insight into the problem. For large N, we rely on simulations by Monte Carlo techniques (with a faster dynamics where a reaction occurs at every step). Generally, the results are in good agreement with predictions from mean field theory, after appropriate rescaling of Monte Carlo time. The theory fails, however, to describe extinction or predict their probabilities. Nevertheless, it can hint at many remarkable behavior associated with extinction, which we discover when studying systems with extremely disparate rates.

[1]Supported in part by NSF-DMR-0705152, 0904999, 1005417.

11:39AM W13.00003 Random inheritance in a stochastic Lotka-Volterra model , ULRICH DOBRAMYSL, Department of Physics, Virginia Tech, GABRIEL MARTINEZ, Department of Computer Science, Virginia Tech, UWE C. TÄUBER, Department of Physics, Virginia Tech — We introduce a stochastic two-species Lotka-Volterra predator-prey model that includes random inheritance features. Specifically, each individual particle takes on a predation rate value which is determined when the particle is created and is dependent on the particle's parent. Thus we arrive at a simple model for evolution due to selection pressure. We employ Monte Carlo simulations to study the time evolution of the predation rate distribution as a function of the prescribed variability. We find that this model yields a steady state with optimized rates for both predator and prey species. Contrary to, e.g., gene expression models, the rates do not experience fixation at extreme values. An approximate description of the resulting data is achieved by means of an effective master equation approach for the predation rate distribution.

11:51AM W13.00004 Time-dependent mechanical response of a network model for the cytoskeleton[1] , NASRIN AFZAL, MICHEL PLEIMLING, Virginia Tech — Motivated by a series of experiments that study the response of the cytoskeleton in living cells to time-dependent mechanical forces, we investigate through Monte Carlo simulations a three-dimensional network subjected to time-dependent perturbations. After having prepared the system in a relaxed state, time-dependent shear or stress is applied and the response is monitored. We discuss the possible implications of our results for the time-dependent mechanical response of the cytoskeleton.

[1]Supported in part by the US National Science Foundation through Grant DMR-0904999.

12:03PM W13.00005 Hopf Bifurcations in a Model for Circadian Rhythms in Arabidopsis Thaliana , ORRIN SHINDELL, RANDALL TAGG, University of Colorado Denver — Arabidopsis thaliana is a plant used for many fundamental studies, including circadian rhythms. Numerically integrating the 7-equation kinetic model of Locke et al. [J. Theor. Bio. 234 (2005) 383], we have mapped regions of parameter space where circadian expression of key mRNA and proteins undergoes limit cycle oscillation. We seek to relate this to the work of Fukuda et al. [Phys. Rev. Lett. 99 (2007) 098102], where a coupled system of cells individually described by Stuart-Landau equations is used phenomenologically to describe experimentally observed spatio-temporal patterns in the plant leaves. To that end we have done a weakly nonlinear analysis of the system of kinetic equations. We also comment on possible experimental directions to further connect the kinetic models to dynamics in this multi-cellular system.

12:15PM W13.00006 Translation with secondary structure: Dynamic blockages in totally asymmetric simple exclusion process , LEAH SHAW, College of William and Mary — The totally asymmetric simple exclusion process (TASEP) is often used as a model for protein synthesis, with the lattice and particles representing the mRNA and ribosomes, respectively. Here we model the effect of secondary structure (folding) of the mRNA by introducing a dynamic blockage region in the lattice. If the region is unoccupied by particles, the blockage can close and prevent upstream particles from moving into it, representing the folding of that section of mRNA. Reopening of the blockage, allowing particles to pass, represents unfolding. We study the effects of the blockage size, closing/opening probabilities, and TASEP parameters on the particle current and blockage switching rates.

12:27PM W13.00007 Rescue Interventions in Biological and Physical Networks , SEAN CORNELIUS, Northwestern University — Gene knockout experiments on single cells have established that expression of most genes is not needed for optimal growth. Yet, environmental and genetic perturbations to these organisms are known to be accompanied by the transient activation of a large number of latent metabolic pathways, suggesting that the temporarily activated reactions increase growth in the presence of perturbations. We have tested this hypothesis computationally and found, surprisingly, that the availability of latent pathways tends in fact to inhibit growth after genetic perturbations. This adverse effect indicates that latent pathway activation is derivative of a suboptimal response and that consequently, growth can actually be improved by removing these pathways from the network. In this talk, I will relate this counterintuitive effect to very recent research showing that a loss in network performance inflicted by an external perturbation can be mitigated by the application of additional perturbations. The challenge is to identify such "rescues" under constraints that limit the type of perturbations that can be made. I will present an approach to identify such eligible rescues for general networks modeled as dynamical systems, and present computational examples for biological and physical networks.

12:39PM W13.00008 Feedback control for stabilizing chaotic spiral waves during cardiac ventricular fibrillation[1] , ILIJA UZELAC, JOHN WIKSWO, Vanderbilt University, RICHARD GRAY, Food and Drug Administration — The cardiac arrhythmias that lead to ventricular fibrillation (VF) arise from electrical spiral waves (SW) rotating within the heart with a characteristic period τ. A single drifting SW can degenerate into a chaotic system of multiple SWs and VF. Hence early SW detection and termination is crucial to prevent VF. Time-delayed feedback control (TDFC) is well known approach for stabilizing unstable periodic orbits embedded in chaotic attractors. We hypothesize that cardiac SWs can be stabilized by TDFC with a time-delay of τ. Implementing this approach will require precise, closed-loop control of the charge delivered to the heart during the defibrillation process. To do this, we have developed a 2 kW arbitrary-waveform voltage-to-current converter (V2CC) with a 1 kHz bandwidth that can deliver up to 5 A at 400 V for 500 ms, and a photodiode system for recording in real time an optical electrocardiogram, OECG(t). The feedback signal driving the V2CC will be the time-difference (OECG(t) - OECG(t-T), where we hypothesize that T is τ, the period of the SW. This may dramatically decrease defibrillation voltages by using a defibrillation waveform customized to the VF event, unlike commercial capacitor defibrillators.

[1]Supported in part by NIH R01 HL58241-11 through ARRA 2009

12:51PM W13.00009 Experimental and theoretical evidence for fluctuation driven activations in an excitable chemical system[1] , HAROLD HASTINGS, SABRINA SOBEL, Hofstra University, RICHARD FIELD, University of Montana, SCOTT MINCHENBERG, NICOLE SPINELLI, KEITH ZAUDERER, Hofstra University — An excitable medium is a system in which small perturbations die out, but sufficiently large perturbations generate large "excitations." Biological examples include neurons and the heart; the latter supports waves of excitation normally generated by the sinus node, but occasionally generated by other mechanisms. The ferroin-catalyzed Belousov-Zhabotinsky reaction is the prototype chemical excitable medium. We present experimental and theoretical evidence for that random fluctuations can generate excitations in the Belousov-Zhabothinsky reaction. Although the heart is significantly different, there are some scaling analogies.

[1]This material is based upon work supported by the Department of Energy under Award Number DE-FG02-08ER64623.

1:03PM W13.00010 The statistical physics of decision-making in insect colonies , PATRICK M. HOGAN, Department of Computer Science, University of Sheffield, UK, THOMAS SCHLEGEL, NIGEL R. FRANKS, School of Biological Sciences, University of Bristol, UK, JAMES A.R. MARSHALL, Department of Computer Science, University of Sheffield, UK — We apply the stochastic methods of statistical physics to analyse collective-decision making in social insect colonies, allowing us to derive the colony-level behaviour from an individual-level model. This contrasts with the traditional approach where a differential equation model, with or without arbitrary noise terms, is assumed. Social insect colonies vary in size from on the order 100 to 10,000,000 individuals, and such a statistical physics approach allows us explicitly to derive equations for both the average behaviour and the noise in the system, across this entire scale. We develop such a framework by building upon an existing stochastic model of opinion formation to model the decision-making processes in emigrating ant colonies. This new model is both driven by and evaluated against results from experiments with rock ants. This allows us to elucidate rigorously the role played by the individual-level phenomena of direct switching in the colony-level decision-making process, which optimality theory has predicted to be of crucial importance, and which we compare with our experimental results. This illustrates the power of the stochastic methods of statistical physics for understanding social insect colonies as complex systems.

1:15PM W13.00011 Thermodynamic efficiency out of equilibrium , DAVID SIVAK, GAVIN CROOKS, Lawrence Berkeley National Laboratory — Molecular-scale machines typically operate far from thermodynamic equilibrium, limiting the applicability of equilibrium statistical mechanics to understand their efficiency. Thermodynamic length analysis relates a non-equilibrium property (dissipation) to equilibrium properties (equilibrium fluctuations and their relaxation time). Herein we demonstrate that the thermodynamic length framework follows directly from the assumptions of linear response theory. Uniting these two frameworks provides thermodynamic length analysis a firmer statistical mechanical grounding, and equips linear response theory with a metric structure to facilitate the prediction and discovery of optimal (minimum dissipation) paths in complicated free energy landscapes. To explore the applicability of this theoretical framework, we examine its accuracy for simple bistable systems, parametrized to model single-molecule force-extension experiments. Through analytic derivation of the equilibrium fluctuations and numerical calculation of the dissipation and relaxation time, we verify that thermodynamic length analysis (though derived in a near-equilibrium limit) provides a strikingly good approximation even far from equilibrium, and thus provides a useful framework for understanding molecular motor efficiency.

1:27PM W13.00012 A simple model for the transmission of malaria , ADRIANA DICKMAN, PUC Minas — We study a simple lattice model describing the transmission of malaria. The transmission of the disease to humans occurs through contact with an infected mosquito, while a healthy mosquito can become infected through contact with an infected human. Recovered individuals are susceptible to re-infection. The mosquitoes diffuse through the lattice, spreading the disease. We show preliminary results for the model obtained via site approximation (mean-field theory).

1:39PM W13.00013 Genearlized force-extension relation for DNA confined in sub-100nm nanoslits , YENG-LONG CHEN, PO-KENG LIN, CHIA-FU CHOU, Institute of Physics and Research Center for Applied Sciences, Academia Sinica — We generalize the force-extension relation of DNA molecules confined in persistence length scale nanoslits. In strong confinement with slit geometry, the segmental correlation length of DNA molecules have two components – in the confined and unconfined dimensions. In the confined dimension, the segmental correlation length is controlled by the slit height. In the unconfined dimension, the segmental correlation length increases as the slit height decreases. We characterize this effect, and generalize how this affects the entropic elasticity of confined DNA molecules. In addition, we investigate the structure of dense strongly confined semi-flexible polymers.

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W14 GSNP: Focus Session: Extreme Mechanics: Elasticity and Deformation III D227

11:15AM W14.00001 A general theory of mechanical instabilities in soft solids , EVAN HOHLFELD, Department of Physics, Harvard University and Chemical Sciences Division, LBNL, L. MAHADEVAN, Engineering and Applied Sciences, Kavli Institute for Nanobio Science and Technology, Harvard University — Some instabilities in soft solids, e.g. buckling and wrinkling, can be detected in linearized analysis. Surprisingly, linearly stable configurations can still have nonlinear instabilities with strictly zero energy barrier. Two examples are cavitation (formation of voids) and sulcification (formation of sharply creased free surface folds), wherein singularities nucleate and grow when a critical strain is achieved. Here we present the first general theory of stability in nonlinearly elastic materials. The theory predicts when singularities spontaneously form, irrespective of linearized analysis, and how these can be controlled with geometry. Such "hidden" instabilities arise from the scale-free geometric and constitutive nonlinearities common in soft materials, and can be understood as scale symmetry breaking processes in simple cases. More deeply, even buckling and wrinkling can be traced back to scale-free linear instabilities (loss of ellipticity at an interface) as was first explained by M. A. Biot. We illustrate the theory with simulations and experiments on sulcification. Time allowing we will also discuss fracture and delamination.

11:27AM W14.00002 Elastocapillary imbibition , CAMILLE DUPRAT, JEFFREY ARISTOFF, HOWARD STONE, Department of Mechanical and Aerospace Engineering, Princeton University, PRINCETON UNIVERSITY TEAM — The deformation of elastic structures under capillary forces (elastocapillarity), and their interaction with fluid flow (elastohyrodynamics), are relevant to many biological, geophysical and engineering processes. Here, we present the dynamics of surface-tension-driven flow into a gap between flexible boundaries (i.e. elastocapillary imbibition). We examine two model systems of elastocapillary imbibition, with and without gravitational effects, using a combination of experiment, theory, and numerical simulation. We identify the characteristic length and time scales, and demonstrate how the prescence of flexible boundaries leads to a departure from classical imbibition. The time to reach equilibrium (if one exists) is determined, and a criterion for the coalescence of the boundaries is established. Good agreement between experiment and theory is obtained.

11:39AM W14.00003 Buckling of swelling gels under constraints , HOWON LEE, University of Illinois at Urbana-Champaign, JIAPING ZHANG, YONGHAO AN, HANQING JIANG, Arizona State University, NICHOLAS FANG, Massachusetts Institute of Technology — Buckling is a traditional topic in mechanics and has been thought to be well studied for the last hundred years. Recently, buckling has drawn new attention in a different perspective; a novel scheme for pattern transformation. Here we present an experimental study on buckling using swelling of gels under constraints. Under critical conditions combined with proper mechanical constraints, non-homogenous stress develops as gel swells, which gives rise to buckling instability. We developed a fabrication technique to make a 3D cylinder-shaped microgel, the bottom end of which is tightly fixed on a rigid substrate to impose constraints. Equilibrium swelling study of such gel structure allowed us to determine a critical geometrical condition for buckling. Furthermore, exploiting slow gel swelling process, we recorded time evolution of buckling as gel swells to study post-buckling morphologies. Numerical simulation also showed close relationship between geometric parameters and resulting buckling pattern. We believe our study on buckling of swelling gels will not only help us better understand the mechanics of soft materials, but it will also contribute to increasing the breadth of possible application of soft materials in many emerging fields such as photonic crystals.

11:51AM W14.00004 Optimal control of growing sheets , GARETH JONES, L. MAHADEVAN, Harvard University — There has been much recent interest in plates and sheets that have the ability to actively swell, grow and bend. In this presentation an inhomogeneously growing plate is modeled by prescribing the in-plane growth strain and the active change-of-curvature function. The plate will then change shape to accommodate the induced strains. For applications of this phenomenon, an important problem is how best to choose these functions in order for the plate to deform to a given target shape. In seeking an answer to this question, we have developed a computational approach, where the growth strains will be found as solutions to a numerical optimization procedure. Example results will be presented which will provide some insight into the mechanical behavior of growing thin structures.

12:03PM W14.00005 Decoupling thermal, chemical, and mechanical strain components in thin films , MEREDITH SILBERSTEIN, ETHAN CRUMLIN, YANG SHAO-HORN, MARY BOYCE, MIT Mechanical Engineering — Many electrochemical systems have performance which is affected by internal strains due to thermal and/or chemical stimuli. The bi-material curvature method is a means to quantify these thermal and chemical strains and their coupling with mechanical stress. In this method, a thin layer of the material of interest is deposited on a substrate of intermediate thickness. The composite assumes a curvature that depends on the mismatch strains between the substrate and film. The Stoney formula provides an explicit expression for the film stress as a function of the elastic substrate properties, film and substrate thickness, and curvature. Here we study two distinct materials systems: Nafion used as the polymer electrolyte in low temperature fuel cells, and epitaxial perovskite thin films used as a catalyst for the oxygen reduction reaction in solid oxide fuel cells. The thermal, chemical, and mechanical strains are quantitatively determined as functions of temperature and atmospheric conditions by monitoring the curvature evolution with changes in these parameters. The extent of coupling of the thermal and chemical strains with mechanical stress is evaluated by conducting the experiment at multiple substrate thicknesses.

12:15PM W14.00006 Plane deformations generating a prescribed finite rotation field , GREGORY RIZZA, JANET BLUME, Brown University — Compatibility conditions for various strain measures are well known in both small and finite strain kinematics. For many problems, such conditions enable boundary value problems to be formulated using strains, stresses, or a generating potential function, as the fundamental dependent variable(s). These methods are effective, as most strain fields fully determine the generating deformations up to an arbitrary rigid deformation. Our research is concerned with the compatibility issue for the rotation field. Although it is not a direct measure of the distortion in a deformation, the rotation associated with a deformation and its variation from point to point within a body turns out to carry quite a bit of information about the actual deformation. For the case of plane deformation, we have been able to show that any suitably smooth plane proper orthogonal tensor field may serve as a finite rotation tensor for a generating deformation. We have developed several examples demonstrating this relationship between material deformation and rotation fields. Our results demonstrate in the case of plane deformation, any skew-symmetric two-dimensional tensor field can serve as a plane rotation field. The relation between the position-dependence of a rotation field and generating deformation information has implications in both mechanical twinning and shear banding.

12:27PM W14.00007 Mechanics of Suture Joints , YANING LI, JUHA SONG, CHRISTINE ORTIZ, MARY BOYCE, MIT, ORTIZ GROUP/DMSE/MIT TEAM, BOYCE GROUP/ME/MIT TEAM — Biological sutures are joints which connect two stiff skeletal or skeletal-like components. These joints possess a wavy geometry with a thin organic layer providing adhesion. Examples of biological sutures include mammalian skulls, the pelvic assembly of the armored fish Gasterosteus aculeatus (the three-spined stickleback), and the suture joints in the shell of the red-eared slider turtle. Biological sutures allow for movement and compliance, control stress concentrations, transmit loads, reduce fatigue stress and absorb energy. In this investigation, the mechanics of the role of suture geometry in providing a naturally optimized joint is explored. In particular, analytical and numerical micromechanical models of the suture joint are constructed. The anisotropic mechanical stiffness and strength are studied as a function of suture wavelength, amplitude and the material properties of the skeletal and organic components, revealing key insights into the optimized nature of these ubiquitous natural joints.

12:39PM W14.00008 Mechanical and thermal stability of adhesive membranes with nonzero bending rigidity , TUOMAS TALLINEN, Harvard University / University of Jyvaskyla, JAN ASTROM, CSC - The Finnish IT Center for Science, PEKKA KEKALAINEN, JUSSI TIMONEN, University of Jyvaskyla — Membranes at a microscopic scale are affected by thermal fluctuations and self-adhesion due to Van der Waals forces. Methods to prepare membranes of even molecular scale, e.g. graphene, have been recently developed, and the question of their mechanical and thermal stability is of crucial importance. To this end we modeled microscopic membranes with a short-range attractive interaction and applied Langevin dynamics. Their behavior was also analyzed under external loading. Even though these membranes folded during isotropic compression as a result of energy minimization, the process at high confinement did not differ much from crumpling of macroscopic thin sheets. The main difference appeared when the external load was released. In such cases, for membranes of sufficiently large size L, folded or scrolled conformations emerged. At high enough temperature T entropic effects made such conformations unfavorable, however. Possible conformations of free-standing membranes ("phase diagrams") were determined in the TL-plane.

12:51PM W14.00009 Universal Shapes formed by Interacting Cracks , MELISSA FENDER, North Carolina State University, FREDERIC LECHENAULT, University of Montpellier, KAREN DANIELS, North Carolina State University — Brittle failure through multiple cracks occurs in a wide variety of contexts, from microscopic failures in dental enamel and cleaved silicon to geological faults and planetary ice crusts. In each of these situations, with complicated curvature and stress geometries, pairwise interactions between approaching cracks nonetheless produce characteristically curved fracture paths known in the geologic literature as en passant cracks. While the fragmentation of solids via many interacting cracks has seen wide investigation, less attention has been paid to the details of individual crack-crack interactions. We investigate the origins of this widely observed crack pattern using a rectangular elastic plate which is notched on each long side and then subjected to quasistatic uniaxial strain from the short side. The two cracks propagate along approximately straight paths until the pass each other, after which they curve and release a lenticular fragment. We find that, for materials with diverse mechanical properties, the shape of this fragment has an aspect ratio of 2:1, with the length scale set by the initial cracks offset s and the time scale set by the ratio of s to the pulling velocity. The cracks have a universal square root shape, which we understand by using a simple geometric model and the crack-crack interaction.

1:03PM W14.00010 Pericyte Actomyosin-Mediated Contraction at the Cell-Material Interface can Modulate the Microvascular Niche , ADAM ZEIGER, MIT, MACIEJ KOTECKI, Tufts University, JOHN MALONEY, MIT, IRA HERMAN, Tufts University, KRYSTYN VAN VLIET, MIT — Here we employ the experimental finding that pericytes can wrinkle a freestanding, underlying membrane via actin-mediated contraction. Pericytes were cultured on deformable silicone substrata. Local stiffness of subcellular domains was investigated by using AFM-enabled nanoindentation. Substratum contraction was quantified by normalized change in wrinkle contour lengths, and a model was used to relate local strain energies to pericyte contractile forces. The nature of pericyte-generated wrinkling and contractile protein-generated force transduction was further explored by the addition of pharmacological cytoskeletal inhibitors that affected contractile forces and the effective elastic moduli of pericyte domains. Actin-mediated forces are sufficient for pericytes to exert an average contraction of 38% on the substrata employed in these in vitro studies. Pericyte generated contractile forces thus serve as a direct mechanical stimulus to adjacent vascular endothelial cells, potentially altering the effective mechanical stiffness of nonlinear-elastic extracellular matrices, to modulate pericyte-endothelial cell interactions that directly influences physiologic angiogenesis.

1:15PM W14.00011 Extraordinary Elasticity of the Distorted Kagome Lattice , ANTON SOUSLOV, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104, KAI SUN, Joint Quantum Institute and Condensed Matter Theory Center, University of Maryland, College Park, MD 20742, XIAOMING MAO, TOM LUBENSKY, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104 — J. C. Maxwell discovered that a system of particles in d-dimensions will be marginally rigid, or *isostatic*, if each particle interacts on average with $2d$ of its neighbors. Isostatic models have been used to describe such diverse soft phenomena as the jamming transition and the elasticity in networks of semi-flexible polymer gels. We develop models based on the isostatic kagome lattice, which has a subextensive number of floppy phonon modes. We show that these can be extended into soft deformations by changing the particle configurations while keeping the bond lengths fixed. Thus, we create families of novel isostatic lattices, which exhibit highly tunable elastic properties as a consequence of isotropic linear elasticity with a zero bulk modulus. They have a negative Poisson ratio, or auxetic (anti-rubber) behavior. Further, we find no bulk soft phonons at large length scales due to conformal symmetry. We discuss the intimate relationship between various symmetries and soft response in these models as well as the relation of these models to other marginally rigid systems.

1:27PM W14.00012 Suppression of Viscous Fingers in Miscible Hele-Shaw Flow , RADHA RAMACHANDRAN, JUSTIN BURTON, SIDNEY NAGEL, University of Chicago — The flow of two immiscible fluids between closely-spaced parallel plates can be highly unstable and produce a series of complex fingering patterns when the less viscous injected fluid invades the more viscous one. Air displacing granular material in such a Hele-Shaw geometry shows similar patterns with sharp features consistent with the granular/air surface tension being virtually zero [1]. Here we investigate the flow of two *miscible* fluids in a radial Hele-Shaw cell, with an inner liquid displacing an outer one of higher viscosity. We use two glycerol- water mixtures so that the viscosity can be tuned by varying the glycerol concentration. We vary the plate spacing and flow rate as well as the fluid viscosites. The non-equilibrium interfacial tension between these two miscible fluids is expected to be nearly zero. However, extrapolating to zero surface tension in the linear theory for Hele-Shaw flow does not describe our results. Specifically, flow becomes *stable* even when the inner liquid has a much lower viscosity than the outer one. At higher velocity, it is possible to see small amplitude fingering patterns develop.

[1] X. Cheng, L. Xu, A. Patterson, H. M. Jaeger and S. R. Nagel *Nature Physics* 4, 234 (2008).

1:39PM W14.00013 Patterns on thin sheets: buckling, wrinkling, crumpling, folding , BENNY DAVIDOVITCH, University of Massachusetts — Recent experiments on thin sheets under various geometric confinements and distributions of exerted forces found a multitude of pattern types. I will discuss the possibility of classifying this diverse phenomenology by generalizing concepts of primary and secondary instabilities, and basic types of symmetry breaking.

1:51PM W14.00014 Mechanics and chemical thermodynamics of a temperature-sensitive hydrogel[1] , SHENGQIANG CAI, Harvard University, ZHIGANG SUO — A temperature-sensitive hydrogel is a network of polymers containing monomers, whose interaction with water molecules can be tuned dramatically by changing temperature. In most cases, the swelling ratio of a temperature-sensitive hydrogel changes discontinuously upon heating above or cooling below a critical temperature, which is called volume phase transition. Interestingly, the coexistence of swollen phases and shrunk phases are frequently observed in the experiments for temperature-sensitive hydrogels and additionally, people have also discovered that a uniaxial force can induce phase transition in a temperature-sensitive gel bar .In order to understand these phenomena, we studied the mechanics and chemical thermodynamics of a temperature-sensitive hydrogel bar, by using the free-energy landscape of a bar made from PNIPAM gel. Following Gibbs, we plot the phase diagram of a temperature-sensitive hydrogel bar under uniaxial force.

[1]This work is supported by the NSF (CMMI-0800161) and by the MRSEC at Harvard University.

2:03PM W14.00015 Mechanics of Curved Folds[1] , MARCELO A. DIAS, CHRISTIAN D. SANTANGELO, University of Massachusetts Amherst — Despite an almost two thousand year history, origami, the art of folding paper, remains a challenge both artistically and scientifically. Traditionally, origami is practiced by folding along straight creases. A whole new set of shapes can be explored, however, if, instead of straight creases, one folds along arbitrary curves. We present a mechanical model for curved fold origami in which the energy of a plastically-deformed crease is balanced by the bending energy of developable regions on either side of the crease. Though geometry requires that a sheet buckle when folded along a closed curve, its shape depends on the elasticity of the sheet.

[1]NSF DMR-0846582

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W15 DMP GMAG FIAP: Focus Session: Spins in Semiconductors - Spin-Orbit Effects and Confinement D171

11:15AM W15.00001 Chern Number Spins of Mn Acceptor Magnets in GaAs , C. M. CANALI[1], Linnaeus University, Kalmar, Sweden — State-of-the-art STM techniques have made it possible to substitute transition metal impurities for individual atoms in semiconductor crystals and have provided detailed information on the nature of the bound acceptor or donor states. Individual coupled acceptor (or donor)-impurity centers represent a new class of nanomagnets which we refer to as *acceptor or donor magnets*. Here we determine the effective total spin $J$of local moments formed from acceptor states bound to Mn ions in GaAs by evaluating their magnetic Chern numbers. When individual Mn atoms are close to the sample surface, the total spin changes from $J = 1$ to $J = 2$, due to quenching of the acceptor orbital moment. For Mn pairs in bulk, the total Jdepends on pair orientation in the GaAs lattice and on the separation between the Mn atoms. We point out that Berry curvature variation as a function of local moment orientation can profoundly influence the quantum-spin dynamics of these magnetic entities.

[1]Work done in collaboration with T. O. Strandberg and A. H. MacDonald.

11:51AM W15.00002 Effect of magnetic field on the local density of states of Mn acceptor magnets in GaAs , M.R. K. MAHANI, C.M. CANALI, Linnaeus University, Kalmar, Sweden, A.H. MACDONALD, University of Texas at Austin — Advances in atomic manipulation, real-space imagining and spectroscopic power of STM techniques have recently made it possible to investigate the local electronic properties of a few substitutional Mn impurities inserted in the GaAs surfaces [1]. Theoretical work [2] predicts that the local density of states in the vicinity of the Mn impurities should depend strongly on the direction of the Mn magnetic moment. In contrast, recent STM experiments [3] from several groups find a negligible dependence of the tunneling LDOS on the magnetic field direction for applied fields up to 7 T. Based on tight- binding calculations we interpret these findings by arguing that large LDOS signals require large angle moment rotations, and that the strength of the magnetic field used in present experiments is not strong enough to substantially modify the magnetic anisotropy landscape of Mn impurities near the GaAs surface.

[1] D. Kitchen et al., Nature, 442, 436 (2006); J. K. Garleff et al., Phys. Rev. B 82, 035303 (2010).
[2] T. O. Strandberg, C. M. Canali, and A. H. MacDonald, Phys. Rev. B 80, 024425 (2009). [3] P. M. Koenraad, Private Communication.

12:03PM W15.00003 Effects of Anisotropy in Magnetic Quantum Dots , RAFAL OSZWALDOWSKI, IGOR ZUTIC, University at Buffalo, ANDRE PETUKHOV, South Dakota School of Mines and Technology — Magnetic ordering in semiconductor Quantum Dots (QDs) doped with Mn is mediated by the confined carriers (typically holes), which interact with Mn through exchange interaction. The ordering can be affected by the QD flat shape [1], and, by the resultant anisotropic g-factor of holes [2]. A reduction of the in-plane symmetry of the QD by an external potential may influence the magnetic alignment as well [3]. We study the magnetic ordering at different degrees of anisotropy. The ordering arises in absence of external magnetic field, e.g., through formation of magnetic polarons. A typical number of Mn in a QD is large, so we replace their spins by classical magnetic moments. We emphasize the limit of full isotropy (electrons) and extreme anisotropy (holes in a flat QD). Supported by DOE-BST, ONR, AFOSR, and NSF-ECCS CAREER.

[1] I. R. Sellers, R. Oszwaldowski, et al., Phys. Rev. B **82**, 195320 (2010)
[2] P. Dorozhkin, et al., Phys. Rev. B **68**, 195313 (2003).
[3] R. M. Abolfath, A. G. Petukhov, and I. Zutic, Phys. Rev. Lett. **101**, 207202 (2008)

12:15PM W15.00004 Incorporation of Mn into Ge Quantum Dots: Growth Strategies to Control Structure and Magnetism[1] , CHRISTOPHER NOLPH, PETRA REINKE, Department of Materials Science and Engineering, University of Virginia — Manganese doped, magnetic germanium quantum dots are important building blocks for the future of spintronic devices. Our goal is to understand and control how the manipulation of the Mn-environment within the Si(100)-Ge wetting layer-Ge QD systems influence the magnetic properties. We investigate several pathways for Mn-doping of Ge QDs which suppress detrimental germanide formation. The first pathway uses a surface-driven approach: Mn is deposited on the Ge QD surface, forms well-defined clusters on the QD and dissolve during annealing. The second pathway uses co-deposition of Ge and Mn (i) throughout the entire QD growth process, and (ii) only during the formation of the wetting layer. The highest concentration of Mn is about 20%, and the Ge QD growth is only marginally perturbed, albeit germanides begin to form. All processes are observed with scanning tunneling microscopy, which yields morphological and electronic structure information of the reaction sequence. A comprehensive model of all processes will be presented. Preliminary magnetism results, obtained with a vibrating sample magnetometer, indicate a ferromagnetic material with a Curie temperature up to 100K.

[1]This work is supported by: NSF CHE-0828318 and DMR-0907234.

12:27PM W15.00005 Control and properties of magnetic nanostructures in nitride semiconductors , ALBERTA BONANNI, Johannes Kepler University, Linz-Austria — We review [1] studies of MOVPE (Ga,Fe)N [2-7] and (Ga,Mn)N [8,9], combining magnetic [2-4,6,8,9], magnetooptical [3], and XANES [4,5,8] investigations with a comprehensive structural and chemical characterization by SIMS, TEM, EDS [2,4,6,8,9], synchrotron-XRD [4,6,8], EXAFS [5,8], and PEEM [7]. We show that the Fe ions aggregate into Fe_xN nanocrystals either by crystallographic or by chemical phase separation, controlled by the growth conditions and by co-doping. Depending on the degree of nitridation, these nanocrystals are either ferromagnetic or antiferromagnetic.

[1] A. Bonanni and T. Dietl, Chem. Soc. Rev. 39, 528 (2010);
[2] A. Bonanni et al., Phys. Rev. B 75, 125210 (2007);
[3] W. Pacuski et al., Phys. Rev. Lett. 100, 037204 (2008);
[4] A. Bonanni et al., Phys. Rev. Lett. 101, 135502 (2008);
[5] M. Rovezzi et al., Phys. Rev. B 79, 195209 (2009);
[6] A. Navarro-Quezada et al., Phys. Rev. B 81, 205206 (2010);
[7] I. Kowalik et al., arXiv:1011.0847;
[8] W. Stefanowicz et al., Phys. Rev. B 81, 235210 (2010);
[9] A. Bonanni et al. arXiv : 1008.2083.

1:03PM W15.00006 From simplicity to complexity: Can transcendental equation and transfer matrix enlighten us about the nature of Rashba physics? , CHIH-PIAO CHUU, University of Texas at Austin, TX, ROLAND WINKLER, Northern Illinois University, IL, QIAN NIU, University of Texas at Austin, TX — We present an analytic model of Rashba spin-splitting of conduction electrons in asymmetric quantum wells based on transcendental equation and transfer matrix approaches. The sources of asymmetries of quantum wells, such as interface discontinuity, conduction and valence band profiles, external field or presence of a potential gradient, related to Rashba spin-splitting will be discussed. We will use type I and type II semiconductor heterostructure quantum wells for demonstration.

1:15PM W15.00007 Signatures of the crystal symmetry after Dyakonov-Perel spin relaxation of photoexcited hot electrons in semiconductor heterostructures[1] , LAN QING, HANAN DERY, Department of Physics and Astronomy, University of Rochester, Rochester, New York 14627 — We reveal unique manifestations of the intimate relation between the crystal structure of zincblende semiconductors and their spin-orbit coupling. We show that reflection of photoexcited hot electrons is capable of tipping the direction of the optically injected net spin vector away from the propagation axis of the exciting circularly polarized beam. The effect is robust even in case of complete electron reflection from a non magnetic target (e.g., GaAs/AlAs). The tipping angle of the net spin vector after spin relaxation is determined by the effective Dyakonov-Perel magnetic field as well as by the momentum alignment and spin-momentum correlation of the initial photoexcited electron population. All of these crystal-structure dependent mechanisms contribute due to the reflection plane induced symmetry breaking. We perform Monte Carlo simulations to calculate the tipping angle and also provide qualitative derivations of the effect. Results are shown for non-magnetic semiconductor heterostructures and for hybrid semiconductor/ferromagnet systems.

[1]This work is supported by AFOSR Contract No. FA9550-09-1-0493 and NSF Contract No. ECCS-0824075.

1:27PM W15.00008 The spin dynamics in the strong spin-orbit coupling regime-A collective Rabi oscillation[1] , XIN LIU, XIONG-JUN LIU, JAIRO SINOVA, Department of Physics, Texas A&M University, College Station, TX 77843-4242, USA — We study the spin evolution in a high-mobility two dimensional electron gas (2DEG) with generic spin-orbit interactions(SOI). A fully understanding of the D'yakonov-Perel's(DP) mechanism is presented by using the microscopic linear response theory from the diffusive to the ballistic regime. We derive a set of spin dynamical equations which capture the characters of the purely exponential and damped oscillatory spin evolution modes in different spin-orbit coupling(SOC) regimes. It is shown that the oscillatory spin dynamics appear when the electron life time is larger than the half of the spin precession time due to the SOI. The Rabi oscillation between two spin bands is the physical origination of the damped oscillatory modes.

[1]NSF under Grant Nos. DMR-0547875 and 0757992.

1:39PM W15.00009 Rasbha Spin-Orbit Interaction in Digital Alloys , JOSEPH PINGENOT, KIERAN MULLEN, The University of Oklahoma Department of Physics and Astronomy — The Rashba spin-orbit interaction couples the electron spatial wavefunction to its spin through breaking the inversion symmetry of a structure. From work by Lange[1], the Rashba spin-orbit effect can be divided into a structural component, originating primarily in the valence band offsets within the nanostructure, and an electric field component, originating primarily in the internal self-consistent electric field and in an applied electric field. A common growth technique, digital alloying, breaks the well into discrete steps and then varies the material composition for each step by constructing a well within the step such that the average material across the step corresponds to the desired percentage, e.g. a $Ga_{0.5}In_{0.5}As$ well would be pure GaAs through half the step, followed by pure InAs for the rest of the step. With digital alloying, the electron wavefunction is approximately the same as is obtained by using a real alloy. The Rashba spin-orbit couplings, however, are considerably smaller for the digital alloy than the real alloy. This comes about because the digital alloy has a series of positive and negative interfaces at each step, whereas the real alloy has a series of identical steps. We calculate the Rashba coefficient for a variety of realistic well geometries, for both digitial and continuous alloying, and discuss how the consequences for experiment. [1] Jens Lange, *Quantentransport in Halbleiter-Heterostrukturen* (1996).

1:51PM W15.00010 Superconductivity in the repulsive Rashba model , LUYANG WANG, OSKAR VAFEK, National High Magnetic Field Laboratory and Department of Physics, Florida State University — We study the superconducting instability of a two dimensional Rashba spin-orbit coupled system with a weak repulsive interaction by a two step renormalization group (RG) method introduced by Raghu et.al. (PRB 81, 224505 (2010)). We present the superconducting transition temperature Tc in terms of the correlation functions of the non-interacting system. The RG flows in the Cooper channel break down below some scale, which we identify with Tc and verify that the Tc is independent of the intermediate cutoff. Finally, we present results of Tc as a function of spin-orbit coupling strength.

2:03PM W15.00011 Kohn-Luttinger superconductivity of two-dimensional electrons in the presence of Rashba spin-orbit coupling , ALI ASHRAFI, DMITRII MASLOV, Department of Physics, University of Florida — We consider a two-dimensional(2D) system of fermions with weak short-range repulsive interac- tion in the presence of Rashba Spin-Orbit coupling(SOC). We show that although Kohn-Luttinger instability in 2D in the absence of SOC occurs only to third order in the interaction, it occurs to second order in the presence of SOC. The critical temperature of the p-wave transition is calculated.

Thursday, March 24, 2011 11:15AM - 1:15PM –

Session W16 DMP GMAG: Focus Session: Bulk Properties of Complex Oxides - Other D173

11:15AM W16.00001 Magnetic Force Microcopy of the Magnetostructural Phases of Mn3O4

, XU WANG, MINJUNG KIM, RAFFI BUDAKIAN, S. L. COOPER, University of Illinois at Urbana-Champaign — In this talk, we report temperature- and field- dependent magnetic force microscopy (MFM) studies of Mn3O4. The spinel Mn3O4 has novel phase structure at low temperatures due to a three-way competition between spin-orbital coupling, geometric frustration and external magnetic field. This competition could lead to complex magnetic pattern formations. A particularly interesting phase exists where the crystal lattice undergoes a transition to resolve the spin frustration due to internal and external magnetic fields. In this phase the spins were expected to be in a disordered state, but local magnetic ordering has not been explored in previous studies. We present results from our investigation of Mn3O4 phase space using a variable temeprature MFM. Measurements were made at temperatures between 4K and 75K and in magnetic fields up to 5 tesla.

11:27AM W16.00002 Magnetic excitations in the geometric frustrated multiferroic $CuCrO_2$

, MATTHIAS FRONTZEK, GEORG EHLERS, ANDREY PODLESNYAK, MASAAKI MATSUDA, ANDREW CHRISTIANSON, NScD, Oak Ridge National Laboratory, 37831 Oak Ridge, USA, RANDY FISHMAN, Materials Science and Technology Division, Oak Ridge National Laboratory, 37831 Oak Ridge, USA, JASON HARALDSEN, Theoretical Division, Los Alamos National Laboratory, 87545 Los Alamos USA, SERGEI BARILO, Institute of Solid State and Semiconductor Physics, Minsk 220 072, Belarus — The delafossite $CuCrO_2$, crystallizing in the rhombohedral $R\bar{3}M$ space group, is an interesting case of a multiferroic compound due to its apparent strong coupling of spin and charge. In contrast to other multiferroic compounds $CuCrO_2$ shows a spontaneous electric polarization upon antiferromagnetic ordering at $T_N \approx 24$ K without an accompanying structural phase transition. Further, $CuCrO_2$ is a rare example where the magnetoelectric properties are tunable by both an electric and a magnetic field. In our contribution we present inelastic neutron scattering experiments on $CuCrO_2$ single crystals. The measured magnetic excitation spectra have been modeled by Monte-Carlo spin wave calculations and allowed the determination of the relevant exchange interaction and anisotropy terms. We will present evidence for a weak ferromagnetic Cr-Cr-interlayer exchange interaction and show that this interaction is relevant for the multiferroic properties of $CuCrO_2$.

11:39AM W16.00003 Charge dynamics in frustrated charge ordered system with strong electron correlation

, MAKOTO NAKA, SUMIO ISHIHARA, Department of Physics, Tohoku University — Electronic ferroelectricity is known as phenomena where the electric polarization is caused by the electronic charge order without inversion symmetry. This is seen in some transition metal oxides, e.g. $LuFe_2O_4$, and charge transfer organic salts. It is suggested from the theoretical works [1,2] that large charge fluctuation and frustration are responsible for the electric polarization. This charge fluctuation is expected to govern dynamical properties and external field effects. Actually, the relaxer like large dielectric fluctuation in some electronic ferroelectricity is observed. Motivated by these experimental and theoretical results, we study charge dynamics in charge ordered fermion system on the layered triangular lattice. We adopt the V-t model where the inter-site electron transfers and the inter-site Coulomb interactions are taken into account. We analyze this model by utilizing the exact diagonalization method and focus on effects of frustration in the charge dynamics. In the 3-fold charge ordered phase associated with the electric polarization, the optical conductivity shows multiple-peak structure in a wide energy range. In the non-polar 2-fold charge ordered phase, a precursor of the 3fold charge order appears in the low energy charge fluctuation around the phase boundary. [1] A. Nagano et al. Phys. Rev. Lett. **99** 217202. [2] M. Naka et al. Phys. Rev. B. **77** 224441.

11:51AM W16.00004 Photo induced spin-state change in itinerant correlated electron systems

, SUMIO ISHIHARA, YU KANAMORI, Tohoku University, HIROAKI MATSUEDA, Sendai National College of Technology — Recently developed ultrafast optical techniques open up a new frontier for research of the phase transition. This is the so-called photo-induced phase transition (PIPT). The spin-state transition between different magnitudes of the spin-angular moment is one of the targets. In particular, the photo-induced spin-state transition is seen in the cobalt oxides with a perovskite structure. The ultrafast optical measurements in the low-temperature low-spin insulators show transient metallic spectra which are completely different from the spectra in the high-temperature high-spin phase. We study theoretically the photo-induced spin-state change in itinerant correlated electron systems. We derive the model Hamiltonians where numbers of photo-excited electron-hole pair are fixed. A bound state of the photo-doped hole and the high-spin state are created inside of the low-spin sites. This bound state brings about a characteristic peak structure in the optical pump-probe spectra which are completely different from the spectra in thermally excited states. The present theory provides a possible scenario in recently observed photo-induced hidden state in perovskite cobaltites.

12:03PM W16.00005 Rapidly fluctuating orbital occupancy above the orbital ordering transition in spin-gap compounds[1]

, FRANCISCO RIVADULLA, BEATRIZ RIVAS-MURIAS, Physical Chemistry Dept. and Center for Research in Biological Chemistry and Molecular Materials, Univ. Santiago Compostela, Spain, HAIDONG ZHOU, National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32306-4005, USA, JOSE RIVAS, Applied Physics Department, University of Santiago de Compostela, Spain — Low-dimensionality spin systems develop a spin-dimer phase within a molecular orbital that competes with long-range antiferromagnetism below TS. Very often, preferential orbital occupancy and ordering are the actual driving force for dimerization, as in the orbitally-driven spin-Peierls (MgTi2O4, CuIr2S4, La4Ru2O10, NaTiSi2O6, etc.). Through a microscopic analysis of the thermal conductivity in La4Ru2O10, we show that the orbital occupancy fluctuates rapidly above TS, resulting in an orbital-liquid state. Strong orbital-lattice coupling introduces dynamic bond-length fluctuations that scatter the phonons to produce a glass-like thermal conductivity above TS. This phonon-glass to phonon-crystal transition occurs in other spin-dimer systems, like NaTiSi2O6, pointing to a general phenomenon.

[1]FR acknowledges support from ERC through Starting Grant 2DTHERMS.

12:15PM W16.00006 Influence of particle size on the magnetic and magnetocaloric properties of nanocrystalline $La_{2/8}Pr_{3/8}Ca_{3/8}MnO_3$

, P. LAMPEN, N.S. BINGHAM, M.H. PHAN, H. SRIKANTH, University of South Florida, T.H. HOANG, H.D. CHINH, Hanoi University of Technology — Bulk manganites $La_{5/8-y}Pr_yCa_{3/8}MnO_3$(LPCMO) exhibit a complex phase diagram due to coexisting and competing charge-ordered (CO) and ferromagnetic (FM) phases. Of particular interest is the CO phase that is unstable under various perturbations, such as carrier doping, strain, magnetic and electric field. We report systematic studies of the influence of particle size on the magnetic and magnetocaloric properties of nanocrystalline LPCMO (y=3/8) synthesized by sol-gel method. The nanocrystalline samples with mean particle sizes of 30 nm, 150 nm, and 250 nm were structurally characterized by XRD, SEM, and TEM. Magnetic and magnetocaloric measurements were conducted using a Quantum Design PPMS. We find that the 150 nm and 250 nm samples exhibit features similar to their bulk counterpart. However, the case is very different for the 30 nm sample where only a paramagnetic to ferromagnetic transition occurs. Size reduction has been found to suppress the CO phase, decrease the magnetization, and strongly modify the magnetocaloric effect in LPCMO.

12:27PM W16.00007 Studies on manganese substituted cobalt ferrite prepared by autocombustion route

, Y. KOLEKAR, Pune University, R. KAMBALE, Shivaji University, Kolhapur, R. GUPTA, P. KAHOL, K. GHOSH, Missouri State University — Compositions of Co1.2-xMnxFe1.8O4 (0 = x = 0.4) were synthesized by autocombustion route keeping oxidizer to fuel ratio at 1. Structural and compositional characterizations of all the samples were performed by XRD, SEM and EDS. Magnetization measurements showed that the Ms increases form 106.5 emu/g for x = 0.0 to 138.5 emu/g for x = 0.2 and then decreases from x = 0.3 (124.71 emu/g for x = 0.3 and 97.78 emu/g for x =0.4), whereas the coercivity (Hc) decreases with manganese (Mn) substitution, except for x = 0.3. Room temperature dielectric properties such as relative dielectric permittivity (er), dielectric loss and ac conductivity, were studied as a function of frequency in the range from 20 Hz to 1 MHz. These studies indicates that the relative dielectric permittivity increasing (from er = 600 for x =0.0 to er = 2400 for x = 0.4) with the increase of Mn content in cobalt ferrite and also all samples show the usual dielectric dispersion which may be due to the Maxwell-Wagner-type of interfacial polarization. Dr. Y. D. Kolekar gratefully acknowledges the award of BOYSCAST fellowship by Department of Science and Technology, India. *On leave from Department of Physics, University of Pune, Pune- 411 007, India.

12:39PM W16.00008 Single magneto-chiral domain observed in langasite $Ba_3NbFe_3Si_2O_{14}$ by non-resonant magnetic X-ray scattering , LAURENT CHAPON, ALESSANDRO BOMBARDI, FEDERICA FABRIZI, CHRIS STOCK, DES MCMORROW, PAOLO RADAELLI, SANG-WOOK CHEONG — The helical magnetic ground state of the chiral langasite compound $Ba_3NbFe_3Si_2O_{14}$ has been investigated using a left-handed single crystal using non resonant x-ray magnetic scattering. This technique, when combined with circularly polarized x-ray and a full polarization analysis of the scattered beam, is sensitive to the chirality of the spiral order previously reported in this compound and it allows an unique determination of the chirality of the magnetic ground state. A topographic map of the sample surface shows that the crystal is made of a single magneto-chiral domain. Azimuthal scans revealed that the long range magnetic order with wave-vector k=(0,0,1/7) is characterized by an elliptical modulation rather than a circular one, as initially reported. We also discuss the possible spin-driven ferroelectric state in this compound.

12:51PM W16.00009 Simple point-ion electrostatic model explains the cation ordering in A2BO4 spinel oxides[1] , VLADAN STEVANOVIC, MAYEUL D'AVEZAC, ALEX ZUNGER, NREL, Golden CO — The A2BO4 spinel oxides are distinguished by having either a normal or an inverse distribution of the A, B cations over the octahedrally and tetrahedrally coordinated sites. While normal spinel represents a single structure (A-octahedral, B-tetrahedral) the inverse spinel is similar to a 50-50 alloy with octahedral sublattice occupied randomly by A and B. We show that a simple point-ion electrostatic (PIE) model parameterized by the oxygen displacement parameter u and by the relative formal cation valencies ZA vs ZB provides a simple rule: if ZA>ZB the structure is normal for u>0.2592 and inverse for u<0.2578, while if ZA<ZB the structure is normal for u<0.2550 and inverse for u>0.2578. This rule is illustrated for the known spinel oxides, proving to be 98 % successful (PRL 105, 075501). Moreover, in inverse spinels the PIE model also explains the origin of the experimentally observed ordered phase that emerges from the random alloy at low T.

[1]This work was supported through the Center for Inverse Design, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

1:03PM W16.00010 Anionogenic Magnetism: Mixed Alkali – Alkaline Earth Metal Oxides , SHIVAKUMARA GIRIYAPURA, SYARIF RIYADI, Solid State Materials for Electronics, Zernike Institute for Advanced Materials, University of Groningen, Groningen,The Netherlands, BAOMIN ZHANG, ROBERT A. DE GROOT, Electronic Structure of Materials, IMM, Radboud University Nijmegen, Nijmegen, The Netherlands, THOMAS T.M. PALSTRA, GRAEME R. BLAKE, Solid State Materials for Electronics, Zernike Institute for Advanced Materials, University of Groningen, Groningen,The Netherlands, S S M E TEAM, IMM COLLABORATION — The scientific and technological potential of materials in which magnetism arises from p-electrons is little explored. Accordingly, we have synthesized the solid solution $Ba_{1-x}K_x(O_2^{2-})_{1-x}(O_2^{-})_x$ which contains a nominal mixture of magnetic superoxide and non magnetic peroxide anions. Magnetization measurements reveal short range antiferromagnetic ordering below ∼65 K for all compositions, with an increasing tendency toward ferromagnetic interactions at lower temperatures, characterized by the opening of magnetic hysteresis loops in applied fields.Field induced reorientation of the dioxygen dumbbells probably occurs, altering the magnetic exchange interactions between nearest neighbor anions.

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W17 GMAG DMP: Focus Session: Magnetic Oxide Thin Films - Cobaltate and Ferrous Oxide Thin Films D174

11:15AM W17.00001 Fist-principles design of magnetic oxides , ARTHUR ERNST, Max Planck Institute of Microstructure Physics — First-principles design of magnetic oxides is one of most ambitious challenges in modern computational physics. The electronic and magnetic properties of these materials are substantially affected by strongly localized electrons, complex crystalline structures, and mixed valencies of magnetic ions. In my talk I shall present an ab-initio Green function method within density functional theory which provides an accurate description of the electronic structure of these materials. In particular, the treatment of strongly localized electrons is improved considerably by applying a self-interaction correction (SIC), thereby removing the spurious interaction of an electron with itself. By localizing a particular electronic configuration using the SIC, we simulate various valencies of magnetic ions. A mixed-valency state can then be efficiently treated within the coherent potential approximation which is implemented in our multiple-scattering Green function code that can be used as well for simulations of any kind of substitutional disorder. In my talk I shall demonstrate the power of our approach on complex magnetic oxidic surfaces and interfaces. In particular, I shall discuss effective exchange interactions in systems with mixed valency and the influence of structural imperfections, such as defects and relaxations, on the electronic and magnetic properties of these materials.

11:51AM W17.00002 Cobalt spin state and hyperfine interaction in ferromagnetic insulating $LaCoO_3$ thin films[1] , RENATA WENTZCOVITCH, HAN HSU, University of Minnesota, PETER BLAHA, TU Vienna, CHRIS LEIGHTON, University of Minnesota — At low temperatures, bulk $LaCoO_3$ is a non-metallic diamagnet. In contrast, thin-film $LaCoO_3$ experiencing a tensile epitaxial strain is a ferromagnetic insulator in the same temperature range. It is difficult to properly describe this phenomenon with density functional theory (DFT) calculations, even with the Hubbard U correction. Previous calculations have found ferromagnetic conducting thin-film $LaCoO_3$ with all Co ions in the intermediate-spin (IS) state, incompatible with experimental data. In this work, using the DFT+U approach, we show that a strained $LaCoO_3$ thin film can be stabilized in a ferromagnetic insulating state. We also predict the electric field gradient (EFG) at the Co nucleus in the magnetic thin film, which can be helpful in identifying Co spin states via nuclear magnetic resonance (NMR) spectroscopy.

[1]This work is primarily supported by the MRSEC Program of NSF under DMR-0212302 and DMR-0819885, and partially supported by EAR-0810212 and EAR-1047629. P.B. was supported by the Austrian Science Fund (P20271-N17). Calculations were performed at MSI.

12:03PM W17.00003 First-principles study of strain-induced ferromagnetism in $LaCoO_3$, HOSUNG SEO, ALEXANDER DEMKOV, The University of Texas at Austin — We study theoretically the effect of biaxial strain on magnetic properties of $LaCoO_3$ (LCO) using density functional theory combined with the Hubbard U method. LCO is normally a non-magnetic insulator with trivalent cobalt ions in low-spin state (t_{2g}^6). Owing to close interplay between orbital, spin, and lattice degrees of freedom, it shows rich magnetic behavior such as temperature-induced spin state transition. Recently, the ferromagnetic tensile-strained LCO films have been reported. The underlying physics of the ferromagnetic state is, however, unclear. Using a large tetragonal cell we calculate full structural response of the system to applied strain for non-magnetic and magnetic solutions. We show that beyond tensile strain of 3.8% the ferromagnetic solution with Co ions in intermediate-spin state (t_{2g}^5 e_g^1) is stabilized accompanied by partial untilting of CoO_6 octahedral network. We also perform the calculation for compressive-strained structures and the difference between these and the tensile strained structures will be presented.

12:15PM W17.00004 Spin-polarized scanning tunneling spectroscopic (SP-STS) studies of the intrinsic electronic heterogeneity in ferromagnetic (FM) cobaltites and manganites , JING SHI, LI ZHANG, WEI-HSUN LIN, HAO CHU, CAMERON HUGHES, NAI-CHANG YEH, California Institute of Technology — The perovskite manganites $Ln_{1-x}A_xMnO_3$ and cobaltites $Ln_{1-x}A_xCoO_3$ (Ln: trivalent rare earth ions; A: divalent alkaline earth ions) exhibit interesting magnetotransport properties in their FM state: the former show colossal magnetoresistance (CMR) and the latter display giant anomalous Hall effect (AHE), where the AHE coefficient peaks near the Curie temperature (T_C). These novel phenomena are associated with the intrinsic electronic heterogeneity resulting from strongly correlated multi-valence multi-spin electronic configurations. We perform SP-STS studies on epitaxial films of $La_{0.7}Ca_{0.3}MnO_3$ and $La_{1-x}A_xCoO_3$ (A = Sr, Ca; $0.4 \leq x \leq 0.6$). In the manganites electronic heterogeneity on the scale of $\sim 10^2$ nm is found to develop below T_C and diminish with increasing magnetic field. A surface FM insulating phase is manifested by the spin filtering effect and is attributed to the MnO_2 surface layer. Similar studies are conducted on the cobaltites to reveal possible correlation between magnetic clustering effects and the Berry phase.

12:27PM W17.00005 Epitaxial growth and characterization of strained $LaCoO_3$ on Si (100) , AGHAM POSADAS, University of Texas at Austin, MORGANN BERG, HOSUNG SEO, DAVID SMITH, ALEXANDER KIRK, DMITRY ZHERNOKLETOV, ROBERT WALLACE, ALEX DE LOZANNE, ALEXANDER DEMKOV — $LaCoO_3$ is a correlated oxide that normally has a diamagnetic ground state in bulk. The material undergoes a spin-state transition and becomes paramagnetic at higher temperatures. In this work, we report the epitaxial growth of strained $LaCoO_3$ on silicon via a fully-relaxed $SrTiO_3$ buffer layer using molecular beam epitaxy (MBE). We confirm that the strained $LaCoO_3$ becomes ferromagnetic with a Curie temperature of 85 K, similar to recent reports for films grown by pulsed laser deposition. We will discuss the issues related to the MBE growth of $LaCoO_3$ and show results of x-ray diffraction, x-ray photoelectron spectroscopy, transmission electron microscopy, and SQUID magnetometry measurements on $LaCoO_3$ films grown on silicon.

12:39PM W17.00006 Control of the Octahedral Tilts in Lanthanum Cobaltite and the Impact on Magnetic Properties , MICHAEL BIEGALSKI, HAILE AMBAYE, VALERIA LAUTER, HANS CHRISTEN, Oak Ridge National Labratory — Strain can be accommodated in two ways in perovskite materials, either via the extension of bond lengths or the rotation of the relatively rigid BO_6 octahedra. To explore the effects of octahedral tilts on magnitism, we have used epitaxy to control the octahedral tilting in the unit cell of $La_{0.5}Sr_{0.5}CoO_3$ by growth on cubic $La_{0.3}Sr_{0.7}Al_{0.65}Ta_{0.35}O_3$ (LSAT) and orthorhombic $NdGaO_3$. From X-ray diffraction, the films grown on LSAT were shown to have a cubic structure whereas the films grown on $NdGaO_3$ show an orthorhombic distortion. Due to the large paramagnetic response of the $NdGaO_3$ polarized neutron reflectometery was used to probe the magnetic structure of the films. The polarized neutron reflectometry demonstrates that changes in the crystal structure due to the epitaxially imposed symmetries alter the magnetism in these materials.

12:51PM W17.00007 Magnetic Phase Separation in Oxygen Doped $SrCoO_{3-y}$[1] , F.J. RUECKERT, C.K. XIE, Y.F. NIE, B.O. WELLS, J.I. BUDNICK, W.A. HINES, University of Connecticut, B. DABROWSKI, Northern Illinois University — $SrCoO_{3-y}$ forms the perovskite structure with oxygen vacancies and is ferromagnetic for $y<0.25$. We have performed a study on polycrystalline samples, controlling the oxidation state using electrochemistry. Under these conditions we have found that magnetically the system segregates into separate, stable phases that correspond to $SrCoO_{2.75}$($T_C = 165$ K), $SrCoO_{2.875}$($T_C = 220$ K), and $SrCoO_3$ ($T_C = 280$ K), with two phase behavior for intermediate oxygen concentrations. Surprisingly, these same samples show only a single structural phase that evolves smoothly. We have recently learned to grow high quality epitaxial films of $SrCoO_y$, allowing for more typical single crystal diffraction experiments. Our initial results indicate that magnetic phase separation is suppressed in the films.

[1]The work is supported by the NSF through contract # DMR-0907197 (UConn) and DMR-0706610 (NIU).

1:03PM W17.00008 Examining the Magnetic Properties of $LaCoO_3$ Thin Films Using Magnetic Force Microscopy[1] , MORGANN BERG, AGHAM POSADAS, ALEX DE LOZANNE, ALEXANDER DEMKOV, Department of Physics, The University of Texas at Austin — In contrast to the non-magnetic ground state of bulk $LaCoO_3$ (LCO) at low temperatures, ferromagnetism has been observed in elastically strained thin film specimens. The origins of ferromagnetism in strained LCO thin films have been obscured by conflicting experimental results. Pulsed laser deposition (PLD) is the current standard of preparation techniques used to grow thin films of LCO, but results from thin film LCO samples prepared by PLD have been questioned on the basis of chemical inhomogeneity and film defects. Using magnetic force microscopy, we investigate the microscale magnetic properties of strained thin films of LCO prepared by molecular beam epitaxy and deposited on lanthanum aluminate and strontium titanate substrates. We observe these properties across a temperature range surrounding the Curie temperature ($T_c \sim 80$K) and compare our results to global magnetic characteristics of these films as measured by a SQUID magnetometer.

[1]Supported by NSF-DMR and NSF-IGERT.

1:15PM W17.00009 Magnetic resonance at the Verwey transition in epitaxial Fe_3O_4[1] , M. PECHAN, B. KASTER, J. DOU, Dept. of Physics, Miami University, Oxford, OH, P. JAYATHILAKA, C. BAUER, C. MILLER, Dept. of Physics, Center for Integrated Functional Materials, University of South Florida, Tampa, Florida — Fe_3O_4 is of interest due to its potential applications in the field of spintronics. Previous studies on magnetite films and Fe_3O_4/Cr/NiFe spin valves indicate the presence of a uniaxial anisotropy when the magnetite is grown in a magnetic field. Two 170 nm thick films of Fe_3O_4 were reactively sputtered simultaneously onto (100) MgO substrates without and with an applied field (100 Oe). Epitaxy was confirmed by in-plane x-ray diffraction and optimal oxygen stoichiometry is confirmed by the 119 K Verwey transition temperature (T_V). Ferromagnetic resonance (FMR) measurements at 35 GHz in the plane of the film revealed four-fold anisotropy confirming high quality (100) epitaxy, with an additional uniaxial contribution present in the field-grown sample. Temperature dependent FMR on the sample grown without field clearly reflects T_V in the linewidth and in-plane and out-of-plane anisotropies. The in-plane uniaxial anisotropy for the sample grown with field exhibits an even stronger temperature response at T_V. Detailed discussions of thermal variations of magnetization, anisotropy and relaxation processes will be presented.

[1]Supported by the US Dept. of Energy at MU, and NSF at USF.

1:27PM W17.00010 LuFe2O4 nanostructures on MgO(111) substrate[1] , XIAOSHAN XU[2], Oak Ridge National Lab, WENBIN WANG, University of Tennessee, GAI ZHENG, PAUL SNIJDER, THOMAZ WARD, JIAN SHEN, Oak Ridge National Lab — $LuFe_2O_4$ nanostructures have been deposited on MgO(111) substrate using pulsed laser deposition. Substrate temperature and gas pressure are found to be very critical to form the $LuFe_2O_4$ phase. Scanning electron microscopy (SEM) and atomic force microscopy (AFM) show very well crystalized morphology with triangular symmetry. The common orientations of the nanosctructurals are consistent with epitaxial growth. X-ray diffraction data show that (001) face of $LuFe_2O_4$ is parrallel to the substrate face MgO(111).

[1]Research supported by US DOE, Office of Basic Energy Science, Masterial Science and Engineering Division

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

1:39PM W17.00011 Edge-Imposed Domain Ordering in Antiferromagnetic LaFeO3 Nanostructures[1] , J.K. GREPSTAD, E. FOLVEN, T. TYBELL, Norwegian University of Science and Technology, A. SCHOLL, A. YOUNG, Advanced Light Source, LBNL, S.T. RETTERER, Oak Ridge National Laboratories, Y. TAKAMURA, University of California, Davis — The antiferromagnetic (AFM) domain structure of submicron-sized $LaFeO_3$ nanostructures was imaged with photoemission electron microscopy in combination with x-ray magnetic linear dichroism. These nanostructures were defined in epitaxial $LaFeO_3$ thin films using e-beam lithography and Ar^+ ion implantation to locally destroy the magnetic order in the surrounding matrix. Extended domains were found to form along the perimeter of rectangular-shaped islands, when their edges were aligned with the in-plane <100> axes of the cubic $SrTiO_3$ substrate. The AFM spin axis of these domains was confined to lie within the film plane, aligned with the edges of the nanostructures. This domain configuration predominated for nanoislands scaled down to 500x500 nm^2. However, no edge-imposed domain ordering was observed for rectangular islands rotated by 45° with respect to the in-plane crystalline axes, suggesting a magnetocrystalline origin of the extended edge-bound AFM domains. These findings may prove important to spintronic devices relying on exchange-biased nanostructures, where domain engineering in antiferromagnets remains relatively unexplored and has the potential to provide new device opportunities.

[1]This work was sponsored by the DoE BES and the Div. of Scientific User Facilities, US DoE, and by the Research Council of Norway.

1:51PM W17.00012 Fe_3O_4/ZnO: a high-quality magnetic oxide-semiconductor heterostructure , ANDREAS MUELLER, MARKUS PAUL, DOMINIK KUFER, SEBASTIAN BRUECK, Experimentelle Physik 4, Universitaet Wuerzburg, EBERHARD GOERING, Max-Planck-Institut fuer Metallforschung, Stuttgart, MARTIN KAMP, Technische Physik, Universitaet Wuerzburg, JO VERBEECK, HE TIAN, Electron Microscopy For Materials Science, University of Antwerp, MICHAEL SING, RALPH CLAESSEN, Experimentelle Physik 4, Universitaet Wuerzburg — Magnetite (Fe_3O_4) is ranked among the most promising materials to use as a spin injector into a semiconducting host. We demonstrate epitaxial growth of Fe_3O_4 films on ZnO which presents a further step towards incorporation of magnetic materials into semiconductor technology. X-ray spectroscopy results evidence that the iron-oxide is phase-pure and nearly stoichiometric magnetite. Diffraction measurements indicate highly oriented epitaxy and almost complete structural relaxation. The microstructure consists of domains separated by anti-phase boundaries or twin boundaries as a result of island-like growth. The magnetic behavior shows a rather slow approach to saturation at high fields in comparison with bulk crystals, which is likely due to antiferromagnetic coupling at the anti-phase boundaries.

2:03PM W17.00013 The control of Morin transition temperature on hematite α-Fe_2O_3(0001) thin film , SEONGHUN PARK, J.-H. PARK, POSTECH, B.-G. PARK, J.-Y. KIM, PAL — The Morin transition of α-Fe_2O_3(0001) thin film was investigated by using soft x-ray absorption spectroscopy (XAS).The epitaxial thin films were grown by cycles of evaporation and post-oxydation method on Al_2O_3(0001) substrate. The x-ray diffraction (XRD) revealed that the strain is changed with variation of the thickness and the buffer layer. The Morin temperature were measured by x-ray magnetic linear dichroism (XMLD).Interestingly, the Morin transition temperature increased up to room temperature in hematite thin film. In addition, the Co metal overlayer suppressed the Morin transition temperature. Finally, we discuss the magnetic anisotropy including the strain and the interlayer exchange interaction.

Thursday, March 24, 2011 11:15AM - 1:39PM –
Session W18 DCOMP: Many Body D172

11:15AM W18.00001 Exact asymptotes of static and dynamic correlation functions of the 1D Bose gas , ADITYA SHASHI, Rice University, LEONID GLAZMAN, Yale University, JEAN-SEBASTIEN CAUX, Institute for Theoretical Physics, Universiteit van Amsterdam, Amsterdam, The Netherlands, ADILET IMAMBEKOV, Rice University — Recent experiments with ultracold atomic gases have provided realizations of one-dimensional systems of bosons with contact interactions, described by the Lieb-Liniger model. These experiments have revived interest in the correlation functions for this model. Since a fully analytical calculation of the correlation functions is still lacking, our results [1] represent a significant step forward. We have combined field theoretical approaches with an analysis of the finite size scaling of exact form factors of the Lieb-Liniger model to analytically calculate "non-universal" prefactors in the long-distance behavior of correlation functions as well as prefactors of singularities in dynamic response functions such as the density structure factor and spectral function. We have also proved the existence of singularities within a continuum spectrum.

[1] A. Shashi, L. I. Glazman, J-S. Caux and A. Imambekov, arXiv:1010.2268.

11:27AM W18.00002 Correlation functions of nonlinear Luttinger liquids as Fredholm determinants , YINBIN MA, ADILET IMAMBEKOV, Rice University — One dimensional quantum liquids are often described within an effective linear hydrodynamic approach known as Luttinger liquid theory. As the principal simplification, a generic spectrum of the constituent particles is replaced by a linear one, which leads to a linear hydrodynamic theory. It has been shown recently [1] that the nonlinearity of the generic spectrum leads to a significant modification of the dynamic response functions. Their description can be achieved within the universal framework of nonlinear Luttinger liquid theory. We show here that correlation functions within such approach can be expressed as Fredholm determinants, and evaluate them in low energy regions for arbitrary interaction strength and small temperatures.

[1] "Universal theory of nonlinear Luttinger liquids," A. Imambekov and L.I. Glazman, Science 323, 228 (2009)

11:39AM W18.00003 Ab initio Low-Dimensional Physics Opened Up by Constrained RPA for Energy and Space: Applications to LaFeAsO and κ-$(BEDT\text{-}TTF)_2X$, KAZUMA NAKAMURA, University of Tokyo, JST-CREST, YOSHIHIDE YOSHIMOTO, Tottori University, YOSHIRO NOHARA, MASATOSHI IMADA, University of Tokyo — Studies on outstanding electron correlation effects such as non-Fermi liquid behavior and unconventional superconductivity discovered in systems with low-dimensional anisotropy have continuously been at a front of condensed matter physics. Analyses for 1D or 2D simplified models have played a primary role in understanding essence of correlation effects, but to a large extent, the studies rely on ad hoc adjustable parameters as in the Hubbard models. We develop a new ab initio downfolding scheme for deriving effective low-energy models with low spatial dimensions [1]. The scheme is based on constrained random-phase-approximations by imposing constraints not only in "energy" but also in "space". We show real applications for 2D-layered superconductors of LaFeAsO and κ-$(BEDT\text{-}TTF)_2X$. The derived interactions in the effective models become short ranged essentially within up to next-nearest neighbors and thus justify multiband 2D Hubbard models as effective models for these materials from first principles. This work is supported from MEXT Japan under grant numbers 22740215 and 22104010.
[1] K. Nakamura, Y. Yoshimoto, Y. Nohara, and M. Imada, arXiv:1007.4429.

11:51AM W18.00004 Beyond Landau Adiabacity: Weak Interaction Quenches in a Fermi Gas

, STEFAN KEHREIN, University of Munich (LMU), Germany, MICHAEL MOECKEL, Max Planck Institute of Quantum Optics, Garching, Germany — The crossover from Landau's Fermi-liquid paradigm with adiabatic switching on of the interaction to a sudden interaction quench is investigated [Phys. Rev. Lett. 100, 175702 (2008); Ann. Phys. 324, 2146 (2009); New J. Phys. 12, 055016 (2010)]. The real time dynamics for weak interactions is calculated in a systematic expansion and one finds three clearly separated time regimes: (i) An initial buildup of correlations where the quasiparticles are formed. (ii) An intermediate quasi-steady prethermalized regime resembling a zero temperature Fermi liquid with a nonequilibrium quasiparticle distribution function. (iii) The long-time limit described by a quantum Boltzmann equation leading to thermalization of the momentum distribution function. This thermalization behavior is contrasted with interaction quenches in 1d models.

12:03PM W18.00005 Dynamical Freezing of Response in Driven Many-Body Quantum System

, ARNAB DAS, Theoretical Division (T-4), Los Alamos National Laboratory, MS-B213, Los Alamos, NM 87545 — We show, that the response of a periodically driven quantum many- body system may freeze drastically, when driven with certain combinations of driving parameters (amplitude and frequency). We demonstrate this effect with analytical results for a broad class of integrable quantum spin models (illustrated particularly for one-dimensional Transverse Ising Model)and direct numerical integration data for large system-size. We show that the immunity of the freezing behavior to external noise can be controlled arbitrarily by controlling the strength of the local (on-site) field.

12:15PM W18.00006 Bethe-Salpeter Equation calculations of transition metal $L_{2,3}$ edge x-ray spectra including multiplet effects[1]

, J. VINSON, U. Washington, E.L. SHIRLEY, NIST, J.J. REHR, U. Washington — Calculations of x-ray spectra at transition metal $L_{2,3}$ edges often present theoretical difficulties due to strong core-hole multiplet effects. Here we discuss an *ab initio* method for treating these effects following the Bethe-Salpeter Equation (BSE) approach of Shirley.[2] The method builds in spin-orbit interactions, intra-atomic Coulomb integrals, core-hole screening, and band-structure effects, and thus accounts for multiplet effects without the need for phenomenological ligand-field parameters. The method has been implemented in the core-level BSE code OCEAN,[3] which uses as input wavefunctions from planewave, pseudopotential DFT calculations and PAW transition matrix elements. Examples are presented for several transition metal systems and compared with experiment.

[1]Supported by DOE BES DMSE Grant DE-FG03-97ER45623 and facilitated by the DOE CMCSN

[2]E. L. Shirley, J. Electron Spectrosc. Relat. Phenom. **144**, 1187 (2005).

[3]J. Vinson, E. L. Shirley, J. J. Rehr, and J. J. Kas, arXiv:1010.0025

12:27PM W18.00007 ABSTRACT WITHDRAWN –

12:39PM W18.00008 Real Space Green's Function Calculations of RIXS[1]

, J.J. KAS, J.J. REHR, U. Washington, J.A. SOININEN, U. Helsinki — We present an *ab initio* theory of resonant inelastic x-ray scattering (RIXS) based on the real-space multiple scattering Green's function (RSGF) formalism and a quasi-boson model Hamiltonian. It is shown that the RIXS spectrum is quasi-local in nature, depending primarily on the Green's function close to the absorbing site. Based on several assumptions, we derive an approximation to the RIXS spectrum in terms of a convolution of the x-ray absorption and x-ray emission spectra. In addition, quasi-particle self-energy and other many-body effects are calculated using a many-pole model dielectric function, and included via a convolution of the RIXS spectrum with an energy dependent spectral function. Core hole effects are also investigated. The method is implemented in an extension of the RSMS code FEFF90[2] and illustrated with several examples. Results are found to be in qualitative agreement with experiment.

[1]Supported by DOE BES Grant DE- FG03-97ER45623 and DOE CMCSN.

[2]J.J. Rehr et al., Comptes Rendus Phys. **10**, 548 (2009)

12:51PM W18.00009 Finite-Temperature Constraint-Pairing Mean Field Theory[1]

, JIANMIN TAO, GUSTAVO SCUSERIA, Rice University — Recently Tsuchimochi and Scuseria have developed a constrained-pairing mean-field theory (CPMFT), based on the Hartree-Fock-Bogoliubov theory. Application to molecular systems shows that CPMFT can accurately describe the binding energy curve in the dissociation of molecules, where electron correlation is strong. However, because CPMFT is a zero-temperature theory, it is not suitable for the description of high-temperature superconductivity and normal state of high-temperature superconductors. Here a finite-temperature generalization is formulated for the thermodynamic state of quantum many-body systems.

[1]This work was supported by NSF under Grant No. CHE-0807194 and the Welch Foundation under Grant No. C-0036.

1:03PM W18.00010 Fermionic duality approach to strongly-interacting lattice models[1]

, JOE MITCHELL, TIGRAN SEDRAKYAN, VICTOR GALITSKI, University of Maryland — We derive an exact Grassmann path-integral representation for strongly interacting fermion systems that is dual to the conventional Hubbard-Stratonovich approach. In contrast to the latter, we decouple the interaction Hamiltonian by introducing additional (dual) fermionic fields. This fermionic decoupling naturally forms in particle-hole channels and leads to alternative order parameters given in terms of the dual fields. The new formalism is tested by calculating the partition function in a simple solvable model with four-fermion interaction and is argued to be very effective for strong or repulsive interactions.

[1]This research is supported by the Department of Energy.

1:15PM W18.00011 ABSTRACT WITHDRAWN –

1:27PM W18.00012 Breakdown of the coherent state path integral: two simple examples[1]

, JUSTIN WILSON, VICTOR GALITSKI, Dept. of Physics, University of Maryland — We show how the time-continuous coherent state path integral breaks down for both the single-site Bose-Hubbard model and the spin path integral. Specifically, when the Hamiltonian is quadratic in a generator of the algebra used to construct coherent states, the path integral fails to produce correct results following from an operator approach. As suggested by previous authors, we note that the problems do not arise in the time-discretized version of the path integral. Further, a naïve use of the semiclassics agrees with our conclusions.

[1]NSF-CAREER award, DMR-0847224

Thursday, March 24, 2011 11:15AM - 2:15PM –
Session W19 GMAG DMP: Focus Session: Novel Magnetic Devices D170

11:15AM W19.00001 Novel Spintronic Device-Terahertz Magnon-Photon Laser , BORIS TANKHILEVICH, Terahertz Technologies LLC — A novel spintronic -based method of generating THz radiation is proposed. The method is based on pumping of non-equilibrium electrons into the upper (spin-down) sub-band of spin-polarized half-metallic ferromagnets or ferromagnetic semiconductors, which makes it possible to build tunable, narrow-band, high-power THz sources. Non-equilibrium electrons pumped into the spin-down subband rapidly emit non-equilibrium magnons with THz frequency, pass into highly excited states of the spin-up subband, and fall into the ground state due to interaction with the equilibrium spin-up electrons or by emitting optical phonons. The mechanism of magnon generation is similar to a three-level conventional laser, and at a critical pumping intensity, which depends on the magnon damping, magnon lasing begins. In this regime the number of excited magnons increases exponentially with time. Merging of two THz magnons with frequency f generates a THz photon with frequency 2f. Thus, a magnon laser becomes a THz photon laser. The proposed one-stage device is capable of generating THz power being of orders of milliwatt and is tunable by tuning the magnetic field and/or the bias. The device has nano-dimensions and can be mass produced on a large scale. Recently THz radiation by spin-polarized current in a ferromagnetic structure was observed. However, the material used in this experiment has not met the conditions for magnon lasing.

11:27AM W19.00002 Micro-Structured Ferromagnetic Tubes for Spin Wave Excitation , ALEXANDER KOZHANOV, DANIEL OUELLETTE, MARK RODWELL, University of California Santa Barbara, DOK WON LEE, SHAN X. WANG, Stanford University, S. JAMES ALLEN, University of California Santa Barbara — Small scale magnetostatic spin wave devices are potentially important for on-chip filters for communication systems and spin wave logic devices. Low efficient coupling the electronic signals into the spin waves as well as coupling-out makes it difficult to build logical circuits especially when structures are scaled down to nanometer sizes. In this work we study the effect of external biasing magnetic field on the propagation of backward volume magnetostatic spin waves (BVMSW) in ferromagnetic CoTaZr stripe with micron sized ferromagnetic tubes fabricated at the ends. Spin waves are excited by shorted coplanar waveguides signal line of which is placed inside the tubes. Ferromagnetic tubes placed at the ends of the stripe form closed magnetic circuit that traps the RF magnetic field produced by the coupling loop. Transmission S-parameters of fabricated structures were measured using a vector network analyzer in the frequency range (0.5-20) GHz and biasing magnetic fields (0-1000) Oe. Experimental data is analyzed with use of theoretical model for BVMSW in ferromagnetic stripe. This work is supported by the Nanoelectronics Research Initiative (NRI) - Western Institute of Nanoelectronics (WIN).

11:39AM W19.00003 Ferromagnetic STM tip operating as a Spin-diode[1] , POLIANA H. PENTEADO, University of São Paulo, FABRICIO M. SOUZA, Federal University of Uberlândia, ANTÔNIO C. SERIDONIO, UNESP, RENATO M. COUTINHO, EDSON VERNEK, Federal University of Uberlândia, J. CARLOS EGUES, University of São Paulo — We study spin-dependent transport in a system composed of a ferromagnetic STM tip coupled to an adsorbed atom (adatom) and to a host metallic (non-magnetic) surface. Electrons can tunnel directly from the tip to the surface or through the adatom. Our calculation is based on the nonequilibrium Green functions technique (Keldysh formalism). We self-consistently calculate the adatom spin occupation and its magnetization as a function of the tip position. We find that the adatom becomes magnetized when the tip approaches it; this magnetization switches sign as the voltage changes from forward to reverse bias. We also calculate the spin-resolved currents. If the tip is near the adatom, we obtain the spin-diode effect [PRB **75**, 165303 (2007)] - i. e., unpolarized current for positive bias and polarized current for reverse bias - when the adatom is singly occupied. We also observe Friedel oscillations in the current as the tip-adatom distance increases [F. M. Souza, P. H. Penteado, et al. - to be submitted].

[1]This work was supported by the funding agencies CNPq, CAPES, FAPEMIG and FAPESP.

11:51AM W19.00004 Spin voltage generation across rare earth spin filter barriers[1] , GUOXING MIAO, MIT, JOONYEON CHANG, KIST, JAGADEESH MOODERA, MIT — When a metal is in close contact with a rare-earth based magnetic compound, strong exchange interaction exists between the localized 4f electrons and the free moving conduction electrons. One important consequence is that the spin degeneracy among the conduction electrons is lifted, showing up as an effective Zeeman splitting higher than tens of Tesla in low dimensional systems such as graphene and other 2DEG. We perform our work using a vertical transport geometry, which consists of double spin filtering barriers based on a ferromagnetic Eu chalcogenide - EuS. A thin Al metallic layer is sandwiched in the middle and its conduction electrons thus experience the strong spin splitting, which is subsequently detected via the spin filtering effect. A spontaneous spin dependent voltage appears across such a device, and its polarity is directly determined by the EuS/Al interface. The voltage level difference between the spin-parallel and -antiparallel configurations is as large as a few mV. Such spin splitting also induces a clear universal behavior in the observed TMR bias dependence. Such spin voltage effect offers a possibility of directly converting magnetic exchange energy into electrical power.

[1]This work is supported by NSF DMR 0504158, ONR N00014-06-1-0235, and KIST-MIT project funds.

12:03PM W19.00005 Generation of spin currents due to mechanical rotation , MAMORU MATSUO, Kyoto Univ., ASRC-JAEA, JUN'ICHI IEDA, ASRC-JAEA, CREAST-JST, EIJI SAITOH, ASRC-JAEA, IMR Tohoku Univ., CREST-JST, SADAMICHI MAEKAWA, ASRC-JAEA, CREST-JST — In the frontier of spintronics, much attention is paid on the control and generation of spin currents. Due to the exciting progress of nanomechatrononics, the importance of mechanical manipulation of electron spin will increase. We discuss theoretically effects of mechanical rotation on spin currents using generally covariant Dirac equation with gauge fields in the non-relativistic limit. We derive semi-classical equations of motion for a wavepacket of electrons in two dimentional planes subject to the spin-orbit interaction argumented by a mechanical rotation. We show that a circular spin current is created by the mechanical rotation with a magnetic field. The magnitude of the spin current becomes $10^8 \mathrm{A/m}^2$ in Pt with the magnetic field $\approx 1\mathrm{T}$ and the rotational velocity $\approx 1\mathrm{kHz}$.

12:15PM W19.00006 Magnetic Field Effects on Mechanical Cantilevers with Deposited Thin Film Micromagnets[1] , ROSA ELIA CÁRDENAS, FRANCISCO MÁRQUEZ, JOHN T. MARKERT, The University of Texas at Austin, Department of Physics — We report on the techniques used to deposit magnetic material onto mechanical cantilevers. The deposition of the magnetic material, permalloy, onto the cantilevers was achieved by using a precise masking technique before mounting the cantilevers inside an electron beam evaporation chamber. This method resulted in a mechanical cantilever with a deposited micromagnet on its tip. A typical size of the resulting micromagnet is 200 nm thick by 20 microns wide by 10 microns in height. Using a laser interferometer, the driven response of the cantilevers with the deposited micromagnets are currently being studied in vacuum as a function of the external magnetic field. We will analyze the magnetic-field-dependent changes in the resonant frequencies and the quality factors of the cantilevers to determine the micromagnet net moment and anisotropy constants.

[1]We acknowledge support from NSF-DMR 0605828 and Welch F-1191.

12:27PM W19.00007 Torque magnetometry of permalloy-coated microcantilevers using higher order vibrational modes , JOSEPH LOSBY, JACOB A.J. BURGESS, Department of Physics, University of Alberta and National Institute for Nanotechnology, DOUGLAS VICK, National Institute for Nanotechnology, JOHN P. DAVIS, Department of Physics, University of Alberta, WAYNE K. HIEBERT, National Institute for Nanotechnology, MARK R. FREEMAN, Department of Physics, University of Alberta — There has been an accumulation of recent interest in the development of magnetometry techniques facilitating the use of nano- and micro-resonators. A finite element model describing the interaction of a magnetic cantilever driven at its fundamental resonance frequency by an external field is described and illustrated for the simple case of a straight domain wall propagating across the cantilever during magnetization reversal. The experimental results are compared to the finite element mechanical transformation of Landau-Lifshits-Gilbert based micromagnetic simulations. This idea is then extended to higher order (flexural and torsional) modes, with the intent of moving towards increased sensitivity and functionalization of magnetometers for the observation of quasi-static magnetization processes.

12:39PM W19.00008 Forces due to Patterned Magnetic Traps within Microfluidic Channels , M. HOWDYSHELL, G. VIEIRA, A. CHEN, M. SIMON, M. POIRIER, R. SOORYAKUMAR — An array of microscopic ferromagnetic disks patterned onto a silicon surface has been previously utilized to trap and transport magnetic microspheres as well as magnetically labeled biological cells across the surface. The transport is activated through programmable weak external magnetic fields that do not damage the cells and enable remote control on the magnitude and direction of the fields. In this talk we present results in which the array of magnetic bits is imprinted within microfluidic channels where now competing hydrodynamic drag forces come into play. The trapping forces on individual microspheres are directly determined from the flow rates required to overcome the local magnetic forces. These findings are compared to results derived from micromagnetic simulations of the magnetic profile of individual disks. The fluid flow within the channel is also used to stretch DNA molecules tethered between two microparticles. With one of the ends trapped on a magnetic disk, the extension is controlled by the fluid flow rate. Comparisons to DNA stretching achieved with conventional magnetic tweezers reported in the literature serve as an additional calibration of the measured forces.

12:51PM W19.00009 Giant Magnetioimpedance in Co-Based Amorphous Ribbons Coated in Magnetic Nanoparticles for Biosensing Applications , N. LAURITA, A. CHATURVEDI, K. STOJAK, S. CHANDRA, M.H. PHAN, H. SRIKANTH, University of South Florida — Giant magnetoimpedance (GMI) is a large change in the ac impedance of a ferromagnetic conductor subject to a dc magnetic field. It forms the basis for developing highly sensitive magnetic sensors. We report studies aimed at developing GMI as a magnetic biosensing technique. We have investigated the GMI effect and its field sensitivity in Co-based amorphous alloys with and without coated magnetic nanoparticles. Fe_3O_4 and $CoFe_2O_4$ nanoparticles (mean size, 5-10 nm) were patterned onto the ribbon surfaces and the number of particle layers was varied from 10 to 80. The influences of particles size, concentration, and layer thickness on the GMI and field sensitivity have been investigated systematically. The coating of the nanoparticles has been shown to enhance the GMI and field sensitivity, both of which increase with increase of particle concentration and layer thickness. Overall, our studies demonstrate the possibility of using GMI as a magnetic biosensor with high sensitivity for applications in biomolecular detection.

1:03PM W19.00010 Correlation between magnetic softness, sample surface and magnetoimpedance in $Co_{69}Fe_{4.5}X_{1.5}Si_{10}B_{15}$ (X = Ni, Al, Cr) amorphous ribbons , A. CHATURVEDI, T. DHAKAL, S. WITANACHCHI, M.H. PHAN, H. SRIKANTH, University of South Florida, A.T. LE, Hanoi University of Technology, Vietnam — In this work we have studied the giant magnetoimpedance (GMI) effect and its field sensitivity (η) in $Co_{69}Fe_{4.5}X_{1.5}Si_{10}B_{15}$ (X = Ni, Al, Cr) amorphous ribbons in the frequency (f) range of 0.1 to 10 MHz. We find that at f $<$ 5 MHz, the GMI effect and η reach the largest values for the Al-containing sample and the smallest values for the Ni-containing sample, while an opposite trend is observed at f $>$ 5 MHz. Magnetization and atomic force microscopy (AFM) experiments reveal that the largest values of the low-frequency GMI effect and η for the Al-containing sample result from the largest value of magnetic permeability, while the largest values of the high-frequency GMI effect and η for the Ni-containing sample are attributed to the smallest surface roughness of this sample. These results point to the importance of the sample surface in determining high-frequency GMI behavior. A correlation between the sample surface and high-frequency GMI is established in the investigated ribbons.

1:15PM W19.00011 Modulating the Magnetic Field to Improve Magnetic Sensors , ALAN EDELSTEIN, JONATHAN PETRIE, JONATHAN FINE, GREG FISCHER, US Army Research Laboratory, JAMES BURNETTE, NIST Gaithersburg, GOPAL SRINIVASAN, SANJAY MANDAL, Oakland University, US ARMY RESEARCH LABORATORY COLLABORATION, NIST GAITHESBURG COLLABORATION, OAKLAND UNIVERSITY COLLABORATION — The sensitivity of most magnetic sensors is affected by $1/f$ noise. Modulating the magnetic field to be detected by magnetic sensors can improve their performance by minimizing the effect of this $1/f$ noise and, in some cases, also have them operate in a narrow frequency band where they have higher sensitivity. We present approaches for modulating the field. One approach is the MEMS flux concentrator can be used with small magnetic sensors and another, based on using a rotating disc containing flux concentrators that can be used with large magnetic sensors, such as magnetoelectric sensors, that have an increased sensitivity at their mechanical resonance frequency. Sidebands observed around the modulation frequency demonstrate the applicability of these approaches. The MEMS flux concentrator has improved the signal to noise ratio in the power spectrum by a factor of 15. The sensors have the potential to achieve sensitivities of a few $pT/Hz^{1/2}$ at 1 Hz.

1:27PM W19.00012 Ultra high sensitivity, room temperature magneto-optic field sensor made of ferromagnetic bismuth rare-earth iron garnet thick films , DONG HO WU, ANTHONY GARZARELLA, Naval Research Laboratory, VINCE FRATELLO, Integrated Photonics, Inc — The ferrimagnetic bismuth rare-earth iron garnet $(BiGdLu)_3(FeGa)_5O_{12}$ thick film has a specific Faraday rotation θ_S of 0.09 $^\circ$/mm at 1550 nm and excellent transparency at infrared wavelengths. Using the thick film we recently have demonstrated a magneto-optic (MO) field sensor with a sensitivity of about $10^{-14}T/Hz^{1/2}$, comparable with SQUID. The sensor is made of all dielectric materials including the bismuth rare-earth iron garnet and optical fibers, and is operated at room temperature without any cooling requirement. The MO field sensor is capable to measure a magnetic field over a very large dynamic range (from a very weak field to a very high magnetic field exceeding several hundred Tesla) and over a very wide frequency range, which may be from DC to a few hundred GHz. However, presently, our MO sensor's frequency range is limited from DC to 2 GHz. We think that this limited frequency range is due to the presence of magnetic domains in the bismuth rare-earth iron garnet film. In this presentation we will report our experimental results obtained from this MO field sensor as well as the effect of magnetic domains.

1:39PM W19.00013 Spin-Flipping at Sputtered Co(90)Fe(10)/Cu Interfaces[1] , HOANG YEN THI NGUYEN, RAKHI ACHARYYA, WILLIAM P. PRATT JR., JACK BASS, Michigan State University — Knowledge of the spin-flipping probability, $P_{F/N} = 1 - \exp[-\delta(F/N)]$, at ferromagnetic/non-magnetic (F/N) interfaces in the Current-Perpendicular-to-Plane (CPP) geometry is minimal [1,2]. We use a new technique [2] to find δ(CoFe/Cu) at 4.2K, where CoFe = Co(90)Fe(10). With thin (3 nm) CoFe layers, the spin-diffusion length of CoFe $\sim$ 12 nm doesn't mask spin-flipping due to δ. Our most important samples, sensitive to δ(CoFe/Cu), have the form FeMn/Py/Cu/X/Cu/Py/FeMn. Here Py = Ni(80)Fe(20), the antiferromagnet FeMn pins the two Py layers to flip at a much higher field than X = $[CoFe(3)/Cu(1.4)]_n CoFe(3)$, and 1.4 nm of Cu couples the CoFe layers ferromagnetically so X reverses as a unit. We measure, versus the number of repeats n, the change in specific resistance, $A\Delta R$ = AR(AP) – AR(P), between states where the X moment is anti-parallel (AP) or parallel (P) to the pinned Py moments. CPP current flows through area A. Our resulting best estimate is δ(CoFe/Cu) $\approx$ 0.2. [1] J. Bass and W.P.Pratt Jr., J. Phys. Cond. Matt. **19**, 183201 (2007). [2] B. Dassonneville et al., Appl. Phys. Lett. **96**, 022509 (2010).

[1]Research supported by NSF- DMR 08-04126 and KIST.

1:51PM W19.00014 Magnetic Properties of Niobium-Permalloy hybrid system , JIYEONG GU, JILL PESTANA, DAVID CHRISTIANSEN, Department of Physics and Astronomy, California State University, Long Beach — Ferromagnet/superconductor hybrid system has been studied intensively due to the proximity effect between ferromagnetism and superconductivity. Not only the superconducting property changes because of the different magnetic configuration, the presence of the superconductivity can also often drastically change the magnetic properties of the ferromagnets. In our current work we focused on the investigation of the magnetic property change of the Nb-Py (Permalloy; NiFe) hybrid system through the superconducting transition. Nb-Py bilayer and trilayers were fabricated using Multi-target sputtering system. Magnetization was measured by Physical Property Measurement System using the Vibrating Sample Magnetometer (VSM) or Alternating Current Measurement System (ACMS) options. In addition to the magnetometry measurement, we also measured magneto optical Kerr effect. Magnetization changed when the system goes through the superconducting transition; however the result varied depending on many parameters, such as magnetic measurement history, cooling or warming rate, and measurement method. Magnetic responses obtained from different methods would be compared and discussed.

2:03PM W19.00015 Localized magnetism on the surface of niobium: experiments and theory[1] , THOMAS PROSLIER, Argonne natl lab, JOHN ZASADZINSKI, Illinois Institute of technology, GIANLUIGI CIOVATI, Jefferson lab, MIKE PELLIN, Argonne natl lab — The presence of magnetic impurities in native niobium oxides have been confirmed by Point contact spectroscopy (PCT), SQUID magnetometry and Electron paramagnetic resonance (EPR). All niobium (Nb) samples displayed a small impurity contribution to the magnetic susceptibility at low temperatures which exhibited Curie-Weiss behavior, indicative of weakly coupled localized paramagnetic moments. By examining Nb samples with widely varying surface-to-volume ratios it was found that the impurity contribution is correlated with surface area. Tunneling measurements which use the native oxide layers as barriers exhibit a zero-bias conductance peak which splits in a magnetic field > 4T, consistent with the Appelbaum model for spin flip tunneling. Viewed together the experiments strongly suggest that the native oxides of Nb are intrinsically defective, and consistently exhibit localized paramagnetic moments caused by oxygen vacancies in Nb_2O_5. The computation of the surface impedance (R_S) in presence of magnetic impurities in the Shiba approximation reveals the saturation at low temperature of Rs, suggesting that magnetic impurities are responsible for the so-called residual resistance.

[1]Work supported by DOE-HEP office, under contract No. DE-AC02-06CH11357.

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W20 DMP GERA FIAP: Focus Session: Thermoelectric Materials: Clathrates and Oxides D168

11:15AM W20.00001 The Atomic Structure of Ga and Ge in Ba-Ga-(Si,Ge) Clathrate , A.N. MANSOUR, NSWCCD, J.B. MARTIN, W. WONG-NG, NIST, G.S. NOLAS, USF — Compression studies on $Sr_8Ga_{16}Ge_{30}$ type I clathrate revealed a 3 fold increase in "ZT" [J. F. Meng et al., J. Appl. Phys., 89, 1730 (2001)]. Substitution of Si for Ge in Ba-Ga-Ge clathrate could mimic the effect of bulk compression, and subsequently enhance "ZT". Recent studies on Si substituted Ba-Ga-Ge clathrate have shown a decrease in the lattice constant and an increase in the power factor with Si substitution. However, the effects of Si on the electronic and local atomic structures of Ga and Ge have not been investigated in detail. We have used XAS to characterize the electronic and local atomic structures of Ga and Ge for a number of samples with varying degree of Si substitution. Analysis of Ga and Ge K-edge XANES spectra revealed that the partial density of p-states was modified for both Ga and Ge with Si substitution with the changes being more pronounced in the case of Ga. Comparisons of Fourier transforms of EXAFS spectra revealed that the local structure of Ga is significantly changed with Si substitution while changes in the local structure of Ge with Si substitution are moderate.

11:27AM W20.00002 Examining Lattice Disorder in Type-I Clathrate $Ba_8Ga_{16}Sn_{30}$ using EXAFS[1] , SCOTT MEDLING, MICHAEL KOZINA, FRANK BRIDGES, UC Santa Cruz, KOICHIRO SUEKUNI, Japan Advanced Institute of Science and Technology, TOSHIRO TAKABATAKE, Hiroshima University — Semiconducting type I clathrates, such as $Ba_8Ga_{16}Ge_{30}$ (BaGaGe) and $Ba_8Ga_{16}Sn_{30}$ (BaGaSn), have a cage-like crystal structure with "rattler" atoms (Ba) located near the center of cages (Ga-Ge/Sn). Such compounds have a low thermal conductivity which is attributed mainly to vibrations of the "rattler" atoms inside the cages which strongly scatter phonons. BaGaSn has a surprising lower thermal conductivity than BaGaGe. To better understand why, we studied samples of BaGaSn using Extended X-ray Absorption Fine Structure (EXAFS). The analysis shows that the average Ga-Sn distance is shorter and the average Sn-Sn distance is longer than the distances found from diffraction; also, the Ba-Ga and Ba-Sn distances have greatly increased disorder. This suggests that the cage-like structure is severely distorted, in contrast to BaGaGe; such a large distortion will strongly scatter phonons, decreasing the thermal conductivity, but unfortunately also will reduce the electrical conductivity. We compare our results for BaGaSn with earlier results for BaGaGe and discuss them in light of recent transport measurements.

[1]NSF grant DMR-1005568

11:39AM W20.00003 Structural, Electronic and Vibrational Properties of $Na_xSi_{136}(0 < x < 24)$ Clathrates , CRAIG HIGGINS, EMMANUEL NENGHABI, CHARLES MYLES, Texas Tech University, KOUSHIK BISWAS, Oak Ridge National Laboratory, MATT BEEKMAN, University of Oregon, GEORGE NOLAS, University of South Florida — CRAIG HIGGINS, EMMANUEL NENGHABI[†], CHARLES W. MYLES, Texas Tech U.; KOUSHIK BISWAS, Oak Ridge National Lab; MATT BEEKMAN, U. of Oregon; GEORGE S. NOLAS, U. of South Florida - Na_xSi_{136} is a Type II clathrate with important thermoelectric properties. It's face-centered cubic lattice contains polyhedral "cages" of silicon atoms with Na atom "guests" in the cages. This material is very interesting because powder X-ray diffraction experiments[1] for differing Na content x have shown that, for increasing x in the range $0 < x < 8$, lattice contraction occurs. After all Si_{28} cages in the unit cell are filled ($x = 8$) and x is increased further, causing a filling of the Si_{20} cages, a contrasting lattice expansion results. Using the local density approximation, we have calculated the x dependences of the structural, electronic and vibrational properties of Na_xSi_{136}. Results are presented for the x dependences of the lattice constant, electronic bands, and vibrational modes. Our results for the x dependence of the lattice constant are in agreement with our X-ray data[1]. [†]Deceased. [1]M. Beekman, E.N. Nenghabi, K. Biswas, C.W. Myles, M. Baitinger, Y. Grin, G.S. Nolas, Inorg. Chem. 49, 5338–5340 (2010).

11:51AM W20.00004 NMR relaxation and phonon rattling in type-I $Ba_8Ga_{16}Sn_{30}$ clathrates , XIANG ZHENG, SERGIO Y. RODRIGUEZ, JOSEPH H. ROSS, JR., Department of Physics and Astronomy, Materials and Engineering Program, Texas A&M University — The atomic motion of guest atoms inside clathrate cages has been considered as one of the important reasons for the observed glasslike thermal behavior. ^{69}Ga and ^{71}Ga Nuclear Magnetic Resonance (NMR) studies of type-I $Ba_8Ga_{16}Sn_{30}$ clathrates show a clear low temperature spin-lattice relaxation peak attributed to the influence of Ba rattling dynamics on the framework-atom resonance. Analysis indicates that the quadrupolar relaxation is the leading contribution. The data are analyzed using a two-phonon Raman process, according to a recent theory involving localized one dimensional anharmonic oscillators. Excellent agreement is obtained using this model, with the parameters corresponding to a double well with very large anharmonicity. We have extended the theory to include a two dimensional anharmonic well, with similar parameters providing the best fit to the data. We also examine the Einstein type peak observed in heat capacity using this model, and compare to previous reported results obtained using different models for the anharmonic oscillator. This work is supported by Robert A. Welch Foundation (A-1526).

12:03PM W20.00005 Zintl stabilization and site preference in Ba-Cu-Ge clathrates , SERGIO Y. RODRIGUEZ, XIANG ZHENG, LAZIZ SARIBAEV, JOSEPH H. ROSS, JR., Department of Physics and Astronomy, Texas A&M University — Sn, Ge and Si clathrates have cage-like structures, and many exhibit enhanced thermoelectric performance. To understand Cu substitution and Zintl stabilization in $Ba_8Cu_xGe_{46-x}$ type-I clathrates with $4 \leq x \leq 6$, we performed NMR measurements coupled with first principles calculations. The ^{63}Cu NMR resonance exhibits a lineshape characteristic of Cu occupation of the high-symmetry 6c site. All electron computational results showed that the lowest energy configuration is the one with all the Cu atoms located in the 6c site, in agreement with NMR and crystallographic analysis. From bandstructure calculations we find that the preferred structure is a semiconductor, consistent with the observed Zintl stabilization in this material. A direct band gap of about 0.27 eV is found within the Generalized Gradient Approximation formalism. The preferred compositions follow quite closely the valence-counting scheme. From an Atoms In Molecules analysis it is seen that the Ba charge is less than 2^+, even though the simple electron-counting argument works well. The framework is seen to be composed of a sp^3 bonded network, with strongly polar bonds for Cu. Ba atoms in the large cages are least strongly bond in the plane of the hexagonal faces, corresponding to ease of rattling as seen for other clathrates. This work is supported by Robert A. Welch Foundation (Grant A-1526).

12:15PM W20.00006 Thermoelectric properties of low-dimensional clathrates from first principles , DEEPA KASINATHAN, HELGE ROSNER, MPI CPfS — Type-I inorganic clathrates are host-guest structures with the guest atoms trapped in the framework of the host structure. From a thermoelectric point of view, they are interesting because they are semiconductors with adjustable bandgaps. Investigations in the past decade have shown that type-I clathrates $X_8Ga_{16}Ge_{30}$(X = Ba, Sr, Eu) may have the unusual property of "phonon glass-electron crystal" for good thermoelectric materials. Among the known clathrates, $Ba_8Ga_{16}Ge_{30}$ has the highest figure of merit (ZT 1). To enable a more widespread usage of thermoelectric technology power generation and heating/cooling applications, ZT of at least 2-3 is required. Two different research approaches have been proposed for developing next generation thermoelectric materials: one investigating new families of advanced bulk materials, and the other studying low-dimensional materials. In our work, we concentrate on understanding the thermoelectric properties of the nanostructured Ba-based clathrates. We use semi-classical Boltzmann transport equations to calculate the various thermoelectric properties as a function of reduced dimensions. We observe that there exists a delicate balance between the electrical conductivity and the electronic part of the thermal conductivity in reduced dimensions. Insights from these results can directly be used to control particle size in nanostructuring experiments.

12:27PM W20.00007 Nanostructured Oxides and Sulfides for Thermoelectrics , KUNIHITO KOUMOTO, Nagoya University — Thermoelectric power generation can be applied to various heat sources, both waste heat and renewable energy, to harvest electricity. Even though each heat source is of a small scale, it would lead to a great deal of energy saving if they are combined and collected, and it would greatly contribute to reducing carbon dioxide emission. We have been engaged in developing novel thermoelectric materials to be used for energy saving and environmental protection and are currently developing nanostructured ceramics for thermoelectric conversion. We have demonstrated a quantum confinement effect giving rise to two dimensional electron gas (2DEG) in a 2D superlattice, STO/STO:Nb (STO: strontium titanate), which could generate giant thermopower while keeping high electrical conductivity. One unit-cell thick Nb-doped well layer was estimated to show ZT=2.4 at 300K. Then, a "synergistic nanostructuring" concept incorporating 2DEG grain boundaries as well as nanosizing of grains has been applied to our STO material and 3D superlattice ceramics was designed and proposed. It was verified by numerical simulation that this 3D superlattice ceramics should be capable of showing ZT=1.0 at 300K which is comparable to or even higher than that of conventional bismuth telluride-based thermoelectrics. We have recently proposed titanium disulfide-based misfit-layered compounds as novel TE materials. Insertion of misfit-layers into the van der Waals gaps in layer-structured titanium disulfide thus forming a natural superlattice gives rise to internal nanointerfaces and dramatically reduces its lattice thermal conductivity. ZT value reaches 0.37 at 673 K even without optimization of electronic properties. Our challenge to further increase ZT by controlling their electronic system and superlattice structures will be presented.

1:03PM W20.00008 Electronic Structure Determination of the Thermoelectric $CuRh_{1-x}Mg_xO_2$ using Soft X-Ray Spectroscopies , ERIC MARTIN, PAOLO VILMERCATI, CHRISTINE CHENEY, Dept. of Physics and Astronomy, University of Tennessee, TAKAO SASAGAWA, Materials and Structures Laboratory, Tokyo Institute of Technology, NORMAN MANNELLA, Dept. of Physics and Astronomy, University of Tennessee — Magnesium-doped rhodium oxides with formula unit $CuRh_{1-x}Mg_xO_2$ and delafossite-type structure exhibit a high thermoelectric figure of merit at elevated temperatures. The electronic structure of $CuRh_{1-x}Mg_xO_2$ has been studied with x-ray emission spectroscopy (XES), x-ray absorption spectroscopy (XAS), and photoemission spectroscopy (PES). The data reveal that the states at the Fermi level are Rh-derived. Measurements carried out by changing the orientation of the linear photon polarization further indicate that the Rh states have a more localized character along the c-axis, consistent with the layered crystal structure. Given the similarity of the electronic configurations of Co and Rh, these data provide solid experimental evidence that the orbital degrees of freedom of the d^6ionic configuration of the states rooted in transport are key for explaining the thermoelectric properties of oxide materials.

1:15PM W20.00009 Thermal Conductivity of Aluminum Oxide from First Principles[1] , MOSES NTAM, JIANJUN DONG, Auburn University, BIN XU, University of Texas at Arlignton — Alumina (Al_2O_3) is a well-known ceramic material. First-principles study of lattice thermal conductivity can assist our understanding in extreme conditions that are difficult to achieve experimentally, as well as analyze the fundamental difference between other materials. We combine density functional theory and the Peierls–Boltzmann transport theory to predict the temperature and pressure dependencies of lattice thermal conductivity of the corundum phase. We use a real space super cell method to extract second force constants and third order lattice anharmonicity tensors. These are then used to directly evaluate the phonon scattering rates due to lattice anharmonicity. Our preliminary results show that at a density of 4.23 g/cm^3 Al_2O_3 has thermal conductivities of 14.8Wm^{-1}K^{-1} at 300K and 5.31Wm^{-1}K^{-1} at 1000K. Moreover, we calculated the thermodynamic properties such as thermal expansion coefficient, bulk modulus and heat capacity, which are in excellent agreement with available measurements and previous theoretical calculations.

[1]NSF EAR-0757847

1:27PM W20.00010 Thermoelectric properties of $Ca_3Co_4O_9$ thin film[1] , ROBERT KLIE, QIAO QIAO, AHMET GULEC, TADAS PAULAUSKAS, University of Illinois - Chicago, STANISLAW KOLESNIK, BOGDAN DABROWSKI, Northern Illinois University, CIHAT BOYRAZ, MEHMET OZDEMIR, DIPANJAN MAZUMDAR, ARUN GUPTA, University of Alabama — Thermoelectric oxides have attracted increasing attention due to their high thermal power and temperature stability. In particular, $Ca_3Co_4O_9$(CCO), a misfit layered structure consisting of single layer hole-doped CoO_2 sandwiched between insulating Ca_2CoO_3 rocksalt layers, exhibits a high Seebeck coefficient at 1000 K. It was suggested that the Seebeck-coefficient can be further increased by growing doped thin films with controlled defects structures. This study combines pulsed layer deposition thin film synthesis of pristine CCO on several oxide substrates, as well as CCO thin films doped with Ti, Bi or La, with aberration-corrected scanning transmission electron microscopy and electron energy loss spectroscopy (EELS) to examine the effects of interfacial strain and doping on the atomic and electronic structures of CCO. The thermoelectric properties will be measured and correlated to the local changes in the atomic and electronic structures. We will further evaluate the role of CoO_2 stacking faults, as well as film thickness on the thermoelectric properties of CCO.

[1]This work is supported by the US Army Research Office (W911NF-10-1-0147) and the National Science Foundation (DMR-0846748).

1:39PM W20.00011 Improvement of the thermoelectric properties of substituted $SrTiO_3$ by synthesis conditions[1] , S. KOLESNIK, S. BOONA, Department of Physics, Northern Illinois University, DeKalb, IL, B. DABROWSKI, Department of Physics, Northern Illinois University, DeKalb, IL, Materials Science Division, Argonne National Laboratory, Argonne IL, K. SWIERCZEK, K. WOJCIECHOWSKI, AGH University of Science and Technology, Cracow, Poland — We have studied thermoelectric properties of polycrystalline $Sr_{1-x}La_xTiO_3$ and $SrTi_{1-x}Nb_xO_3$ (x<=0.2) synthesized by a solid state synthesis method in a H_2/Ar atmosphere. The incorporation of La and Nb into the crystal structure was confirmed by x-ray diffraction and energy dispersive x-ray spectroscopy. By increasing the synthesis temperature (up to $\sim$1570^{o}C) and decreasing the partial pressure of oxygen, we were able to optimize the thermoelectric properties of the studied materials. The determined values of the thermoelectric figure of merit ZT$\sim$0.1 at 400 K and $\sim$0.3 at 800 K are comparable to those of single crystals of La- and Nb- substituted compounds. Our results show that the synthesis conditions play a crucial role in tailoring of the thermoelectric properties of substituted strontium titanates.

[1]Work at NIU was supported by the NSF (DMR-0706610) and at ANL by the U.S. DOE under contract No. DE-AC02-06CH11357.

1:51PM W20.00012 Thermoelectric Properties of a-InGaZnOx , D.S. WILLIAMS, STEPHAN PIOTROWSKI, B.E. WHITE, Binghamton University — Primarily known as an active layer in thin film transistors, the electrical and thermal properties of a-InGaZnOx indicate promise as a thermoelectric material. In contrast to most phonon-blocking, electron-transmitting thermoelectric materials, a-InGaZnOx is a structurally amorphous material that maintains relatively high electron mobility (10-50 cm2/V-s) and optical transparency. Here we report on the electrical conductivity, thermal conductivity, and Seebeck coefficient of this material as a function of charge carrier concentration. Carrier concentration is modulated through thin film annealing in a reducing ambient. Room temperature thermal conductivity is found to be 0.35 W/m-K with a Seebeck coefficient of approximately 200μV/K. These data suggest room temperature thermoelectric figures of merit in the range of 0.1-0.3 are achievable with these materials, offering the possibility of transparent thermoelectric energy generation.

2:03PM W20.00013 ABSTRACT WITHDRAWN –

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W21 GIMS: Novel Imaging Techniques and Calorimetry D161

11:15AM W21.00001 Particle distribution and dynamics in a complex fluid suspension studied by an image-analysis light-scattering technique , SAAD ALGARNI, H. KASHURI, GERMANO IANNACCHIONE, WPI — A relatively unique approach is described to analyze the scattered laser light from a complex fluid suspension for both static and dynamic behavior. Recent development of speckle analysis using CCD recorded direct imaging of the scattered coherent light has opened many new avenues for the application of static and dynamic light scattering experiments. The straightforward nature of this approach is somewhat offset by the constraints of the CCD chip size and placement to probe wide (or narrow) ranges of the wave vector. An alternative, and greatly simplified variation of this technique, is to convert the scattered light into diffuse scattering using a translucent screen placed at a desired location down beam then imaging the resulting pattern on the screen. A thru-beam stop and axis scales can be easily placed on the screen and recorded to improve the image quality and later analysis. One of many possible applications is the study of the particle (7nm diam aerosil SiO2 spheres) distribution and dynamics due to Brownian motion as well as sedimentation in a complex fluid (glycerol).

11:27AM W21.00002 ABSTRACT WITHDRAWN –

11:39AM W21.00003 3D Optical Field Mapping of a Focused Cylindrical Vector Beam Using Rayleigh Nanoparticles[1] , LIANGCHENG ZHOU, Lehigh University, QIWEN ZHAN, University of Dayton, H. DANIEL OU-YANG, Lehigh University — We report a novel method of mapping the optical field distribution of a focused cylindrical vector beam (CVB) using optically trapped Rayleigh nanoparticles. By using an ensemble method to measure the potential energy of nanoparticles in a CVB trap, optical trapping energy as low as 0.05 k_BT was measured. We demonstrated that the absolute intensity of a highly localized optical field is measured *in situ* using low concentration of polystyrene nanoparticles sized at 48 nm acting as optical nanoprobes. Their collective behavior in the focal volume gives very accurate reading of the optical field distribution, which shows excellent consistency with numerical simulations.

[1]This project is supported in part by NSF DMR 0923299, Pennsylvania Department of Commerce and Economic Development through the Center for Optical Technologies at Lehigh University and the Pennsylvania Department of Health CURE Formula Funds.

11:51AM W21.00004 High Resolution Micro-Optical Wall Shear Stress Sensor Based on Whispering Gallery Modes of Dielectric Microspheres , ULAS AYAZ, TINDARO IOPPOLO, VOLKAN OTUGEN, Southern Methodist University — We report the performance of a photonic wall shear stress sensor based on Whispering gallery mode (WGM) shifts of dielectric microsphere resonators. In particular, issues related to the sensitivity, resolution, frequency response and cross-axis sensitivity of the sensor are investigated experimentally. The sensor used in this prototype is a dielectric hollow microsphere made of Polydimethylsyloxane (PDMS). The wall shear stress acting on a sensing element of 125 μm diameter, is transmitted mechanically to the microsphere and the transmitted stress leads to shifts in the WGMs of the microsphere. By monitoring these WGM shifts, the magnitude as well as the direction of the wall shear stress are measured. Measurement resolutions better than 1 mPa have been observed.

12:03PM W21.00005 An effect of probe current on ADF image intensity of Si crystal , SUHYUN KIM, Tokyo Institute of Technology, YOSHIFUMI OSHIMA, YASUMASA TANISHIRO, KUNIO TAKAYANAGI — Annular dark field (ADF) scanning transmission electron microscope has been used to identify elements in the crystal. To analyze ADF image intensity more quantitatively, simulation of ADF image is required. However, the simulation has been known to overestimate the intensity because source size used in the simulation is assumed to be a point. Therefore, finite effective source size has been taken into an account by convolving Gaussian function to simulation. And, the Gaussian convolution has been usefully used to solve the mismatch in intensity, providing us a way of quantitative analysis for ADF image. Here, we quantitatively estimated an effective size of the cold field emission source. We obtained different Gaussian convolution size for ADF image acquired with various probe current by comparing ADF image contrast between experiment and simulation. As a result, we found that the effective source size which is needed for explaining contrast of ADF image decreased with decreasing probe current.

12:15PM W21.00006 Fast and Computationally Efficient Boundary Detection Technique for Medical Images , ARPITA DAS, PARTHA GOSWAMI, SUSANTA SEN, Calcutta University, India — Detection of edge is a fundamental procedure of image processing. Many edge detection algorithms have been developed based on computation of the intensity gradient. In medical images, boundaries of the objects are vague for gradual change of intensities. Therefore need exists to develop a computationally efficient and accurate edge detection approach. We have presented such algorithm using modified global threshold technique. In our work, the boundaries are highlighted from the background by selecting a threshold (**T**) that separates object and background. In the image, where object to background or vice-verse transition occurs, pixel intensity either rises greater or equal to **T** (background to object transition) or falls less than **T** (object to background). We have marked these transition regions as object boundary and enhanced the corresponding intensity. The value of **T** may be specified heuristically or by following specific algorithm. Conventional global threshold algorithm computes the value of **T** automatically. But this approach is not computationally efficient and required a large memory. In this study, we have proposed a parameter for which computation of **T** is very easy and fast. We have also proved that a fixed size memory [256×4Byte] is enough to compute this algorithm.

12:27PM W21.00007 Integrated instrument for holographic optical trapping and multicolor holographic video microscopy , BHASKAR JYOTI KRISHNATREYA, DAVID G. GRIER, Department of Physics and Center for Soft Matter Research, New York University, New York, NY 10003 — We designed and constructed an integrated holographic materials characterization and processing workstation that combines dynamical holographic optical trapping with multicolor holographic video microscopy. Unlike previously described systems, which are based on conventional light microscopes, our holographic workstation features a rigid, compact, adaptable, and modular design that can be replicated easily using standard off-the-shelf optical components. We demonstrate enhanced efficiency in micro-manipulation of colloidal materials using our instrument. By illuminating these colloidal particles with multiple laser wavelengths concurrently and analyzing the multicolor holograms independently for each color, we can acquire complementary information about the particles' size, position, and composition, and also gain insights into their material-dependent properties.

12:39PM W21.00008 Graded Index Lens Design for Aqueous Applications[1] , THEODORE MARTIN, MICHAEL NICHOLAS, GREGORY ORRIS, Naval Research Laboratory, LIANG-WU CAI, Kansas State University, DANIEL TORRENT, JOSE SANCHEZ-DEHESA, Universidad Politecnica de Valencia — A graded refractive index (GRIN) provides a means of controlling wave propagation within the bulk of a material without relying on curved interfaces between dissimilar materials. We report the design and experimental testing of a GRIN metamaterial that behaves as a lens for acoustic waves in water. The graded index is achieved using a regular array of cylindrical scatterers with an anisotropic distribution of sizes. The metamaterial lens operates at sonic frequencies and has flat interfaces. We demonstrate that this metamaterial design focuses acoustic signals in the same manner as an ideal optical lens. By comparing with calculations using multiple scattering theory and finite difference time domain methods we show that the elastic properties of the scatterers are important for achieving an accurate model of the transmitted signal. We consider perturbations of the metamaterial design and their impact on the transmission.

[1]Supported by the Office of Naval Research

12:51PM W21.00009 WASTED at work: the Webcam Alpha Spectrometer Experiment Demonstrator , ARTHUR PALLONE, NICOLE NEWTON[1], Murray State University — Ion beam analysis (IBA) methods are commonly used to determine the composition or other properties of samples. The scanning of micrometer diameter and smaller ion beams across sample surfaces produces spatial distribution maps of those properties for the samples. Electron microscope providers offer radiation-hardened CMOS camera options to directly image sample areas as a complement to scanning the electron beam. A modified webcam operated in the radiographic mode of transmission ion microscopy (TIM), with alpha particles in place of electrons, has been shown to be an effective low-cost alternative to that camera for TIM. IBA under ambient pressure is still not commonly practiced. Even less common is the use of a radioactive source of ions, such as Po-210, in IBA. The synthesis of these three ideas – the direct imaging by a modified webcam of Po-210 alpha particles that first pass through a sample under ambient pressure – is explored with the Webcam Alpha Spectrometer Experiment Demonstrator (WASTED). A description of the experiment, first results, conclusions and future work will be presented.

[1]undergraduate student

1:03PM W21.00010 Fourier phase contrast microscopy technique for real time imaging of phase and fluorescence features simultaneously[1] , CHANDRA YELLLESWARAPU, ALEXEY VERAKSA, BHARGAB DAS, DEVULAPALLI RAO[2], University of Massachusetts Boston, DEPARTMENT OF PHYSICS TEAM, DEPARTMENT OF BIOLOGY COLLABORATION — Understanding of biological cell response is facilitated by microscopy techniques, but has been limited by our ability to image cell structure and function at the same time. Current procedure is to obtain separate images, such as phase and fluorescence features, using different imaging techniques one after the other and digitally register the resulting images together. Mostly this procedure requires switching between the light sources and the associated optical paths, making it difficult to image biological events at short time scales. Recently we developed a novel optical Fourier phase contrast microscopy technique for real time display of phase and fluorescence features of biological specimens at the same time. We were able to image the brightfield+fluorescence, phase+fluorescence, and edge enhanced+fluorescence features of the *Drosophila* embryo at once without the need for digital image registration and fusion. This comprehensive microscope has the capability of simultaneously providing both structural and functional information.

[1]Supported by NIH-NCRR 1R21RR024429 grant
[2]Presenter

1:15PM W21.00011 Atomic Resolution imaging with non-contact Atomic Force Microscope (nc-AFM) in a closed liquid cell , UMIT CELIK, Istanbul Technical University, DEMET CATCAT, NanoMagnetics Instruments Ltd./Hacettepe University, H. OZGUR OZER, Istanbul Technical University, AHMET ORAL, Sabanci University, ISTANBUL TECHNICAL UNIVERSITY TEAM, NANOMAGNETICS INSTRUMENTS LTD. TEAM, HACETTEPE UNIVERSITY TEAM, SABANCI UNIVERSITY TEAM — We have designed a non-contact Atomic Force Microscope, which can achieve true atomic resolution in a closed liquid cell, which does not suffer from evaporation of fluids during imaging. We have designed a closed liquid cell, where we can flow the fluid using a syringe or a peristaltic pump. The AFM cantilever holder was designed to eliminate acoustical resonances. We can obtain resonance curves without spurious acoustic peaks in liquid using a piezoactuator. We have used an RF modulated 635 nm low noise diode laser. RF modulation is effective to reduce the optical feedback noise and the optical interference noise. Deflection noise density of designed system is $\sim$20 fm/$\sqrt{\text{Hz}}$ in air and $\sim$25 fm/$\sqrt{\text{Hz}}$ in water. The observed frequency noise at the PLL output was $\sim 1\text{Hz}_{pp}$ in water using a 300kHz, 32N/m cantilever oscillated at 0.9nm amplitude with Q$\sim$11. Force sensitivity of our system is demonstrated by imaging cleaved mica surface in water environment with atomic resolution.

1:27PM W21.00012 Scanning Tunneling Microscope Study of Atomic Steps in Gold Films on Muscovite Mica[1] , OLESYA SITNIKOVA, RAMESH MANI, Georgia State University — We are carrying Scanning Tunneling Microscope (STM) studies of gold on Muscovite mica to observe the atomic step migration and test the functionality of our STM. The experiment was performed by using a RHK ultra-high-vacuum STM. The gold sample was prepared in low pressure vacuum chamber, and the films were grown at constant rate of 0.1 nm/sec to the desired thickness. After deposition, the films were thermally annealed to produce flat terraces which are being studied. The migration of atomic steps over time is being observed and the results are presented.

[1]Work has been supported by the ARO under W911NF-07-01-0158, and by the DOE under DE-SC0001762

1:39PM W21.00013 X-Ray Fluorescence Imaging of Ancient Artifacts , ROBERT THORNE, ETHAN GEIL, Cornell University, KATHRYN HUDSON, CHARLES CROWTHER, Oxford University — Many archaeological artifacts feature inscribed and/or painted text or figures which, through erosion and aging, have become difficult or impossible to read with conventional methods. Often, however, the pigments in paints contain metallic elements, and traces may remain even after visible markings are gone. A promising non-destructive technique for revealing these remnants is X-ray fluorescence (XRF) imaging, in which a tightly focused beam of monochromatic synchrotron radiation is raster scanned across a sample. At each pixel, an energy-dispersive detector records a fluorescence spectrum, which is then analyzed to determine element concentrations. In this way, a map of various elements is made across a region of interest. We have succesfully XRF imaged ancient Greek, Roman, and Mayan artifacts, and in many cases, the element maps have revealed significant new information, including previously invisible painted lines and traces of iron from tools used to carve stone tablets. X-ray imaging can be used to determine an object's provenance, including the region where it was produced and whether it is authentic or a copy.

1:51PM W21.00014 Measuring the Imaginary Part of the Permittivity Using Calorimetry[1] , HEKTOR KASHURI, KRISHNA SIGDEL, KLAIDA KASHURI, GERMANO S. IANNACCHIONE — Modulated or AC calorimetry is a well established technique for measuring the temperature dependence of the heat capacity of many complex fluids. Employing a dielectric or RF heating method, the heat capacity, thermal conductivity, and the dielectric properties of the sample are all probed simultaneously. Combining the results obtained by this technique for the liquid crystal 4-n-pentyl-4-cyanophenyl (5CB) with those obtained by our novel AC calorimetric technique employing RF (dielectric) heating, we have been able to directly measure the temperature dependence of the imaginary part of the permittivity of this liquid crystal. Measurements were performed over a temperature range from 303 to 313 K, spanning the nematic to isotropic phase transition, as well as radio frequencies from 10 to 30 MHz

[1]Worcester Polytechnic Institute (WPI)

2:03PM W21.00015 Calorimetry of epitaxial thin films[1] , FRANCES HELLMAN, DAVID COOKE, University of California at Berkeley, JAMES GROVES, BRUCE CLEMENS, Stanford University — Thin film growth allows for the manipulation of material on the nanoscale, allowing for the creation of metastable phases not seen in the bulk. Heat capacity provides a direct way of measuring thermodynamic properties of these new materials, but traditional bulk calorimetric techniques are inappropriate for such a small amount of material. Micro- and nanocalorimetry techniques exist for the measurements of thin films but rely on an amorphous membrane platform, limiting the types of films which can be measured. In this work, ion-beam-assisted deposition is used to provide a biaxially-oriented MgO template on a suspended membrane microcalorimeter. Synchrotron X-ray diffraction was used to successfully assess the biaxial order of the MgO template. X-ray diffraction was also used to prove the high level of epitaxy of a film grown onto this MgO template. The contribution of the MgO layer to the technique will be discussed. An $Fe_{.49}Rh_{.51}$ film grown epitaxially onto the device was measured, comparing favorably to literature data on bulk crystals. This shows the viability of the MgO microcalorimeter as a way of measuring the thermodynamic properties of epitaxial thin films.

[1]This work was supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231

Thursday, March 24, 2011 11:15AM - 2:15PM –
Session W22 DCMP: Magnetic Phase Transitions II D163

11:15AM W22.00001 Bound states and E8 symmetry effects in perturbed quantum Ising chains , JONAS KJALL, University of California, Berkeley, FRANK POLLMANN, University of California, Berkeley and Academia Sinica, JOEL MOORE, University of California, Berkeley and Lawrence Berkeley National Laboratory — In a recent experiment on $CoNb_2O_6$, Coldea et al. found for the first time experimental evidence of the exceptional Lie algebra E_8. The emergence of this symmetry was theoretically predicted long ago for the transverse quantum Ising chain in the presence of a weak longitudinal field. We consider an accurate microscopic model of $CoNb_2O_6$ incorporating additional couplings and calculate numerically the dynamical structure function using a recently developed matrix-product-state method. We compare the signatures of this model to those found in the transverse Ising chain in a longitudinal field and to experimental data, with focus on how far the effects of integrability extends and how robust they are to the additional interactions. The excitation spectra show bound states characteristic of the weakly broken E_8 symmetry and a bound state continuum carrying spectral weight comparable to the higher bound states.

11:27AM W22.00002 Comparison between two simple models for the magnetoelectric interaction in multiferroics , G.E. BARBERIS, IFGW, Unicamp, Brazil, C.J. CALDERON FILHO, IFGW Unicamp, Brazil — We developed numerical calculations to simulate the magnetoelectric coupling in multiferroic compounds, using the Monte Carlo technique. Two simple models were used to simulate the compounds. In the first one, the magnetic ions are represented by a spin 1/2 2D Ising lattice of ions, and the electric lattice by classical moments, coupled one to one with the magnetic moments. The coupling between both lattices allows to the leading lattice, that is, the magnetic one, to change the orientation of the electrical dipoles in one direction perpendicular to the magnetic dipoles. This direction was chosen to accomplish the symmetry requirements of the magnetoelectric effect. In the second case, the magnetic lattice is also a 2D Ising lattice, but the electric momenta are in a lattice that also behaves as an Ising lattice, perpendicular to the magnetic moments. In this case, the one-to-one coupling of the electric and magnetic momenta is represented by a two-valued energy parameter, allowing the possibility of independent transition temperatures for both lattices. Both models contain three independent parameters. We studied the physical properties obtained with both models, as functions of the ratio of the three parameters. The results in both cases allowed us to compare changes in the physics of the models, and with the physics of compounds measured experimentally.

11:39AM W22.00003 The itinerant ferromagnetic phase of the Hubbard model , GIUSEPPE CARLEO, SAVERIO MORONI, FEDERICO BECCA, STEFANO BARONI, SISSA and CNR-IOM DEMOCRITOS - Trieste, Italy — Using a newly developed quantum Monte Carlo technique, we provide strong evidence for the stability of a saturated ferromagnetic phase in the high-density regime of the two-dimensional infinite-U Hubbard model. By decreasing the electron density, a discontinuous transition to a paramagnetic phase is observed, accompanied by a divergence of the susceptibility on the paramagnetic side. This behavior, resulting from a high degeneracy among different spin sectors, is consistent with an infinite-order phase transition. The remarkable stability of itinerant ferromagnetism renews the hope to describe this phenomenon within a purely kinetic mechanism and will facilitate the validation of experimental quantum simulators with cold atoms loaded in optical lattices.

11:51AM W22.00004 Two species Bosonic Hubbard model in a two-dimensional optical lattice , KALANI HETTIARACHCHILAGE, VALY ROUSSEAU, JUANA MORENO, MARK JARRELL, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803, USA — We study a two-component hardcore bosonic Hubbard model in a two- dimensional optical lattice by performing Quantum Monte Carlo (QMC) simulations. Our model contains a repulsive interspecies interaction between the two species of bosons and a hopping term between nearest neighbors. The phase diagram shows magnetic orderings, insulatings and superfluid phases as a function of doping for balanced populations. We predict the appearance of a first order phase transition from an antiferromagnetic phase to a superfluid phase near half filling. A phase transition from superfluid to an exotic phase occurs away from half filling at very low temperature.

12:03PM W22.00005 An Anomalously Elastic, Intermediate Phase in Randomly Layered Planar Magnets, Superfluids, and Superconductors , THOMAS VOJTA, Missouri University of Science and Technology, PAUL GOLDBART, University of Illinois at Urbana-Champaign, PRIYANKA MOHAN, RAJESH NARAYANAN, Indian Institute of Technology Madras, JOHN TONER, University of Oregon — We show that layered quenched randomness in planar magnets leads to an unusual intermediate phase between the conventional ferromagnetic low-temperature and paramagnetic high-temperature phases. In this intermediate phase, which is part of the Griffiths region, the spin-wave stiffness perpendicular to the random layers displays anomalous scaling behavior, with a continuously variable anomalous exponent, while the magnetization and the stiffness parallel to the layers both remain finite. Analogous results hold for superfluids and superconductors. We study the two phase transitions into the anomalous elastic phase, and we discuss the universality of these results, and implications of finite sample size as well as possible experiments.

12:15PM W22.00006 Quantum fidelity in the thermodynamic limit[1] , MAREK RAMS, BOGDAN DAMSKI, Los Alamos National Laboratory — A quantum phase transition happens when dramatic changes in the ground state properties of a quantum system can be induced by a tiny variation of an external parameter (e.g., a magnetic field in spin systems). Quantum fidelity – the overlap between two ground states calculated at slightly different values of the external parameter – provides the most basic probe into the dramatic change of the wave-function. In this talk I will discuss quantum fidelity focusing on thermodynamic regime. I will present novel analytical results for quantum fidelity of the Ising chain, a paradigmatic model of quantum phase transitions, and discuss a theory extending these findings to systems characterized by other universality classes. In particular, I will show how quantum fidelity approaches a non-analytic limit, quantify how the Anderson catastrophe takes place in quantum critical systems, and discuss scaling properties of quantum fidelity when it cannot be approximated by the popular fidelity susceptibility approach. This approach provides a promising way of characterizing quantum phase transition in strongly correlated systems. The work is summarized in M.M. Rams, B. Damski, arXiv:1010:1048

[1]This work was supported by U.S. Department of Energy through the LANL/LDRD Program.

12:27PM W22.00007 Finite-Temperature Fidelity Susceptibility for One-Dimensional Quantum Systems[1] , JESKO SIRKER, TU Kaiserslautern — We calculate the fidelity susceptibility χ_f for the Luttinger model and show that there is a universal contribution linear in temperature T (or inverse length $1/L$) by using conformal field theory. Furthermore, we develop an algorithm - based on a lattice path integral approach - to calculate the fidelity $F(T)$ in the thermodynamic limit for one-dimensional quantum systems. We check the Luttinger model predictions by calculating $\chi_f(T)$ analytically for free spinless fermions and numerically for the XXZ chain. Finally, we study χ_f at the two phase transitions in this model.

J. Sirker, PRL **105**, 117203 (2010)

[1]Financial support by the MATCOR school of excellence is gratefully acknowledged.

12:39PM W22.00008 Thermodynamics of itinerant metamagnetic transitions , ANDREW BERRIDGE, University of St Andrews — Itinerant metamagnetic transitions may be driven by features in the electronic density of states. These features produce signatures in the entropy and specific heat near to the transition. We study these signatures for a variety of different cases, identifying the key features which differ from naive expectations, such as enhanced critical fields and 'non-Fermi liquid' temperature dependencies above the transition. We will consider the generic case of a logarithmically divergent density of states, as caused by a van Hove singularity in 2D. We also study a specific model for the bandstructure of $Sr_3Ru_2O_7$, a material with a well-studied metamagnetic transition and quantum critical endpoint. We consider how far the behaviour of the system can be explained by the density of states rather than quantum fluctuations, and the distinctive features of this mechanism. The most intriguing feature of $Sr_3Ru_2O_7$ is an unusual phase with a higher entropy than its surroundings, we consider how this may arise in the context of a density of states picture and find that we can reproduce the observed thermodynamic behaviour and first-order phase transitions.

12:51PM W22.00009 Low-energy behavior of the generalized Golden chain at an integrable point , PAATA KAKASHVILI, EDDY ARDONNE, NORDITA — Recently, properties of collective states of interacting non-Abelian anyons have attracted a considerable attention. In particular, it has been shown to that the generalization of the Golden chain, a chain of interacting Fibonacci anyons, has a rich phase diagram with various critical and gapped phases. In additions, several integrable points have also been studied. We identify a new integrable point in the parameter space of the model and diagonalize the Hamiltonian exactly using the Bethe Ansatz method. To describe the corresponding low-energy conformal field theory, we perform the finite-size analysis to calculate the central charge and critical exponents.

1:03PM W22.00010 Tensor renormalization group: Local magnetizations, correlation functions, and phase diagrams of systems with quenched randomness[1] , CAN GÜVEN, MICHAEL HINCZEWSKI, University of Maryland, A. NIHAT BERKER, Sabanci University — The tensor renormalization-group method, developed by Levin and Nave, brings systematic improvability to the position-space renormalization-group method and yields essentially exact results for phase diagrams and entire thermodynamic functions. The method, previously used on systems with no quenched randomness, is extended in this study to systems with quenched randomness [1]. Local magnetizations and correlation functions as a function of spin separation are calculated as tensor products subject to renormalization-group transformation. Phase diagrams are extracted from the long-distance behavior of the correlation functions. The approach is illustrated with the quenched bond-diluted Ising model on the triangular lattice. An accurate phase diagram is obtained in temperature and bond-dilution probability for the entire temperature range down to the percolation threshold at zero temperature.

[1] C. Güven, M. Hinczewski, and A.N. Berker, Phys. Rev. E 82, 051110 (2010).

[1]This research was supported by the Alexander von Humboldt Foundation, the Scientific and Technological Research Council of Turkey (TÜBITAK), and the Academy of Sciences of Turkey.

1:15PM W22.00011 Nature of Fermi Systems near l=0 Pomeranchuk Instability: A Tractable Crossing Symmetric Equation Approach , KELLY REIDY, KHANDKER QUADER, Kent State University, KEVIN BEDELL, Boston College — In Fermi liquids, a Pomeranchuk instability occurs when one of the Landau parameters $F_\ell^{a,s} \to -(2\ell+1)$. The Pomeranchuk instabilities at $F_0^{a,s} = -1$ are related to respectively to a ferromagnetic transition (a), and to a density wave or charge instability resulting in phase separation (s). We use the tractable crossing symmetric equations (TSCE) method to explore the nature of quantum fluctuations, excitations and pairing in a 3D Fermi system, around these points. We obtain interesting limiting results at zero and finite momentum (q), and in the limits of large and small coupling strengths. We develop methods to deal with a set of finite-q singularities in the competing quantum fluctuation terms contained in TSCE; these may have physical significance. Using graphical and numerical methods to solve coupled non-linear integral equations that arise in the TSCE scheme, we obtain results for the behavior of spin and density excitations, and pairing properties around the instability points. Our results may have relevance to ferromagnetic superconductors.

1:27PM W22.00012 Microscopic model for the $Sr_{n+1}Ir_nO_{3n+1}$ Ruddlesden-Popper series of materials , JEAN-MICHEL CARTER, HAE-YOUNG KEE, University of Toronto — The $Sr_{n+1}Ir_nO_{3n+1}$ family of materials displays an insulator to metal transition as the number of layers (n) increases. The presence of large spin-orbit coupling is believed to be a significant ingredient for the novel $J_{eff} = 1/2$ state found in Sr_2IrO_4. We offer a microscopic tight-binding Hamiltonian with spin-orbit coupling and Hubbard interactions, and compare our results with experimentally observed phases.

1:39PM W22.00013 Protecting clean critical points by local disorder correlations[1] , J.A. HOYOS, Universidade de São Paulo, NICOLAS LAFLORENCIE, Universite Paris-Sud, ANDRÉ VIEIRA, Universidade de São Paulo, THOMAS VOJTA, Missouri University of Science and Technology — We show that a broad class of quantum critical points can be stable against locally correlated disorder even if they are unstable against uncorrelated disorder. Although this result seemingly contradicts the Harris criterion, it follows naturally from the absence of a random-mass term in the associated order-parameter field theory. We illustrate the general concept with explicit calculations for quantum spin-chain models. Instead of the infinite-randomness physics induced by uncorrelated disorder, we find that weak locally correlated disorder is irrelevant. For larger disorder, we find a line of critical points with unusual properties such as an increase of the entanglement entropy with the disorder strength. We also propose experimental realizations in the context of quantum magnetism and cold-atom physics.

[1]Financial support: Fapesp, CNPq, NSF, and Research Corporation

1:51PM W22.00014 Quantum antiferromagnet on a Bethe lattice at percolation I. Low-energy states, DMRG, and diagnostics , HITESH CHANGLANI, SHIVAM GHOSH, C.L. HENLEY, Cornell University — We investigate ground and excited state properties of randomly diluted spin-1/2, exchange-coupled Heisenberg antiferromagnets on the Bethe lattice with coordination 3. In the case of square lattice percolation clusters, previous Quantum Monte Carlo (QMC) calculations [1] found that the singlet-triplet gaps scaled "anomalously," being much smaller than the $1/N$ scaling expected from the tower of "quantum rotor" states (due to $E = M^2/2N\chi$). The low energies were attributed to the interaction of distant "dangling spins," forced by the local imbalance of even and odd sites. In the present study we further study this effect on the Bethe lattice, using Exact Diagonalization and density-matrix RG. (DMRG applies naturally since the Bethe lattice lacks loops). We introduce inter-site correlation and susceptibility matrices as diagnostics to identify the spatial locations of the low-energy degrees of freedom, and to understand interactions between them. These matrices have been computed within the harmonic spin-wave theory, in order to highlight the deviations seen in the spin-1/2 system. In addition to the above, we propose a simple effective Hamiltonian which explains the magnitude of the singlet-triplet gap.

[1] L. Wang and A. Sandvik, Phys. Rev. B 81, 054417 (2010).

2:03PM W22.00015 Quantum antiferromagnet on a Bethe lattice at percolation II.Effective Hamiltonian for dangling spins , SHIVAM GHOSH, HITESH CHANGLANI, SUMIRAN PUJARI, C.L. HENLEY, Cornell University — The lowest energy excitations of spin 1/2 Heisenberg antiferromagnets on percolation clusters (about the Neel ordered state) were believed to be "quantum rotor states" scaling with cluster size as 1/N, until Wang and Sandvik [Wang et al, Phys. Rev. B 81, 054417 (2010)] discovered a class of states in the diluted square lattice that had even lower energies and had a different finite size scaling of the gap exponent. They conjectured these anomalous states were due to local even/odd sublattice imbalances, leading to emergent local moments called "dangling spins" that interact over large distances, mediated through intervening spins. We have pursued this question on the z=3 Bethe lattice at the percolation threshold. Exact diagonalization shows, forevery cluster, a split-off group of low-energy states having the same quantum numbers as can be made using the dangling spins. We identify these with the Wang-Sandvik anomalous states and model their energies using an effective pair Hamiltonian coupling the "dangling spins." The couplings are a function of separation and geometry; the parameters are solved by fitting to a database of different clusters.The separation dependence of these interactions can be related to the gap scaling with N. We will also compare the effective Hamiltonian predictions to the intersite susceptibility matrix of each cluster.

Thursday, March 24, 2011 11:15AM - 2:03PM –
Session W23 DCMP: Superconductivity: Mesoscopic and Nanometer Scale Phenomena D165

11:15AM W23.00001 Fluxoid Quantization in Superconducting Al Nano-Rings[1] , STEPHEN SNYDER, ALLEN GOLDMAN, University of Minnesota — The Little-Parks experiment on superconducting cylinders is an important demonstration of fluxoid quantization in superconductors. The transition temperature oscillations in magnetic field have a period of $h/2e$ for the micro cylinders in their studies, which was further evidence for Cooper paring at the time [W. A. Little, R. D. Parks, PRL 1964, 9, 9]. However recent theoretical works have suggested that in superconducting loops smaller than the coherence length this period changes from $h/2e$ to h/e, for details see [F. Loder, et al. PRB, 2008, 78, 174526] and references therein. We present experimental work in an effort to achieve this limit with Al nano-rings prepared by electron beam lithography. The rings presented here are smaller than others reported in the literature by as much as a factor of two or three [H. Wang, et al. PRB, 2007, 75, 064509].

[1]This work was supported by the U.S. Department of Energy under Grant No. DE-FG02-02ER46004.

11:27AM W23.00002 Destructive regime in Al loops prepared by e-beam lithography , NEAL STALEY, YING LIU, Department of Physics and Materials Research Institute, The Pennsylvania State University — For doubly connected superconductors, cylinders, loops, or rings, the fundamental fluxoid quantization leads to oscillations in the superconducting transition temperature (T_c) with the applied flux. This is known as the Little-Parks effect. For sufficiently small loops, with a circumference smaller than $\pi\xi(0)$, where $\xi(0)$ is the zero temperature coherence length, superconductivity is completely destroyed near the half-flux quanta. This "destructive regime" emerges because of the competition between the kinetic energy carried by the supercurrent, and the condensation energy of the system. Theoretically, it has been shown that adding a tail to the loop can increase the condensation energy and possibly eliminate the destructive regime. We present electrical transport measurements on Al loops defined by e-beam lithography with a size comparable to $\xi(0)$. The loops were varied to have different condensation energies by adding explicit tails, and by lengthening and shortening the measurement leads. We observed strongly enhanced Little-Parks oscillations due to the reduction of the sample size, and the transition to the destructive regime when the size of sample was further reduced. These experimental results will be examined in the context of the competition between the kinetic and condensed energies. Work supported by NSF.

11:39AM W23.00003 Superconducting nanowires as nonlinear inductive elements for qubits[1] , JASEUNG KU, University of Illinois at Urbana-Champaign, VLADIMIR MANUCHARYAN, Yale University, ALEXEY BEZRYADIN, University of Illinois at Urbana-Champaign — We report microwave transmission measurements of superconducting Fabry-Perot resonators, having a superconducting nanowire placed at a supercurrent antinode. As the plasma oscillation is excited, the supercurrent is forced to flow through the nanowire. The microwave transmission of the resonator-nanowire device shows a nonlinear resonance behavior, significantly dependent on the amplitude of the supercurrent oscillation. We show that such amplitude-dependent response is due to the nonlinearity of the current-phase relationship of the nanowire. The results are explained within a nonlinear oscillator model of the Duffing oscillator, in which the nanowire acts as a purely inductive element, in the limit of low temperatures and low amplitudes. The low-quality factor sample exhibits a "crater" at the resonance peak at higher driving power, which is due to dissipation. We observe a hysteretic bifurcation behavior of the transmission response to frequency sweep in a sample with a higher quality factor. The Duffing model is used to explain the Duffing bistability diagram.

[1]NSF DMR-1005645, DOE DO-FG02-07ER46453

11:51AM W23.00004 Electrical transport properties of topological insulator Bi2Te3 nanowires contacted with superconducting electrodes[1] , MINGLIANG TIAN, JIAN WANG, MEENAKSHI SINGH, MOSES CHAN, PENN STATE UNIVERSITY TEAM — Single-crystal Bi2Te3 nanowires were fabricated by template-assisted electrochemical deposition. The electrical transport properties of the nanowires in the temperature range 1.8-300 K were investigated by connecting nonsuperconducting or superconducting electrodes. When the wire was connected to focused-ions beam deposited W-electrodes, a series of exotic quasi-periodic oscillations were found and the amplitude of the oscillations was unusually enhanced near 3.5 K below the Tc, 4.5 K, of W-electrodes. When the wire was connected to nonsuperconducting Pt electrodes, the wire showed positive magnetoresistance accompanied with random fluctuations.

[1]This work was supported bythe center for nanoscale science (Penn State MRSEC) funded by NSF under Grant No. DMR-0820404.

12:03PM W23.00005 Observation of Little-Parks Oscillations of the Kinetic Inductance at Low Temperatures Using a GHz Resonator with Two Parallel Superconducting Nanowires[1] , ANDREY BELKIN, MATTHEW BRENNER, THOMAS AREF, JASEUNG KU, ALEXEY BEZRYADIN, University of Illinois at Urbana-Champaign — Little-Parks (LP) effect manifests the phenomenon of the fluxoid quantization in doubly connected superconductors. Usually it is observed at high temperatures, i.e. slightly below the critical temperature (Tc). We demonstrated that a thin-film Fabry-Perot superconducting resonator with a pair of nanowires inserted at the point of supercurrent antinode can be used to reveal LP effect even at temperatures much lower than Tc. As magnetic field (H) is applied, the Meissner current develops, changing the kinetic inductance of the wires and, correspondingly, the resonance frequency of the resonator and its transmission S21 measured at the fixed frequency. The periodicity of the LP effect is revealed as a periodic set of distorted parabolas S21(H) corresponding to the states with different vorticities. The transition from one state to another corresponds to a Little's phase slip. We suggest a theoretical explanation to the shape of the observed parabolas. We also report a statistical analysis of the jumps between the parabolas.

[1]This work was supported by DOE Grant No. DO-FG02-07ER46453 and NSF Grant No. DMR-1005645.

12:15PM W23.00006 Spin Resonance and dc Current Generation in a Quantum Wire , PENG ZHOU[1], ARTEM ABANOV[2], WAYNE SASLOW[3], VALERY POKROVSKY[4], Texas A&M Univ. — We show that in a quantum wire the spin-orbit interaction leads to a narrow spin resonance at low temperatures, even in the absence of an external magnetic field. A relatively weak dc magnetic field of a definite direction strongly increases the resonance absorption. Linearly polarized resonance radiation produces dynamic magnetization as well as electric and spin currents. The effect strongly depends on the external magnetic field.

[1]Graduate Student
[2]Professor
[3]Professor
[4]Professor

12:27PM W23.00007 Large oscillations of the magnetoresistance in nano-patterned high-temperature superconducting films , ILYA SOCHNIKOV, AVNER SHAULOV, YOSEF YESHURUN, Bar-Ilan University, GENNADY LOGVENOV, IVAN BOZOVIC, Brookhaven National Laboratory — Measurements on nano-scale structures made of high-temperature superconductors are expected to shed light on the origin of superconductivity in these materials. The size of loops made of these compounds was so far limited to the submicron scale. We report the results of measurements on loops of $La_{1.84}Sr_{0.16}CuO_4$, with dimensions down to tens of nanometers. We observe oscillations in the loops resistance as a function of the magnetic flux through the loops. The oscillations have a period of $h/2e$ and their amplitude is much larger than the amplitude of resistance oscillations expected from the Little-Parks effect [1-2]. Unlike the Little-Parks oscillations, caused by periodic changes in the superconducting transition temperature, the oscillations we observe are caused by periodic changes in the interaction between thermally-excited moving vortices and the oscillating persistent current induced in the loops. Despite the enhanced amplitude of these oscillations, we have not detected oscillations with a period of h/e, as recently predicted for nanoscale loops of superconductors with d-wave symmetry, or with a period of $h/4e$, as predicted for superconductors that exhibit stripes. [1] I. Sochnikov *et al.*, Nature Nano. **5**, 516 (2010). [2] I. Sochnikov *et al.*, PRB **82,** 094513 (2010).

12:39PM W23.00008 Penetration Depth of Superconductors with Random Superfluid Density , THOMAS LIPPMAN, KATHRYN MOLER, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, CA 94025, USA. — Electronic inhomogeneity is inevitable in doped superconductors, due simply to the random nature of the doping process. We argue that when the superconducting coherence length is not much larger than the lattice scale, this creates spatial randomness in the superconducting properties. In particular, we expect the superfluid density to be stochastic, which modifies the measured diamagnetic response. We approximate the London equation with random superfluid density as a modified equation for the disorder averaged field response, and speculate on implications for the interpretation of measurements of the penetration depth.

12:51PM W23.00009 MBE Growth for Qubit Devices , ANTHONY MEGRANT, ALEX KOZHANOV, LUDWIG FEIGL, MARTIN WEIDES, JIAN ZHAO, YI YIN, JAMES WENNER, ANDREW CLELAND, CHRIS PALMSTROM, JOHN MARTINIS — A major component of the UCSB research program is to find and understand proper growth conditions and procedures for epitaxial Re and sapphire thin films. Separately, we are taking what we have learned from this research and applying it to develop growth-optimized procedures in our dedicated MBE chamber for qubit devices. I will report on important parameters that need to be adjusted to obtain optimum growth, some of which include: temperature, deposition rate and surface preparation. Measurement tools such as in-situ RHEED and ex-situ XRD and AFM are used to characterize the quality of the films, as well as the fabrication of resonators to measure the quality factor.

1:03PM W23.00010 Single Electron Turnstiles: Improving Performance for a Quantum Metrological Current Standard , THOMAS AREF, Aalto Univ, Low Temp Lab, Espoo, Finland, VILLE MAISI, MIKES, Espoo, Finland, OLLI-PENTTI SAIRA, Aalto Univ, Low Temp Lab, Espoo, Finland, ANTTI KEMPPINEN, MIKES, Espoo, Finland, JUKKA PEKOLA, Aalto Univ, Low Temp Lab, Espoo, Finland — A top priority in metrology is to develop measurement standards that are based on fundamental physical constants. Although such standards exist for resistance and voltage (the quantum Hall effect and the Josephson effect respectively), no such standard exists for the unit of current, the ampere, at the present time. The best candidate for a quantum metrological standard for current is a single electron turnstile. Such turnstiles allow electrons through one at a time. When operated at a specific frequency, they produce a proportional current traceable to the single electron charge. Our turnstiles are based on a normal metal copper island contacted through insulating barriers by superconducting aluminum electrodes. By engineering improvements such as on-chip filtering and increased charging energy, we have improved our turnstiles to suppress both first order leakage and second order Andreev currents thus approaching the required accuracy for a new quantum metrological current standard. This current standard would allow the closing of the quantum metrological triangle created by voltage, resistance and current.

1:15PM W23.00011 Tunneling spectroscopy of the Andreev Bound States in a Carbon Nanotube[1] , JEAN-DAMIEN PILLET, CEA-Saclay, CHARIS QUAY, CRISTINA BENA, LPS Orsay, ALFREDO LEVY YEYATI, Universidad Autónoma de Madrid, PHILIPPE JOYEZ, CEA-Saclay — Carbon nanotubes are not intrinsically superconducting but they can carry a supercurrent when connected to superconducting electrodes. This supercurrent is mainly transmitted by discrete entangled (electron-hole) states confined to the nanotube, called Andreev Bound States. These states are a key concept in mesoscopic superconductivity as they provide a universal description of Josephson-like effects in quantum-coherent nanostructures (e.g. molecules, nanowires, magnetic or normal metallic layers) connected to superconducting leads. We report here the first tunneling spectroscopy of individually resolved ABS, in a nanotube-superconductor device. Analyzing the evolution of the ABS spectrum with a gate voltage, we show that the ABS arise from the discrete electronic levels of the molecule and that they reveal detailed information about the energies of these levels, their relative spin orientation and the coupling to the leads.

[1]This work was partially supported by ANR project ANR-07-BLAN-0240 SEMAFAET, C'Nano project SPLONA and Spanish MICINN under contracts NAN2007-29366 and FIS2008-04209.

1:27PM W23.00012 Quantum impurity model for microwave photons , MOSHE GOLDSTEIN, Department of Physics, Yale University, 217 Prospect Street, New Haven, CT 06520, USA, MICHEL DEVORET, Departments of Physics and Applied Physics, Yale University, New Haven, CT 06520, USA, MANUEL HOUZET, SPSMS, UMR-E 9001, CEA-INAC/UJF-Grenoble 1, F-38054 Grenoble, France, LEONID GLAZMAN, Department of Physics, Yale University, 217 Prospect Street, New Haven, CT 06520, USA — We consider propagation of microwave photons along an array of superconducting grains with a set of weakly-coupled grains at its center. Quantum fluctuations of charge on the weakly- coupled grains make the process of "photon splitting" effective. In such a process, an incoming photon may be split into a number of photons of lower energy. The minimal number of photons created in such process depends on the symmetry properties of the corresponding quantum impurity model. As an example, we consider a specific circuit allowing quantum fluctuations between two charge configurations of two weakly- coupled grains, thus mimicking the behavior of an anisotropic Kondo impurity. Both ferromagnetic and antiferromagnetic Kondo regimes may be reached this way. We relate the rate of conversion of the incoming photons into the lower-energy ones to the dynamic spin susceptibility of the Kondo model.

1:39PM W23.00013 Elliptic billiard is a nontrivial integrable system , TAO MA, ROSTISLAV SEROTA, University of Cincinnati — We investigate the semiclassical energy spectrum of quantum elliptic billiards. The nearest neighbor spacing distribution, level number variance and spectral rigidity support the notion that the elliptic billiard is a generic integrable system. A classical simulation shows that all periodic orbits, except two, are not isolated. From Fourier analysis of the spectrum, all peaks correspond to periodic orbits. The two isolated periodic orbits have relatively small contribution to the fluctuations of the level density as compared to non-isolated periodic orbits. We argue that elliptic billiard is a nontrivial classically integrable system that enables us to gain new insights into their properties.

1:51PM W23.00014 Measurement of the statistical properties of the persistent current in normal metal rings , MANUEL CASTELLANOS BELTRAN, WILL SHANKS, DUSTIN NGO, Yale University, ANIA BLESZYNSKI-JAYICH, UCSB, JACK HARRIS, Yale University — A striking manifestation of quantum mechanics at the mesoscopic scale is the existence of an equilibrium persistent current in normal metal rings threaded by a magnetic flux. A theory of non-interacting diffusive electrons predicts that the amplitude of these currents is a stochastic function of the disorder profile of the specific ring. Thus the persistent current is different from sample to sample, with a Gaussian distribution. Due to the difficulty of measuring these currents, experiments to determine the form of the persistent current distribution had not yet been performed. However, our group recently developed a technique for measuring persistent currents in normal metal rings with high SNR, low measurement back-action, excellent background rejection, and over a large range of magnetic fields. We have measured a total of roughly 100 independent realizations of persistent current amplitudes in single rings. Within the statistical limits of our data, we corroborate that the first five cumulants are consistent with a Gaussian distribution. As a further test of the higher-order statistical properties of the persistent current, we also show that the quadrature amplitudes of the current's Aharonov-Bohm oscillations are uncorrelated.

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W24 DCOMP: Density Functional Theory I D167

11:15AM W24.00001 A conventional, massively parallel eigensolver for electronic structure theory[1] , V. BLUM, M. SCHEFFLER, Fritz Haber Institute, Berlin, Germany, R. JOHANNI, H. LEDERER, RZ Garching, TH. AUCKENTHALER, TH. HUCKLE, H.-J. BUNGARTZ, TU Munich, L. KRÄMER, P. WILLEMS, B. LANG, BU Wuppertal, V. HAVU, TKK Helsinki — We demonstrate a robust large-scale, massively parallel conventional eigensolver for first-principles theory of molecules and materials. Despite much research into $O(N)$ methods, standard approaches (Kohn-Sham or Hartree-Fock theory and excited-state formalisms) must still rely on conventional but robust $O(N^3)$ solvers for many system classes, most notably metals. Our eigensolver overcomes especially parallel scalability limitations, where standard implementations of certain steps (reduction to tridiagonal form, solution of reduced tridiagonal eigenproblem) can be a serious bottleneck already for a few hundred CPUs. We demonstrate scalable implementations of these and all other steps of the full generalized eigenvalue problem. Our largest example is a production run with 1046 Pt (heavy-metal) atoms [1] with converged all-electron accuracy in the numeric atom-centered orbital code FHI-aims,[2] but the implementation is generic and should easily be portable to other codes. [1] P. Havu *et al.*, Phys. Rev. B **82**, 161418 (2010). [2] V. Blum *et al.*, Comp. Phys. Comm. **180**, 2175 (2009).

[1]ELPA research consortium, funded by German Ministry of Research and Education (BMBF). http://elpa.rzg.mpg.de

11:27AM W24.00002 GPAW on Blue Gene/P[1] , NICHOLS ROMERO, Argonne National Laboratory, JUSSI ENKOVAARA, CSC - IT Center for Science Ltd., MARCIN DULAK, CHRISTIAN GLINSVAD, ASK LARSEN, JENS MORTENSEN, Technical University of Denmark, SAMEER SHENDE, University of Oregon, VITALI MOROZOV, JEFFREY GREELEY, Argonne National Laboratory — Density function theory (DFT) is the most widely employed electronic structure method due to its favorable scaling with system size and accuracy for a broad range of molecular and condensed-phase systems. The advent of massively parallel supercomputers have enhanced the scientific community's ability to study larger system sizes. Ground state DFT calculations of systems with $O(10^3)$ valence electrons can be routinely performed on present-day supercomputers. The performance of these massively parallel DFT codes at the scale of 1 - 10K execution threads are not well understood; even experienced DFT users are unaware of Amdahl's Law and the non-trivial scaling bottlenecks that are present in standard $O(N^3)$ DFT algorithms. The GPAW code was ported an optimized for the Blue Gene/P. We present our algorithmic parallelization strategy and interpret the results for a number of benchmark tests cases. Lastly, I will describe opportunities for computer allocations at the Argonne Leadership Computing Facility.

[1]This work has been supported by the Academy of Finland (Project 110013) , Tekes MASI-program, Danish Center for Scientific Computing, Lundbeck Foundation, Office of Science of the U.S. Department of Energy under contract DE-AC02-06CH11357.

11:39AM W24.00003 Application of partition density-functional theory to model systems[1] , LARRY BOYER, George Mason University, MICHAEL MEHL, Naval Research Laboratory — Elliott et al.[2] have introduced a method called partition density-functional theory (PDFT) for expressing the Kohn-Sham charge density as a sum of overlapping fragment densities, which promises accuracy and efficiency along with a framework for developing and testing useful approximations for kinetic-energy functionals, T[n]. They illustrate their method using results obtained for non-interacting electrons in a one-dimensional model potential. Following their approach, we apply PDFT to similar models which examine its usefulness in developing approximations for T. We also discuss how PDFT compares with the self-consistent atomic deformation[3] method.

[1]Supported by the U.S. Office of Naval Research
[2]P. Elliott, K. Burke. M. H. Cohen and A. Wasserman, Phys. Rev. A **82**, 024501 (2010)
[3]L. L. Boyer, H. T. Stokes, M. M. Ossowski and M. J. Mehl, Phys. Rev. B **78**, 045121 (2008)

11:51AM W24.00004 Simple Impurity Embedded in a Spherical Jellium: Approximations of Density Functional Theory compared to Quantum Monte Carlo Benchmarks , MICHAL BAJDICH, MSTD, ORNL, Oak Ridge, TN 37831, JEOGNIM KIM, NCSA, UIUC, Urbana, IL 61801, USA, PAUL R.C. KENT, CNMS, ORNL, Oak Ridge, TN 37831, FERNANDO A. REBOREDO, MSTD, ORNL, Oak Ridge, TN 37831 — We study the electronic structure of a simple Gaussian impurity embedded in a spherical jellium in order to mimic the localization effects present in d- and f-electron compounds. We use quantum Monte Carlo benchmarks to validate approximations of density functional theory (DFT), such as local density approximation (LDA) and generalized gradient approximation (GGA) as well as the Hartree–Fock (HF) method. We identify distinct transitions between delocalized and localized states in the phase space of realistic densities ($1 \leq r_s \leq 5$) and moderate depths of the Gaussian impurity. We also extend the previous fixed-node diffusion Monte Carlo calculations of impurity-free jellium spheres and extract very accurate jellium surface exchange-correlation energies. Computer resources supported by DOE, Office of Science under contract DE-AC05-00OR22725 (NCCS). Research sponsored by DOE, BES, Materials Sciences and Engineering Division (FAR) and LDRD program (MB) and DOE SUF, CNMS (PRCK).

12:03PM W24.00005 Periodic Density Functional Theory Solver using Multiresolution Analysis with MADNESS[1] , ROBERT HARRISON, Oak Ridge National Laboratory, WILLIAM THORNTON, University of Tennessee — We describe the first implementation of the all-electron Kohn-Sham density functional periodic solver (DFT) using multi-wavelets and fast integral equations using MADNESS (multiresolution adaptive numerical environment for scientific simulation; http://code.google.com/p/m-a-d-n-e-s-s). The multiresolution nature of a multi-wavelet basis allows for fast computation with guaranteed precision. By reformulating the Kohn-Sham eigenvalue equation into the Lippmann-Schwinger equation, we can avoid using the derivative operator which allows better control of overall precision for the all-electron problem. Other highlights include the development of periodic integral operators with low-rank separation, an adaptable model potential for nuclear potential, and an implementation for Hartree Fock exchange.

[1]This work was supported by NSF project OCI-0904972 and made use of resources at the Center for Computational Sciences at Oak Ridge National Laboratory under contract DE-AC05-00OR22725.

12:15PM W24.00006 A Robust Spectrum Slicing Method Applied to the Kohn-Sham Equation for the Liquid/Solid Silicon Interface[1] , GRADY SCHOFIELD, JAMES CHELIKOWSKY, University of Texas at Austin — A difficult aspect of solving the Kohn Sham equation is the super-linear scaling of eigensolvers with the number of valence orbitals desired. We present a robust spectrum slicing technique that calculates the valence orbitals in a divide and conquer fashion through the use of smooth Chebyshev-Jackson filters. This algorithm allows for a "parallel" implementation of the eigensolver. Our calculations are done in the real-space density functional framework implemented in the program PARSEC. We apply this method to examine the liquid-solid silicon interface.

[1]Supported by the National Science Foundation OCI-1047997, DMR-0941645 and the Welch Foundation (F-1708)

12:27PM W24.00007 Beyond the LDA in density functional theory: empirical Laplacian-based models for the exchange-correlation energy[1]

, ANTONIO C. CANCIO, CHRISTOPHER E. WAGNER, Ball State University — We report recent work in developing a GGA-level density functional theory using primarily the Laplacian of the density $\nabla^2 n$ as an input beyond the LDA. Our starting point and motivation is a model fit to the exchange-correlation energy density of the valence shell of the Si crystal and other systems, as calculated by quantum Monte Carlo simulations, which show a strong, roughly linear dependence of this quantity on the Laplacian. The model respects the Lieb-Oxford bound for large positive Laplacian but suffers from a pole at negative values. A better treatment of $\nabla^2 n$ in this limit can be used to construct an all-electron extension of our model, and as an added benefit, avoid the singularity in the Kohn-Sham potential that gradient-based models suffer due to the cusp in electron density at the nucleus. Using an expansion in $1/\nabla^2 n$ we fit exchange energy densities in the cusp region accurately; obtaining reasonable potentials is a harder task but made easier by keeping the gradient of the density.

[1]Work support by National Science Foundation grant DMR-0812195.

12:39PM W24.00008 Better GGA and meta-GGA Functionals: VT84, meta-VMT, meta-VT84[1]

, ALBERTO VELA, Cinvestav, Mexico DF Mexico, J. MARTIN DEL CAMPO, J.L. GAZQUEZ, Univ. Autonoma Metropolitana I., Mexico, S.B. TRICKEY, Physics, QTP, Univ. Florida — The goal of fast DFT calculations on large families of highly complicated systems (e.g. large clusters, biomolecules) implicitly conflicts with the heavy emphasis of recent years on inclusion of exact exchange. In response we have worked on improving non-empirical GGA X functionals. Here we report extension of our VMT GGA functional (J. Chem. Phys. **130** 244103 (2009)) to satisfy a relevant asymptotic constraint, yielding the VT{84} X functional. With the PBE C functional, VT{84} gives about 10% improvement over VMT in energetics on the G3 223 molecule set. At the meta-GGA level of complexity, we have both meta-VMT and meta-{84}. The former is about 10% better on the G3 set than the TPSS meta-GGA, while meta-VT{84} gives roughly 10% further improvement over meta-VMT. Details of these assessments, including improvements in chemical shifts, will be presented.

[1]SBT acknowledges US DOE Grant DE-SC0002139

12:51PM W24.00009 All-Electron and Pseudopotential Orbital-Free Density Functional Calculations[1]

, VALENTIN KARASIEV, T. SJOSTROM, S.B. TRICKEY, Physics, QTP, Univ. Florida — Generalized gradient approximation (GGA) and modified-conjoint GGA kinetic energy functionals, proposed recently, have been implemented in an all-electron diatomic molecule code and in a periodic boundary condition code which uses local pseudopotentials. Self-consistent OF-DFT calculations confirm earlier non-self-consistent results. The GGA KE functionals give qualitatively incorrect total energy surfaces in the attractive region (isolated molecule) and the equilibrium crystalline cell volume is strongly expanded. In contrast, the mcGGA functional predicts a qualitatively correct energy surface for isolated systems, and the equilibrium geometry for pseudopotential calculations is in agreement with the Kohn-Sham results. We show the closeness in behavior between GGA-based functionals and simpler approximations defined by mixing of the Thomas-Fermi and the von Weizsäcker KE functionals. Effects of the pseudopotential in OF-DFT calculations also are discussed.

[1]We acknowledge support from US DoE Grant DE-SC0002139.

1:03PM W24.00010 Contributions to the Non-interacting Free Energy Density Functional[1]

, S.B. TRICKEY, Physics, QTP, U. Florida, JAMES DUFTY, Physics, U. Florida, T. SJOSTROM, Physics, QTP, U. Florida — Phenomenological models for the T=0 non-interacting kinetic energy density functional often use a linear combination of the von Weizsäcker (vW) and Thomas-Fermi (TF) functionals. A more systemmatic approach, for any temperature follows from extracting the vW functional from the exact free energy density functional, and analyzing the remainder in a local density approximation. We show that the vW functional is a lower bound for the free energy functional, extending a well-known T=0 result and indicating its priority in the decomposition. The exact remainder involves gradients of the off-diagonal one-body Fermi density matrix, for which a local density approximation is ambiguous. We discuss the extent to which a TF contribution can be extracted. Extension of the original vW phenomenological approach gives complementary insight. Modeling the orbitals as modulated plane waves, with coefficients identified in terms of the density and its gradients leads to vW and TF functionals plus higher-order gradient and temperature corrections.

[1]Supported in part by US DOE Grant DE-SC00002139.

1:15PM W24.00011 Finite-size correction in many-body electronic structure calculations of spin polarized systems[1]

, FENGJIE MA, SHIWEI ZHANG, HENRY KRAKAUER, Department of Physics, The College of William and Mary — We extend the post-processing finite-size (FS) correction method, developed by Kwee, Zhang, and Krakauer[2], to spin polarized systems. The method estimates the FS effects in many-body (MB) electronic structure calculations by a modified density functional theory (DFT) calculation, without having to repeat expensive MB simulations. We construct a unified FS DFT exchange-correlation functional for spin unpolarized and fully spin polarized systems, and then interpolate the results to arbitrary spin polarizations using the formula of Perdew and Wang[3] or that of Perdew and Zunger.[4] The application of this FS correction method to several typical magnetic systems with varying supercell sizes demonstrates that it consistently removes most of the FS errors, leading to rapid convergence of the MB results to the infinite size limit.

[1]Supported by DOE, NSF, ONR.

[2]H. Kwee, S. Zhang, and H. Krakauer, Phys. Rev. Lett. **100**, 126404 (2008)

[3]J. P. Perdew and Y. Wang, Phys. Rev. B **45**, 13244 (1992)

[4]J. P. Perdew and A. Zunger, Phys. Rev. B **23**, 5048 (1981)

1:27PM W24.00012 Generalization of the Hohenberg-Kohn theorem to the case of the presence of a magnetic field[1]

, VIRAHT SAHNI, Brooklyn College, CUNY, XIAOYIN PAN, Ningbo University — We generalize the HK theorem for the nondegenerate ground state of electrons in an external electrostatic field $\mathbf{E}(\mathbf{r}) = -\boldsymbol{\nabla} v(\mathbf{r})$ to the presence of an additional external magnetostatic field $\mathbf{B}(\mathbf{r}) = \boldsymbol{\nabla} \times \mathbf{A}(\mathbf{r})$. We prove that the nondegenerate ground state wave function Ψ is a functional of the ground state density $\rho(\mathbf{r})$, the physical current density $\mathbf{j}(\mathbf{r})$, and a gauge function $\alpha(\mathbf{R})$, with $\mathbf{R} = \{\mathbf{r}\}$. In other words, the basic variables, viz. those that uniquely determine the external potentials $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$, are $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$. As the choice of $\alpha(\mathbf{R})$ is arbitrary, it is possible to construct a $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ functional theory, as well as the corresponding Kohn-Sham and quantal density functional theories.

[1]Supported by RF CUNY and National NSF, China.

1:39PM W24.00013 Quantal density functional theory (QDFT) in the presence of a magnetic field[1] , XIAOYIN PAN, TAO YANG, Ningbo University, VIRAHT SAHNI, Brooklyn College, CUNY — We present the QDFT of electrons in an external electrostatic $\mathbf{E}(\mathbf{r}) = -\boldsymbol{\nabla} v(\mathbf{r})$ and magnetostatic $\mathbf{B}(\mathbf{r}) = \boldsymbol{\nabla} \times \mathbf{A}(\mathbf{r})$ field. This is the mapping from the interacting system of electrons to one of noninteracting fermions with the same density $\rho(\mathbf{r})$ and physical current density $\mathbf{j}(\mathbf{r})$. The mapping, based on the 'quantal Newtonian' first law, is in terms of 'classical' fields and quantal sources, the fields being separately representative of electron correlations due to the Pauli exclusion principle and Coulomb repulsion, and correlation-kinetic and correlation-magnetic effects. The theory is valid for ground and excited states. It is explicated by application to a ground state of the exactly solvable Hooke's atom in the presence of a magnetic field.

[1]Supported by National NSF, China and RF CUNY.

1:51PM W24.00014 Quantum Continuum Mechanics for Many-Electron Systems in a Strong Magnetic Field[1] , STEFANO PITTALIS, University of Missouri-Columbia, U.S.A., I.V. TOKATLY, Universidad del Pais Vasco and KERBASQUE, Basque Foundation for Science, Spain, G. VIGNALE, University of Missouri-Columbia, U.S.A. — A quantum continuum mechanics approach for the determination of the excitation energies of many-electron systems in strong magnetic field is introduced by means of linear response theory (LRT) and time-dependent deformation-functional theory (TD-DefT). In the high-frequency (anti-adiabatic) limit the collective modes of the system appear as the small oscillations of an elastic body in the presence of non-inertial forces reminiscent of the Coriolis and centrifugal forces. Interestingly, the complexity of the problem does not increase significantly with the particle number and only ground state properties are needed as an input. Further results, together with elementary and illustrative examples, may be presented as well.

[1]S.P. and G.V. are supported by DOE grant DE-FG02-05ER46203.

2:03PM W24.00015 First principles finite temperature magnetism of defects in Fe using Wang-Landau method[1] , AURELIAN RUSANU, Materials Science and Technology Division, ORNL, D.M. NICHOLSON, Computational Science and Mathematics Division, ORNL, KH. ODBADRAKH, Materials Science and Technology Division, ORNL, GREGORY BROWN, Florida State University, MARKUS EISENBACH, National Center for Computational Sciences, ORNL — Magnetic structure of materials with defects presents a strong dependence on local atomic arrangements. This dependence affects mechanical, magneto-caloric, and magnetization properties. Insights into thermodynamic and magnetic fluctuations at defects in Fe are obtained from first principle analysis by deploying the first principle local self consistent multiple scattering method(LSMS) and Wang-Landau statistical method. The computation of thermodynamic properties requires the sampling of a large number of configurations. To reduce the computational effort a Heisenberg model will be used to speed the configuration sampling procedures. The approach will be demonstrated for Fe systems and will address the magnetic structure of defects.

[1]This work was supported by the Center for Defect Physics, an Energy Frontier Research Center funded by the US DoE, Office of Science, Office of Basic Energy Sciences. Calculations performed at the National Center for Computational Sciences.

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W25 DCMP: Novel Superconductors I D166

11:15AM W25.00001 Parallels and contrasts in the pairing mechanism between cuprate and organic superconductors , THOMAS MAIER, Oak Ridge National Laboratory — The organic superconductors share many characteristics with the cuprates, such as the existence of antiferromagnetism, unconventional superconductivity and Mott insulating behavior. In addition, despite their complexity, their physics can be approximated by a single-band Hubbard model on a two-dimensional lattice. Here, we will present dynamic cluster quantum Monte Carlo simulations of a half-filled "dimer" Hubbard model on an anisotropic triangular lattice, which find a transition from an antiferromagnetic phase to a d-wave superconducting phase with increasing frustration. In particular, we will discuss commonalities and differences in the nature of the superconducting behavior between the dimer Hubbard model of the organic compounds and the standard Hubbard model of the cuprate materials.

11:27AM W25.00002 Can simple hydrocarbon molecular solids superconduct? A theoretical investigation of superconductivity in K_3Picene , XUHUI LUO, UIC & NIST, SERDAR OGUT, UIC, TANER YILDIRIM, UPenn & NIST — Unlike many well established high temperature (T_c) superconductors such as cuprates, M_3C_{60}, MgB_2 and iron-pnictides, the possibility of superconductivity in molecular hydrocarbon solids remains a controversial issue. This topic became active again by a recent study reporting superconductivity up to $T_c \sim$ 17 K in potassium doped Picene [1], a wide-bandgap semiconducting solid hydrocarbon. However, there is no theoretical study about possible mechanism of superconductivity. In this talk, we present a detailed first-principles study of the electron-phonon (el-ph) coupling in doped organic molecular solids. Due to large system size, the calculation of el-ph coupling using the standard linear response theory is not feasible. Hence, we have developed a finite-displacement method where both the phonon energies and el-ph coupling can be easily calculated for large systems. We have tested our code for well-established superconductors such as K_3C_{60} and MgB_2. As a comparison, we have also studied the el-ph coupling in alkali-doped Pentacene, a similar well-studied hydrocarbon in which no superconductivity has been observed. We discuss the effect of charge transfer as well as pressure on $T_c$for solid Picene and make predictions for future possible experiments.
[1] Mitsuhashi et al. Nature, 464, p. 76 (March, 2010).

11:39AM W25.00003 Electronic structure and magnetic properties of the hydrocarbon K_3picene superconductor near the metal-insulator transition , MINJAE KIM, B.I. MIN, Department of Physics, PCTP, Pohang University of Science and Technology, GEUNSIK LEE, HEE JAE KWON, Y.M. RHEE, JI HOON SHIM, Department of Chemistry, Pohang University of Science and Technology — Superconductivity has recently been observed in K-doped picene, K_3picene, which is a first organic superconductor in the hydrocarbon system with high transition temperature Tc=18K [1]. We have investigated the electronic structures and magnetic properties of K_3picene by density-functional theory. We have shown that the metal-insulator transition (MIT) is driven in K_3picene by 5% volume enhancement with a formation of local magnetic moment. Active bands for superconductivity near the Fermi level (E_F) are found to have hybridized character of LUMO and LUMO+1 picene molecular orbitals. Fermi surfaces of K_3picene manifest neither prominent nesting feature nor marked two-dimensional behavior. By estimating the ratio of the Coulomb interaction $U$and the band width $W$of the active bands near E_F , U/W, we have demonstrated that K_3picene is located in the vicinity of the Mott transition.

[1] R. Mitsuhashi *et. al.* Nature. 464, 76 (2010)

11:51AM W25.00004 Slow-Motion ^1H NMR Study of κ-$(ET)_2Cu[N(CN)_2]Br$[1] , J.C. GEZO, TAK-KEI LUI, R.W. GIANNETTA, C.P. SLICHTER, Loomis Laboratory of Physics, University of Illinois at Urbana-Champaign, J.A. SCHLEUTER, Materials Sciences Division, Argonne National Laboratory — The recent discovery of an anomalous Nernst signal in the pseudogap phase of organic superconductor κ-$(ET)_2Cu[N(CN)_2]Br$ suggests the presence of magnetic flux vortices above T_c.[2] We report spin-locked and line-narrowed proton NMR data on the pseudogap phase of this material. These experiments are sensitive to magnetic fluctuations, and probe far slower timescales (10^{-6}-10^{-3}s) than the previously explored NMR parameter space. Other experiments[3] have suggested that vortices leave an NMR fingerprint at these low frequencies.

[1]Work at UIUC supported by NSF DMR 10-05708 and the Center for Emergent Superconductivity, USDOE Award No. DE-AC0298CH1088. Work at Argonne supported by UChicago Argonne, LLC, Operator of Argonne National Laboratory, DOE Contract No. DE-AC02-06CH11357.
[2]M. S. Nam et al, Nature 449, 584-587 (2007)
[3]C. H. Recchia et al, Phys. Rev. Lett. 78, 3543-3546 (1997)

12:03PM W25.00005 NMR Study of κ-$(ET)_2Cu[N(CN)_2]Br$[1] , TAK-KEI LUI, J.C. GEZO, R.W. GIANNETTA, C.P. SLICHTER, University of Illinois at Urbana-Champaign, IL 61801, J.A. SCHLUETER, Material Sciences Division, Argonne National Laboratory, Argonne, IL 60439 — We report measurements of the ^{13}C spin-lattice relaxation rate, $(T_1T)^{-1}$ of κ-$(ET)_2Cu[N(CN)_2]Br$, an organic superconductor with $T_C = 11.9\,K$. The shape of the $(T_1T)^{-1}$versus T graph suggests the existence of a finite spin singlet-triplet gap[2]. Knight shifts were measured to search for a two-component electronic system. We also report measurements using an "S-shape" pulse sequence[3] that inverts half of the absorption line, permitting one to study slow motions and spin density waves.

[1]Work at UIUC supported by NSF DMR 10-05708, and Center for Emergent Superconductivity USDOE Award No. DE-AC02-98CH10886, Work at Argonne supported by UChicago Argonne, LLC, Operator of Argonne National Laboratory, DOE Contract No. DE-AC02-06CH11357.
[2]C. P. Slichter, Experimental Evidence for Spin Fluctuations in High Temperature Superconductors, in *Strongly Correlated Electronic Materials*: A Los Alamos Symposium, pp. 427-479, ed. K.S. Bedell *et al.*, Addison-Wesley (1994)
[3]L. R. Becerra, C. A. Klug, C. P. Slichter, and J. H. Sinfelt, J. Phys. Chem. **97**, 12014 (1993)

12:15PM W25.00006 13C NMR measurements of Zeeman limited superconductivity in κ-(BEDT-TTF)2Cu(NCS)2 , JEFFREY WRIGHT, UCLA , JAMES BRUGGER, UCLA Dept. of Physics & Astronomy, JOHN SCHLUETER, Argonne National Laboratory, REIZO KATO, RIKEN, STUART BROWN, UCLA — The class of superconductors formulated by the BEDT-TTF molecule offers a unique ability to study superconductivity which is Zeeman limited, utilizing their qausi-2D layered structure. The critical field H_{c2}, which usually limits superconductivity due to orbital screening currents, can be suppressed by aligning the applied magnetic field parallel to the conducting layers. In this orientation, the field penetrates in the form of Josephson vortices, and the dominant effect of the magnetic field is from the Zeeman interaction with quasiparticles. We present 13C NMR measurements of the spin lattice relaxation rate as a function of applied field on a single crystal of κ-(BEDT-TTF)2Cu(NCS)2 after aligning the field in this orientation. A quadratic dependence is observed: $R(B) \sim B^2$, which gives clear evidence of k-space nodes in the superconducting gap. Extending these measurements to field strengths near and above the Pauli limit, we observe a phase transition within the superconducting state at B=21.5T, and we comment on the compatibility of these results with the sought after FFLO state.

12:27PM W25.00007 Upper Critical Field in the Molecular Organic Superconductor $(DMET)_2I_3$[1] , PASHUPATI DHAKAL[2], Boston College, HARUKAZU YOSHINO, Osaka City University, JEONG IL OH, Boston College, KOICHI KIKUCHI, Tokyo Metropolitan University, MICHAEL J. NAUGHTON, Boston College — We report the temperature dependence of the upper critical magnetic field in the quasi-one-dimensional molecular organic superconductor $(DMET)_2I_3$, for magnetic field applied along the intrachain, interchain, and interplane directions. The upper critical field tends to saturation at low temperature for field in all directions and does not exceed the Pauli paramagnetic limit. Thus the superconductivity appears to be conventional spin singlet, in contrast to the status of the isostructural Bechgaard salts. Furthermore, we will discuss a magnetic field-induced dimensional crossover effect in the normal metallic state leading to a magnetoresistance minimum for the field parallel to the most conducting plane. This result will be useful to understand the nature of superconductivity in the molecular organic conductors.

[1]This work was supported by NSF Grant No. DMR 0605339.
[2]Current Address: Jefferson Lab, Newport News, VA

12:39PM W25.00008 London penetration depth of λ-$(BETS)_2GaCl_4$ superconductor , JASON MURPHY, H. KIM, K. CHO, M.A. TANTAR, Iowa State University/Ames Laboratory, A. KOBAYASHI, University of Tokyo, Japan, H. KOBAYASHI, Department of Chemistry, Nihon University, Japan, R. PROZOROV, Iowa State University/Ames Laboratory — After many years of study, it is still unclear whether the superconductivity of organic charge transfer salts is conventional or not. In particular, symmetry of the superconducting gap is an important unresolved question. The gap anisotropy and nodal structure can be probed via precision measurements of London penetration depth, $\lambda(T)$, for which tunnel-diode resonator has been developed over past 20 years. Here we report $\lambda(T)$ in λ-$(BETS)_2GaCl_4$ crystals ($T_c \sim 5$ K) measured down to 400 mK. We find that different samples exhibit different widths of superconducting transition, ΔT_c. It is known for organic superconductors that cooling rate from room temperature is important for the properties probed at the low temperatures. We discuss observed variation of ΔT_c with the cooling rate as well as sample size and aspect ratio. Results are compared with thermal conductivity measurements [1].

[1] M. A. Tanatar, T. Ishiguro, H. Tanaka, H. Kobayashi, Phys.Rev. B **66**, 134503 (2002).

12:51PM W25.00009 Thermodynamic study of the superconducting gap structure of $(TMTSF)_2ClO_4$, SHINGO YONEZAWA, YOSHITERU MAENO, Department of Physics, Graduate School of Science, Kyoto University, KLAUS BECHGAARD, Department of Chemistry, Oersted Institute, Copenhagen, Denmark, DENIS JEROME, Laboratoire de Physique des Solides, Univ. Paris-Sud, Orsay, France — We have studied the superconducting (SC) gap structure of the quasi-one-dimensional molecular conductor $(TMTSF)_2ClO_4$ based on our high-resolution heat capacity measurement. We developed a new calorimeter, which allowed us field-angle resolved calorimetry using one single crystal weighing as small as 76 μg. From our results, we investigate the SC gap structure in the k-space as well as in the spin space. Comparison between the SC phase diagram deduced from the present results and those obtained from previous resistivity measurements are also discussed.

1:03PM W25.00010 Superconducting energy gap features of MgB_2 thin films on different substrates and orientations , WENQING DAI, QI LI, Department of Physics, The Pennsylvania State University, University Park, PA 16802, KE CHEN, XIAOXING XI, Department of Physics, Temple University, Philadelphia, PA 19122 — We report a detailed study of tunneling spectra of MgB_2/I/Pb planar junctions with MgB_2 films on various substrates and of various doping levels. Planar trilayer junctions were fabricated using MgB_2 films with native oxide barrier grown by the Hybrid Physical-Chemical Vapor Deposition technique. Both π and σ bands contribute to the tunneling spectra of tilted-axis films on MgO (211) substrate and mainly π band was observed on c-axis MgB_2 films on SiC (0001), MgO (111) and c-sapphire substrates. We observed σ gap value of $\sim$7.9 meV in MgB_2 films on SiC substrates which display higher T_c due to the lattice strain. This is larger than 7.4 meV on unstrained substrates. However, the π gap value of all samples is $\sim$2.3 meV. We concluded that the strain in MgB_2 films on SiC substrates mainly affects the σ band of MgB_2. In addition, small amount of nitrogen gas was added during film growth to introduce more scattering in MgB_2 films. We systematically studied the change of two gaps with nitrogen doping from the tunneling spectra of MgB2/I/Pb junctions.

1:15PM W25.00011 Measurements of Multiple Gap Substructure in MgB_2 Below 1 Kelvin[1] , STEVEN CARABELLO, JOSEPH LAMBERT, ROBERTO RAMOS, Department of Physics, Drexel University — The two superconducting energy gaps of magnesium diboride (MgB_2) are well established. First-principles calculations have also predicted substructure within the sigma- and pi-band gaps. However, due to anticipated intraband impurity scattering, there is controversy as to whether these finer structures can be observed in real samples. Prior experimental evidence above 1 Kelvin has provided evidence supportive of these features. We have performed tunneling spectroscopy experiments on MgB_2/insulator/Pb Josephson junctions on SiC substrates, at temperatures as low as 20 mK. By measuring differential conductance at low temperatures, and by using extremely clean MgB_2 thin films, we have resolved features within the energy gaps to under 1 meV. We report results of these experiments, which are in remarkable agreement with theoretical predictions for this substructure.

[1]We wish to thank Profs. Xiaoxing Xi and Ke Chen for providing high quality MgB_2 Josephson junctions and many helpful insights.

1:27PM W25.00012 Time Dependent Transport Properties of Superconducting MgB_2 , MURAT OLUTAS, ATILGAN ALTINKOK, ATILLA KILIC, KIVILCIM KILIC, Abant Izzet Baysal University — The time dependent transport properties of polycrystalline superconducting MgB_2 sample was investigated in details by means of current-voltage (I – V curves) measurements with different current sweep rates (dI/dt) and transport relaxation (V – t curves) measurements. The corresponding measurements were carried out as functions of temperature (T), transport current (I) and external magnetic field (H). Upon cycling of the transport current, it was observed that the hysteresis effects in I – V curves are negligible. Further, for slow or fast sweep rates (dI/dt) of the transport current, the measured voltage dissipation at a given transport current is approximately stable and does not change much with time. Analysis of the I – V curves shows that the pinning potential is also practically independent of dI/dt. The time evolution of sample voltage reveals that the increase in sample voltage is quite a sharp and non-linear. The V – t curves were interpreted in terms of re-organization of flux lines and suppression of the effective superconducting order parameter along the sample as the time progresses. The quenched state created in V – t curves was correlated to the supercooling of flux lines. Finally, the experimental results of polycrystalline MgB_2 sample were compared to previous similar studies on superconducting $Y_1Ba_2Cu_3O_{7-x}$ and $Bi_{1.7}Pb_{0.3}Sr_2Ca_2Cu_3O_x$ polycrystalline samples.

1:39PM W25.00013 Measurement of Hc1 in MgB2 thin films and multilayer structures by a microwave absorption technique , CHENGGANG ZHUANG, KE CHEN, Temple Univ., SOM TYAGI, Drexel Univ., XIAOXING XI, Temple Univ. — For superconducting RF applications, Gurevich suggested a route to enhance the vortex penetration field, Hc1, and thermal breakdown field by a multilayer structure consisting of alternating insulator and superconductor layers with thicknesses smaller than the penetration depth. We have measured Hc1 of MgB2 thin films and multilayer structures by measuring the microwave absorption of the sample at 9.3 GHz in a TE102 rectangular cavity under an applied magnetic field. The magnetic fluxon penetration into the sample as the applied field is increased to greater than Hc1 leads to an increase in the microwave absorption. Preliminary results indicate an enhancement of Hc1 in the MgB2 thin films from the bulk value, consistent with Gurevich's thickness effect model, which is very promising for RF applications of MgB2.

1:51PM W25.00014 Magnetic force microscopy study of the penetration depth in MgB_2 thin films , JEEHOON KIM, LEONARDO CIVALE, MPA Division, Los Alamos National Laboratory, EVGUENI NAZARETSKI, Brookhaven National Laboratory, Upton, NY, NESTOR HABERKORN, MPA Division, Los Alamos National Laboratory, JOSH THIBODAUX, ILYA VEKHTER, Dept of Physics and Astronomy, Louisiana State University, BRIAN MOECKLY, Superconductor Technologies, Inc., Santa Barbara, JOE D. THOMPSON, ROMAN MOVSHOVICH, MPA Division, Los Alamos National Laboratory — We performed magnetic force microscopy (MFM) investigations of superconducting vortices in thin films of MgB_2. Our MFM instrument has the capability of scanning multiple samples. Prior to imaging vortices in MgB_2, vortex imaging in a Nb thin film was performed to characterize the cantilever's tip. This procedure allows extraction of the penetration depth with only one fitting parameter. Images of two MgB_2 films with different thickness were taken as a function of temperature, together with periodic checks of the condition of the magnetic tip via imaging of vortices in the Nb reference sample, during a single cooldown. The temperature dependent penetration depth determined by MFM will be compared to that obtained via SQUID magnetometry on the same samples.

2:03PM W25.00015 Metastable Vortex Lattice Phases in MgB_2 , C. RASTOVSKI, K. SCHLESINGER, P. DAS, M.R. ESKILDSEN, University of Notre Dame, IN, US, L. DEBEER-SCHMITT, Oak Ridge National Laboratory, TN, USA, N. ZHIGADLO, J. KARPINSKI, ETH Zurich, Switzerland — We present small-angle neutron scattering (SANS) studies of vortex lattice (VL) metastability in MgB_2. Three different VL phases are observed, all of which have a triangular symmetry. At low fields the VL is aligned with the crystalline a-axis. At intermediate fields the VL rotates away from the a-axis, leading to two degenerate domain orientations. Once the rotation reaches 30° a single domain, high field VL is reformed, now aligned along the a^*-axis. Metastable configurations are obtained when crossing the equilibrium VL transition lines by cooling or heating in a constant field. At any given field and temperature the equilibrium VL can be obtained by inducing vortex motion. We have explored the details of how the metastable VL transitions to the ground state, and established that the equilibrium VL phase propagate from the edge of the sample towards the center as the magnetic field is reduced. We have successfully prepared samples with a coexistence of metastable and ground state VL domains, and explored how large field changes are necessary to completely suppress the metastable VL phase. The SANS results are compared to measurements of the critical current obtained from magnetization measurements. This work was supported by DOE BES award no. DE-SC0005051.

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W26 DMP DCOMP: Focus Session: Iron Based Superconductors – Tuning Magnetism and Superconductivity D162/164

11:15AM W26.00001 ABSTRACT WITHDRAWN –

11:27AM W26.00002 Superconductivity in (Sr,Ba)Fe2As2 single crystals by Pt substitution[1] , TYLER DRYE, SHANTA SAHA, KEVIN KIRSHENBAUM, NICHOLAS BUTCH, JOHNPIERRE PAGLIONE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park, MD, PETER ZAVALIJ, Department of Chemistry and Biochemistry, University of Maryland, College Park, MD — Iron-based superconducting materials with the ThCr2Si2 tetragonal crystal structure appear to show a maximum superconducting transition temperature of Tc $\sim$ 20-25 K when transition metals (e.g., Co, Ni, Ru, Rh, Pd, or Ir) are substituted for Fe, effectively doping d-electrons and suppressing the antiferromagnetic order of the parent compounds. However, this trend is known to be broken in the case of SrFe2-xNixAs2 and SrFe2-xPdxAs2, which both have lower optimal Tc values near 10 K. We will present our recent work on Pt substitution in single crystalline BaFe2As2 and SrFe2As2, which induces a maximum Tc of 23 K and 17 K, respectively. The relation between Pt substitution in these systems and the related cases of isoelectronic Ni and Pd substitution will be discussed.

[1]This work was supported by AFOSR MURI Grant FA9550-09-1-0603.

11:39AM W26.00003 Tetragonal lattice collapse in $SrFe_2As_2$ - a combined experimental and theoretical study , HELGE ROSNER, DEEPA KASINATHAN, MIRIAM SCHMITT, ALIM ORMECI, KATRIN MEIER, ULRICH SCHWARZ, MPI CPfS Dresden, MICHAEL HANFLAND, ESRF Grenoble, KLAUS KOEPERNIK, IFW Dresden, YURI GRIN, ANDREAS LEITHE-JASPER, MPI CPfS Dresden — In a joint experimental and theoretical study we investigate the crystal structure of the Fe pnictide compounds $SrFe_2As_2$ under applied hydrostatic pressure. Applying high pressure X-ray diffractyion, for a critical pressure of about 10 GPa we observe a sudden collapse of the tetragonal c axis, accompagnied by a small expansion of the basal plane. This results in a drastic reduction of the c/a ratio and a significant decrease of the unit cell volume. This tetragonal collapse is well described by DFT band structure calculations and can be assigne d to the formation of an additional As-As bond along the tetragonal c axis.

11:51AM W26.00004 Structural tuning of superconductivity and magnetism in intermetallic iron-pnictide materials[1] , JOHNPIERRE PAGLIONE, University of Maryland — The relationship between superconductivity, magnetism and crystallographic structure remains as one of the intriguing properties of the new family of iron-based superconducting materials. A well established requirement for high-temperature superconductivity in these systems is a substructure of iron ions tetrahedrally coordinated with either pnictogen or chalcogen anions stacked together to form a layered material, suggesting that both tetrahedral geometry and quasi-two-dimensionality are key ingredients. Through an investigation of solid solutions of (Ba,Sr,Ca)Fe_2As_2 series of parent compounds, we present a study of the importance of internal tetrahedral structure in stabilizing both magnetic and superconducting ground states in these materials, revealing an intimate relationship between the energy scale that dictates magnetic order and the internal structure of the $FeAs_4$ tetrahedra even far above the magnetic ordering temperature. In addition, interlayer coupling is investigated by exploiting the "collapse" of the tetragonal unit cell of $CaFe_2As_2$ under pressure, where interlayer pnictogen-pnictigen bonding changes dramatically. We investigate the effect of this collapse on superconductivity via chemical substitution, demonstrating an intriguing interplay of structure, magnetic and superconducting properties.

[1]This work is supported by AFOSR-MURI grant #FA9550-09-1-0603.

12:27PM W26.00005 Magnetic ordering in $EuCo_2As_2$[1] , BALAZS SIPOS, ATHENA S. SEFAT, BRIAN C. SALES, OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TENNESSEE 37831, USA TEAM — We have synthesized and studied $EuCo_2As_2$ single crystals by resistivity, magnetoresistance, and susceptibility measurements. We found antiferromagnetic (AFM) ordering of the Eu spins at $T_N = 50$ K. Upon applying a magnetic field $H \| ab$ at $T = 2$ K this phase exhibits a metamagnetic (MM) transition at $H_{MM} = 3.5$ T. In case of $H \| c$ the magnetisation increases linearly up to 7 T. The same AFM to MM transition was found at 0.5 T in $EuFe_2As_2$ where it was found to be due to the reorientation of the Eu spin. We found that replacing Fe with Co strengthens the coupling between the Eu moments resulting in a higher T_N and H_{MM}.

[1]Research sponsored by the Material Science and Engineering Division Office of Basic Energy Sciences, U. S. Department of Energy.

12:39PM W26.00006 High Magnetic Field Studies of Pressure-induced Superconductor $EuFe_2As_2$, NOBUYUKI KURITA, MOTOI KIMATA, KOTA KODAMA, ATSUSHI HARADA, HIROYUKI SUZUKI, TAKEHIKO MATSUMOTO, SHINYA UJI, TAICHI TERASHIMA, National Institute for Materials Science, KEIZO MURATA, Graduate School of Science, Osaka City University — We have performed resistivity and susceptibility measurements of the pressure-induced superconductor $EuFe_2As_2$ under high magnetic fields up to 27 T. The upper critical field B_{c2} and its pressure evolution up to 3.2 GPa were determined in a wide temperature range down to 1.6 K. At 2.5 GPa, nearly the optimal pressure with T_c=30 K, $B_{c2}(0)$ obtained by the onset of resistive transitions are 25 T and 22 T for $B \parallel ab$ and $B \parallel c$, respectively, which are appreciably smaller than those for other Fe-based superconductors with similar T_c. The small $B_{c2}(0)$ values and the peculiar $B_{c2}(T)$ curves in $EuFe_2As_2$ can be explained by a multiple pair-breaking model including the exchange field due to the magnetic Eu^{2+} moments. We will also present the results of quantum oscillations observed above the optimal pressure.

12:51PM W26.00007 Pressure shift of the superconducting T_c of $(Pr_{1-x}Sr_x)FeAsO$ and $Sm(O_{1-x}F_x)FeAs$, KALYAN SASMAL, Department of Physics, TcSUH, University of Houston, G. MU, H.-H. WEN, Institute of Physics, Chinese Academy of Sciences, B. LORENZ, Department of Physics, TcSUH, University of Houston, CHING-WU CHU, Department of Physics, TcSUH, University of Houston and Lawrence Berkeley National Laboratory — Pressure plays important role in discovery and unraveling physics of novel superconductors.High Tc iron-based layered compounds can be obtained by hole/electron-doping.To determine if a symmetry between electron and hole-doping exists,we investigated pressure-induced shift in T_c by carryingout resistivity measurements under hydrostatic pressure on hole-doped $Pr_{1-x}Sr_xFeAsO$ up to 1.8GPa using piston-cylinder clamp cell device.The coexistence of superconductivity & spin-density wave behavior were observed and pressure effects on both being investigated. Four probe resistance measurements show T_c increases ($+dT_c/dP$) with pressure for under-doped $Pr_{1-x}Sr_xFeAsO$ similar to high-T_c cuprates. High pressure can compress crystalline structure of material and force its layers to be closer,which might increase material's T_c by improving pressure-induced charge transfer between (Fe_2As_2) and (Pr/Sr)O layers. The pressure effect on T_c of $Pr_{1-x}Sr_xFeAsO$ is being compared with that of electron doped $Sm(O_{1-x}F_x)FeAs$. The results suggest a symmetry appear to exist between electron and hole-doping Fe-pnictide superconductors.

1:03PM W26.00008 Pressure induced superconductivity in LaFeAsO: the role of anionic height and magnetic ordering[1] , RAVHI KUMAR, HiPSEC and Dep. Physics, University of Nevada Las Vegas, JAMES HAMLIN, Department of Physics, University of California San Diego, YUMING XIAO, STANISLAV SINOGEIKIN, PAUL CHOW, HPCAT and Carnegie Institution of Washington, BRIAN MAPLE, Department of Physics, University of California San Diego, YUSHENG ZHAO, HiPSEC and Dep. Physics, University of Nevada Las Vegas, ANDREW CORNELIUS, HiPSEC and Dep.Physics, University of Nevada Las Vegas — We have investigated the pressure effect on the crystal structure and magnetic ordering of LaFeAsO at low emperature ($\sim$18K) using high pressure powder x-ray diffraction (HPXRD) and nuclear forward scattering (NFS) to pressures up to 40 GPa. We demonstrate a continuous suppression of the long range antiferromagnetic ordering in this compound under pressure. Furthermore we show here a direct correlation between the pressure induced changes in the anionic height parameter to the transition temperature (Tc) and is first observed in the 1111 class of iron arsenide compounds under pressure. Our findings suggest that pressure induced suppression of magnetic ordering and the anionic height variation both play important roles in the origin of pressure induced superconductivity in LaFeAsO.

[1]HiPSEC is supported by NNSA, and DOE (DE-FC52-06NA26274).

1:15PM W26.00009 The Pressure Effects on $SmFeAsO_{0.85}$ and $PrFe_{0.925}Co_{0.075}AsO$ Superconductors , X.L. DONG, W. LU, J. YANG, W. YI, Z.C. LI, C. ZHANG, Z.A. REN, G.C. CHE, L.L. SUN, F. ZHOU, X.J. ZHOU, Z.X. ZHAO, National Laboratory for Superconductivity, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, CAS, Beijing 100190 — We have measured magnetic susceptibility of iron pnictide superconductors $SmFeAsO_{0.85}$ and $PrFe_{0.925}Co_{0.075}AsO$ under hydrostatic pressure up to 1.15 GPa. Our results indicate that the pressure dependences of T_C and superfluid density in both systems are positively correlated which suggests that these quaternary iron-based superconductors are not conventional BCS ones.

1:27PM W26.00010 Valence change of europium and its relation to superconductivity in $EuFe_2As_{1.4}P_{0.6}$ and compressed $EuFe_2As_2$, LILING SUN, JING GUO, GENFU CHEN, XIANHUI CHEN, XIAOLI DONG, WEI LU, CHAO ZHANG, ZHENG JIANG, YANG ZUO, SHUO ZHANG, YUYING HUANG, QI WU, XI DAI, YUANCHUN LI, JING LIU, ZHONGXIAN ZHAO — Superconductivity can be realized in Eu-containing pnictides by applying chemical (internal) and physical (external) pressure, the intrinsic physical mechanism of which attracts much attention in the studies of pnictide superconductors. Here we present the experimental evidence for the pressure-induced valence change of europium in $EuFe_2As_{1.4}P_{0.6}$ exposed to ambient pressure and $EuFe_2As_2$ to high pressure by x-ray absorption measurements on L_3-Eu edge. We found that the absorption spectrum of $EuFe_2As_{1.4}P_{0.6}$ showed a clear spectra weight transfer from divalent to trivalent state. Furthermore, a similar behavior of valence transition as in $EuFe_2As_{1.4}P_{0.6}$ was also observed in $EuFe_2As_2$ when pressure was applied. This is the first to report the observation of valence change in pnictide superconductors and the analysis of its influence on superconductivity in $EuFe_2As_{1.4}P_{0.6}$ and compressed $EuFe_2As_2$.

1:39PM W26.00011 Pressure effects on strained $FeSe_{0.5}Te_{0.5}$ thin films , MELISSA GOOCH, BERND LORENZ, Department of Physics and TcSUH at the University of Houston, SUNXIANG HUANG, CHIA-LING CHIEN, Department of Physics and Astronomy at John Hopkins University, PAUL CHU, Department of Physics and TcSUH at the University of Houston; Lawrence Berkeley National Laboratory — FeSe is the simplest structure in the family of the iron pnictides, with a reported superconducting transition of 8K for the α-PbO- type structure. With the substitution of Te for Se, $FeSe_{0.5}Te_{0.5}$, was found to have an increased superconducting transition up to 15.2 K. To investigate the strain effect on the superconducting properties of the $FeSe_{0.5}Te_{0.5}$, thin films were grown under different conditions. The Tc and the normal state properties show a correlation to the induced strain of the system. The application of external pressure resulted in an increase of T_c, but at different rates depending on the pre-existent strain in the system.

1:51PM W26.00012 Enhanced SDW transition temperature under hydrostatic pressure in Fe1.02Se0.10Te0.90 , NAOYUKI KATAYAMA, University of Virginia, KAZUYUKI MATSUBAYASHI, University of Tokyo, JUSCELINO LEAO, NIST, SUNGDAE JI, University of Virginia, SUNG CHANG, NIST, YOSHIYA UWATOKO, TAKU SATO, University of Tokyo, SEUNGHUN LEE, University of Virginia, UNIVERSITY OF VIRGINIA TEAM, UNIVERSITY OF TOKYO COLLABORATION, NIST COLLABORATION — We will present the spin glass (SG) to spin density wave (SDW) transition in Fe1.02Se0.10Te0.90 under hydrostatic pressure. At ambient pressure, the present compound shows SG transition, characterized by a broad weak magnetic peak. By applying hydrostatic pressure, SG develops to SDW at Pc $\sim$ 0.5 GPa and the sharp strong magnetic Bragg peak appears. The SDW transition temperature is increased up to $\sim$ 250 K at 8 GPa, which is sharply contrast to the results of pressure experiments in LaFeAsO families and BaFe2As2 families.

2:03PM W26.00013 Competition between magnetic order and superconductivity in Fe oxypnictides , SAMUELE SANNA, Physics Department and CNISM University of Pavia, Italy, P. CARRETTA, G. PRANDO, A. RIGAMONTI, R. DE RENZI, T. SHIROKA, G. LAMURA, M. PUTTI, A. MARTINELLI, R. CIMBERLE, M. TROPEANO, C. FERDEGHINI, A. PALENZONA, UNIVERSITY OF PAVIA TEAM, UNIVERSITY OF PARMA TEAM, UNIVERSITY OF GENOVA AND SPIN-CNR TEAM, ETH OF ZURICH TEAM — We have microscopically investigated the interplay between magnetism (M) and superconductivity (SC) of the RFeAsO (1111) oxy-pnictide for R=La, Sm and Ce as a function of F doping, isoelectronic Fe/Ru substitution and external pressure. In contrast to earlier data, our results suggest a unique behaviour in different 1111 families at the M-SC crossover, showing a sharp crossover between the two types of order as a function of F doping [1-3]. In the optimally e^--doped $SmFe_{1-x}Ru_xAsO_{0.85}F_{0.15}$ compound, magnetic order appears in the FeAs layers for $0.1 < x < 0.5$, together with a concomitant dramatic reduction of the superconducting transition temperature [3]. Both these features suggest a strong competition between the magnetic and superconducting order parameters within the FeAs layers of 1111 oxypnictides.

[1] S. Sanna et al., PRB 80 (2009) 052503.
[2] S. Sanna et al., PRB 82 (2010) 060508R.
[3] Manuscript in preparation.

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W27 GQI: Focus Session: Semiconductor Qubits- Optical Control, Donors, and Hybrid Systems C155

11:15AM W27.00001 Ultrafast optical entanglement control between two quantum dot spins

, SAM CARTER, DANNY KIM, ALEX GREILICH, ALLAN BRACKER, DANIEL GAMMON, Naval Research Laboratory — A single electron spin in an InAs quantum dot is very attractive as a qubit since this system is potentially scalable and allows complete quantum control on an ultrafast timescale using optical pulses. While great progress has been achieved with single spin qubits, it is essential for quantum information applications to move toward entangled multi-qubit systems. Two-qubit systems have been studied in electrostatically-defined quantum dots, but their optical functionality remains unexplored. Here we demonstrate ultrafast optical control of two interacting qubits consisting of two electron spins in separate InAs dots. We initialize the system into a spin singlet state using a cw laser. We then manipulate the entangled state of the two spins with single qubit gates (acting only on one spin) by using pulses faster than the exchange interaction. This allows us to generate all four Bell states. Two-qubit gates are obtained either by the natural exchange precession or by using a longer laser pulse that induces a phase shift in the precession. The two-qubit exchange rate (30 GHz) here gives SWAP gate times of 16 ps, the fastest of any candidate for quantum information processing.

11:27AM W27.00002 Complete ultrafast optical coherent control and spin echo of single InAs quantum dot spins

, KRISTIAAN DE GREVE, PETER MCMAHON, DAVID PRESS, Ginzton Labs, Stanford University, THADDEUS LADD[1], Ginzton Labs, Stanford University and National Institute of Informatics (NII), Tokyo, CHRISTIAN SCHNEIDER, DIRK BISPING, MARTIN KAMP, LUKAS WORSCHECH, SVEN HOEFLING, ALFRED FORCHEL, Technische Physik, Physikalisches Institut, Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, YOSHIHISA YAMAMOTO, Ginzton labs, Stanford University and National Institute of Informatics (NII), Tokyo — We report on recent progress on the complete ultrafast optical coherent control of individual InAs quantum dot spin qubits. We demonstrate Rabi-oscillations and Ramsey-fringes, and implement a spin echo to overcome time-averaged dephasing.[2] We probe the hyperfine interaction of a single spin using optical pulse control. Interesting non-Markovian dynamics could be observed in the single electron spin free-induction decay, resulting from feedback between the strong electron spin Overhauser shift and spin dependent nuclear relaxation.[3]

[1]currently at HRL Laboratories, LLC, Malibu, CA 90265

[2]D. Press, K. De Greve, P. McMahon *et al.*, Nat. Phot. **4**, 367 (2010)

[3]T. D. Ladd, D. Press, K. De Greve *et al.*, Phys. Rev. Lett. 105, 107401 (2010)

11:39AM W27.00003 Control of exciton relaxation channels in quantum dot molecules

, KUSHAL C. WIJESUNDARA, JUAN E. ROLON, SERGIO E. ULLOA, ERIC A. STINAFF, Department of Physics and Astronomy, and Nanoscale and Quantum Phenomena Institute, Ohio University, Athens, OH 45701, USA, ALLAN BRACKER, DAN GAMMON, Naval Research Laboratory, Washington, DC 20375, USA — We observe modulations in radiative lifetimes and intensities of the spatially indirect exciton as the InAs/GaAs coupled quantum dot system is tuned between molecular and atomic like states. With standard time-resolved single photon counting techniques the measured lifetimes were found to vary between 0.3 and 2.0 ns which resulted in modulations of the observed photoluminescence intensity of the indirect exciton. These modulations can be attributed to phonon mediated relaxations and carrier tunneling processes in good agreement with the modeled results. We clearly see the structure of the acoustic phonon distribution as shown in recent theoretical predictions. Tuning the relative energy levels in coupled quantum dots results in controllable modulation of exciton relaxation channels that may provide new directions in engineering decoherence in these systems.

11:51AM W27.00004 Charge dynamics and phonon induced oscillatory relaxation rates of indirect excitons in quantum dot molecules[1]

, J.E. ROLON, K.C. WIJESUNDARA, E.A. STINAFF, S.E. ULLOA, Ohio University — Optoelectronic control of quantum dots is a thriving area of research with impact on fundamental physics and quantum information devices. Time-resolved photoluminescence experiments, carried out in charge tunable coupled quantum dots, have demonstrated non-monotonic behavior of neutral indirect exciton lifetimes over a wide range of applied electric fields [1]. We present a model for neutral indirect exciton lifetimes in electric field tunable quantum dot molecules. Our model includes field-dependent oscillatory phonon-induced relaxation rates [2], carrier tunneling rates, and carrier relaxation into nearby charged exciton states. To this end we have used a multi-excitonic Hamiltonian, and calculated the exciton population dynamics using a master equation with electric field dependent rates. We find that lifetime suppression is dominated by scattering with LA phonons at low fields, and that the maximum lifetime gives information on the effective dimensions of the molecule. In contrast, at high fields the lifetime suppression is dominated by the interplay of carrier population exchange with nearby charged excitons. This prompts for ways of controlling exciton lifetimes and possible decoherence in quantum dots. [1] K. C. Wijesundara et al., (unpublished), [2] J. I. Climente et al., Phys. Rev. B 74, 035313 (2006).

[1]Supported by CONACYT and NSF PIRE and MWN/CIAM.

12:03PM W27.00005 Ultralong Coherence of Phosphorus Donors in High-Purity ^{28}Si Silicon

, S.A. LYON, A.M. TYRYSHKIN, Princeton University, S. TOJO, K.M. ITOH, Keio University, J.J.L. MORTON, Oxford University, T. SCHENKEL, Lawrence Berkeley National Laboratory, M.L.W. THEWALT, Simon Fraser University, H. RIEMANN, N.V. ABROSIMOV, Institute for Crystal Growth, IKZ, P. BECKER, PTB Braunschweig, H.-J. POHL, VITCON Projectconsult GmbH — We report on electron spin coherence measurements for phosphorus donors in high purity, highly-enriched ^{28}Si, with residual ^{29}Si of less than 50 ppm. At this low ^{29}Si density, spectral diffusion processes by nuclear spin flip-flops are suppressed, and therefore other relaxation processes become prominent. By examining a series of ^{28}Si crystals with a donor concentration of 1×10^{14} to 3×10^{15}/cm^3, we identified three decoherence mechanisms, all related to dipole interactions between donors: (1) instantaneous diffusion, caused by flips of donor spins induced by the applied microwave pulses; (2) spectral diffusion caused by T_1-induced flips of neighboring donors; (3) spectral diffusion caused by donor spin flip-flops. We demonstrate how all three mechanisms can be suppressed, leading to measured coherence times extrapolating to T_2 $\sim$10 sec. The work was funded by DOE and LPS.

12:15PM W27.00006 Electrical Control of the high spin system Mn2+ in ZnO

, RICHARD GEORGE, JOHN MORTON, ARZHANG ARDAVAN, University of Oxford, JAMES EDWARDS, University of Cambridge — We examine the high spin impurity Mn^{2+} in single crystal ZnO (S=5/2, I=5/2), and report a strong linear coupling (K = 52.3 rad/V/m) of the manganese electrical and magnetic moments that preserves quantum coherence. We combine pulsed EPR and electric field techniques to manipulate the Mn states and study electron spin lifetimes, finding T_{2e} and T_{1e} times of 0.8ms and 100ms at 2K in the natural material. We investigate the 'forbidden' transitions that become allowed in the low symmetry environment and use these to manipulate the nuclear spin state on a sub-microsecond timescale that is inaccessible via ENDOR and RF techniques. Finally, we explore the existence of subspaces that are robust against strain-induced decoherence and the application of this material as an entanglement-based field sensor.

12:27PM W27.00007 Electron spin coherence and electron nuclear double resonance of Bi donors in natural Si , JOHN MORTON, STEPHANIE SIMMONS, RICHARD GEORGE, Oxford University, WAYNE WITZEL, Sandia National Labs, H. RIEMANN, NIKOLAI ABROSIMOV, N. NOTZEL, Institute for Crystal Growth, Berlin, MIKE THEWALT, Simon Fraser University — We have shown that the electron spin coherence times of Si:Bi donors in natural silicon are limited by the same mechanism of spectral diffusion as seen in Si:P, though the smaller Bohr radius of the Bi donor leads to $\sim 30\%$ longer T_2 times (up to 0.8 ms). We have mapped out the 36 ENDOR transitions observable at X-band arising from the $I = 9/2$ nuclear spin of ^{209}Bi, going up to 1.3 GHz. We also demonstrate the transfer of electron spin coherence to and from the ^{209}Bi nuclear spin with a fidelity of $\sim 63\%$. Using pulsed ESR at W-band (100 GHz), we observe optically-induced dynamic nuclear polarisation, consistent with the mechanism of exciton capture proposed in by T. Sekiguchi *et al.*. Finally, we explore the zero-field splitting of 7.5 GHz in this system, within the context of coupling to superconducting resonators.

12:39PM W27.00008 Neutral donors interacting with a two-dimensional electron gas measured by electrically detected magnetic resonance up to 94GHz , C.C. LO, J. BOKOR, University of California, Berkeley, V. LANG, R.E. GEORGE, J.J.L. MORTON, University of Oxford, A.M. TYRYSHKIN, S.A. LYON, Princeton University, T. SCHENKEL, Lawrence Berkeley National Laboratory — Electrically detected magnetic resonance of a silicon field-effect transistor with channel-implanted donors is measured in a W-band (94 GHz, 3.36 T) resonant microwave cavity. It is found that the two-dimensional electron gas (2DEG) resonance signal intensity increases by two orders of magnitude compared with conventional low-field X-band (9.7 GHz, 0.35 T) measurements. On the other hand, the neutral donor resonance signals increase by over one order of magnitude. We interpret the results in terms of direct spin-dependent scattering and a polarization transfer from the donors to the 2DEG spin system.

12:51PM W27.00009 Electrical Manipulation of Spin Qubits in Li-doped Si , ANDRE PETUKHOV, LUKE PENDO, ERIN HANDBERG, South Dakota School of Mines, VADIM SMELYANSKIY, NASA Ames Research Center — We propose a complete quantum computing scheme based on Li donors in Si under external biaxial stress. The qubits are encoded on the ground state Zeeman doublets and coupled via long-range spin-spin interaction mediated by acoustic phonons. This interaction is unique for Li donors in Si due to their inverted electronic structure. Our scheme takes advantage of the fact that the energy level spacing in $1s$ Li-donor manifold is comparable with the magnitude of the spin-orbit interaction. As a result the Li spin qubits can be placed 100 nm apart and manipulated by a combination of external electric field and microwave field impulses. We present a specially-designed sequence of the electric field impulses which allows for a typical time of a two-qubit gate ~ 1 μs and a quality factor $\sim 10^{-6}$. These estimates are derived from detailed microscopic calculations of the quadratic Stark effect and electron-phonon decoherence times.

1:03PM W27.00010 Entanglement in a Solid State Spin Ensemble , STEPHANIE SIMMONS, RICHARD BROWN, Oxford University, HELGE RIEMANN, NIKOLAI ABROSIMOV, Leibniz Institut, PETER BECKER, PTB Braunschweig, HANS-JOACHIM POHL, VITCON Projectconsult GmbH, MIKE THEWALT, Simon Fraser University, KOHEI ITOH, Keio University, JOHN MORTON, Oxford University — Entanglement is a both a fascinating phenomenon and a critical ingredient in most emerging quantum technologies. Spin ensembles manipulated using magnetic resonance have demonstrated the most advanced quantum algorithms to date, however these studies contain no entanglement and hence constitute classical simulations of quantum algorithms. Here we report the on-demand generation of entanglement between an ensemble of electron and nuclear spins in isotopically engineered phosphorus-doped silicon. High field/low temperature electron spin resonance (3.4 T, 2.9 K) was used in conjunction with a hyperpolarisation sequence to reduce the spin entropy to a level sufficient to form an inseparable state. The generated entanglement was confirmed by measuring the state's density matrix which displayed a fidelity of 98% compared to the ideal state at this field and temperature. The entanglement operation was performed simultaneously, with high fidelity, to 10^{10} spin pairs, and represents an essential requirement of a silicon- based quantum information processor.

1:15PM W27.00011 Optimized Electron-spin-cavity coupling in a double quantum dot[1] , XUEDONG HU, University at Buffalo, SUNY, YU-XI LIU, Tsinghua University, China, FRANCO NORI, RIKEN, Japan — We search for the optimal regime to couple an electron spin in a semiconductor double quantum dot to a superconducting stripline resonator via the electrically driven spin resonance technique. In particular, we calculate the spin relaxation rate in the regime when spin-photon coupling is strong, so that we can identify system parameters that allow the electron spin to reach the strong coupling limit.

[1]We thank support by NSA/LPS through ARO.

1:27PM W27.00012 Near Field Photon Emission and Revival in Quantum Dot Qubits[1] , S. TAFUR, M.N. LEUENBERGER, Dept of Physics, University of Central Florida — Modeling the spontaneous emission of photons coupled to the electronic states of quantum dots is important for understanding quantum interactions and entanglement in condensed matter as applied to proposed solid-state quantum computers, quantum networks, single photon emitters, and single photon detectors. A quantum dot initially in an excited state can be experimentally observed to decay to its ground state and the observed homodyne tomography of the emitted photon can yield information about the qubit state of the emitter. Though the characteristic lifetime of photon emission is traditionally modeled via the Weisskopf-Wigner approximation, we seek to model the fully quantized spontaneous emission, including near field effects, of a photon from the excited state of a quantum dot beyond the Markovian limit. We further investigate subsequent interactions between the emitted photon and adjacent quantum dots in an effort to describe multipartite entanglement. We propose the use of discretized central-difference approximations of space and time partial derivatives, similar to finite-difference time domain models, to describe single photon states via single photon operators. Additionally, within the future scope of this model, we seek results in the Purcell and Rabi regimes for spontaneous emission events from quantum dots embedded in micro-cavities.

[1]NSF (Grant No. ECCS-0725514), DARPA/MTO (Grant No. HR0011-08-1-0059), NSF (Grant No. ECCS-0901784), and AFOSR (Grant No. FA9550-09-1-0450)

1:39PM W27.00013 A Theoretical Model of Single Photon Source at Room Temperature , AHMED ELHALAWANY, MICHAEL LEUENBERGER, University of Central Florida — In this work we present a theoretical model for an electrically injected single photon source at room temperature. The source is made of three regions. The region containing the source is n-doped, the middle region is an intrinsic semiconductor heterostructure. The region containing the drain is p-doped. The conguration of the intrinsic region is designed to trap a single pair of electron and hole; this is due to Pauli Exclusion Principle and Coulomb blockage. This is achieved by applying a reverse voltage to neutralize the intrinsic electric field between the n- and p-doped regions. Based on the calculated tunneling time of the electron/hole, the reverse voltage will be switched o. For the kinetics at the room temperature operation is calculated by means of the Master equations. For this we use an eective Hamiltonian in the tight-binding approximation. The results show that a single electron and a single hole are trapped simultaneously for an adequate period of time until they recombine.

1:51PM W27.00014 Phonons and solid-state qubits for quantum technology , Ö.O. SOYKAL, RUSKO RUSKOV, University of Maryland, College Park, MD 20742, CHARLES TAHAN, Laboratory for Physical Sciences, College Park, MD 20740 — Phonons in the context of quantum information processing are traditionally negatives. They induce relaxation or decoherence of or between qubit states. Learning to control phonons for positive purposes, both as supporting technology for quantum information processing, and for other quantum devices is of great possible interest. Already, acoustic waves are used as a supporting technology in microelectronics and optoelectronics (e.g. their slow speed can be useful in certain contexts). Here we consider some methods for making phonons useful and describe the physics of such systems in several potential solid-state systems including silicon. Our results may also be of interest to the optomechanics community.

2:03PM W27.00015 Towards electrons floating over diamond[1] , M.P. RAY, J.W. BALDWIN, M.K. ZALALUTDINOV, J.L. SHAW, J.E. BUTLER, B.B. PATE, Naval Research Laboratory, T.I. FEYGELSON, SAIC Inc. — The opportunities for development of a 2D electron system of image potential surface electrons over negative electron affinity diamond are examined. Image potential surface electron states, located spatially outside the solid, are well established on a variety of surfaces (metals, semiconductors and dielectrics). In particular, laterally confined electrons above liquid helium have been demonstrated and proposed for advanced computing applications [1,2]. Unlike the surface of liquid helium, the electron affinity of the diamond surface can be varied [3], providing the ability to lithographically pattern surface electron 'pools' and 'wires'. We present candidate structures for lateral charge control that make use of buried and surface features patterned in and on diamond. Electronic properties and spectroscopy of electrons over diamond in our fabricated structures are discussed.

[1] S. A. Lyon, Phys. Rev. A **74**, 052338 (2006).
[2] P. M. Platzman and M. I. Dykman, Science **284**, 1967(1999).
[3] J. Ristein, Surf. Sci. **600**, 3677 (2006).

[1]Work supported by the Office of Naval Research.

Thursday, March 24, 2011 11:15AM - 2:15PM –
Session W28 DCMP: Graphene: Nanoribbons and Electronic Transport C156

11:15AM W28.00001 Low Bias Negative Differential Resistance in Graphene Nanoribbon Superlattices[1] , GERSON J. FERREIRA, Universidade de São Paulo, MICHAEL N. LEUENBERGER, University of Central Florida, DANIEL LOSS, University of Basel, J. CARLOS EGUES, Universidade de São Paulo — We theoretically investigate negative differential resistance (NDR) for ballistic transport in semiconducting armchair graphene nanoribbon superlattices at low bias voltages V_{SD}. We combine the modulated graphene-Dirac hamiltonian with the Landauer formalism to calculate the current I_{SD} through the system. This description is expected to be valid at low biases and for narrow samples. We find three distinct transport regimes in which NDR occurs: (i) a "classical regime" in which the transport across the crossings of barrier and valley bandgaps is suppressed; (ii) a quantum regime dominated by superlattice miniband conduction, with current suppression arising from the misalignment of miniband states with increasing V_{SD}; (iii) a Wannier-Stark ladder regime with current peaks occurring at the crossings of Wannier-Stark rungs from distinct ladders. We emphasize that all the above mechanisms show NDR at voltages lower than 500 mV. Interestingly, within the miniband transport regime the NDR occurs at biases as low as 10 mV, i.e., comparable to the miniband width.

[1]This work was supported by FAPESP, CNPq, NSF/USA, DARPA/MTO, AFOSR, Swiss NSF, and NCCR Nanoscience.

11:27AM W28.00002 A finite difference method for transport of massless Dirac fermions: The case of graphene nanoribbons[1] , CAIO LEWENKOPF, Universidade Federal Fluminense - Brazil, ALEXIS HERNANDEZ, Pontificia Universidade Catolica do Rio de Janeiro - Brazil — We develop a new finite difference scheme to numerically compute the scattering matrix of two-dimensional massless Dirac fermions propagating in a ribbon geometry. The method is nonlocal, avoids the fermion doubling problem, and is suitable for introducing different kinds of boundary conditions. To illustrate its utility we compute the Landauer conductance of a monolayer graphene sheets with zig-zag boundary conditions in presence of a perpendicular magnetic field. The method is particularly useful in the study of long range disorder effects (much larger than the lattice spacing) in large graphene strips. In passing, we also show how the method works in the description of electronic transport at the surface of three-dimensional topological insulators.

[1]supported by FAPERJ and CNPq-Brazil

11:39AM W28.00003 ABSTRACT WITHDRAWN –

11:51AM W28.00004 Graphene edge from A to Z , YUANYUE LIU, SOMNATH BHOWMICK, BORIS I. YAKOBSON, Rice University — We introduce an energy decomposition anzats, which leads to an analytical expression for the edge energy G(X) of arbitrary direction-cut angle X in two dimensional materials [1]. We further show that thermodynamic conditions at the edge simply add a "chemical phase shift" C, G(X) = cos(X + C), making the favorable shapes controllable, according to the Wulff construction. Direct atomistic computations and analysis for graphene, as well as 2D boron nitride (h-BN), and zinic oxide (ZnO) support the universal nature of the relationship.

[1] Y. Liu, A. Dobrinsky, and B.I. Yakobson, Phys. Rev. Lett., in press (Dec 10 2010 issue).

12:03PM W28.00005 Boron nitride nanoribbons become metallic , ALEJANDRO LOPEZ-BEZANILLA, JING-SONG HUANG, HUMBERTO TERRONES, BOBBY SUMPTER, Oak Ridge National Laboratory — Boron nitride (BN) sheets can be grown on nickel substrates, similar to graphene, and BN domains coexist with graphene. The synthesis of zig-zag BN nanoribbons (zBNNRs) brings interesting possibilities regarding edge chemistry: since both boron and nitrogen atoms are exposed on each edge the functionality of the nanostructure is enriched. We report first principles calculations on the electronic properties of zBNNR nanoribbons with several types of functionalization. Sulfur and oxygen edge doping and topological one-dimensional defects are studied and the possibility of having half metallicity is also analysed. Sulfur and oxygen edge passivation converts zBNNRs into a metallic material which offers several possibilities for new applications in electronics, molecular sensing and spintronics.

12:15PM W28.00006 Graphene valley pseudospin filter using an extended line defect[1] , DANIEL GUNLYCKE, CARTER WHITE, Naval Research Laboratory — Although graphene exhibits excellent electron and thermal transport properties, it does not have an intrinsic band gap, required to use graphene as a replacement material for silicon and other semiconductors in conventional electronics. The band structure of graphene with its two cones near the Fermi level, however, offers opportunities to develop non-traditional applications. One such avenue is to exploit the valley degeneracy in graphene to develop valleytronics. A central component in valleytronics is the valley filter, just as the spin filter is central in spintronics. Herein, we present a two-dimensional valley filter based on scattering of electrons and holes off a recently observed extended line defect [Nat. Nanotech. **5**, 326 (2010)] within graphene. The transmission probability depends strongly on the valley pseudospin and the angle of incidence of the incident quasiparticles. Quasiparticles arriving at the line defect at a high angle of incidence lead to a valley polarization of the transmitted beam that is near 100 percent.

[1]This work was supported by ONR, directly and through NRL.

12:27PM W28.00007 Zero Landau level in folded graphene nanoribbons[1] , ELSA PRADA, Instituto de Ciencia de Materiales de Madrid-CSIC, PABLO SAN-JOSE, Instituto de Estructura de la Materia-CSIC, LUIS BREY, Instituto de Ciencia de Materiales de Madrid-CSIC — Graphene nanoribbons can be folded into a double layer system keeping the two layers decoupled. In the Quantum Hall regime folds behave as a new type of Hall bar edge. We show that the symmetry properties of the zero Landau level in metallic nanoribbons dictate that the zero energy edge states traversing a fold are perfectly transmitted onto the opposite layer. This result is valid irrespective of fold geometry, magnetic field strength and crystallographic orientation of the nanoribbon. Backscattering suppression on the N=0 Hall plateau is ultimately due to the orthogonality of forward and backward channels, much like in the Klein paradox.

[1]We acknowledge financial support from MICINN (Spain), through grants FIS2009-08744 and FIS2008-00124.

12:39PM W28.00008 Effective time-reversal symmetry breaking in the spin relaxation in a graphene quantum dot , PHILIPP STRUCK, GUIDO BURKARD, University of Konstanz — We study the relaxation of a single electron spin in a circular gate-tunable quantum dot in gapped graphene [1]. Direct coupling of the spin to out-of-plane phonons via the intrinsic spin-orbit coupling leads to a lowered relaxation time T_1 at intermediate B-fields. At low fields, T_1 increases as $\propto B^{-2}$ due to the suppression of the phonon density of states at long wavelengths in a finite system. We also find that Rashba spin-orbit induced admixture of opposite spin states in combination with the emission of in-plane phonons provides various further relaxation channels via deformation potential and bond-length change. In the absence of valley mixing, spin relaxation takes place within each valley separately and thus time-reversal symmetry is effectively broken, thus inhibiting the van Vleck cancellation at $B = 0$ known from GaAs quantum dots. Both the absence of the van Vleck cancellation as well as the out-of-plane phonons lead to a behavior of the spin relaxation rate at low magnetic and intermediate fields which is markedly different from the known results for GaAs. At high fields there is a crossover to $T_1 \propto B^{-2}$ or $\propto B^{-4}$.

[1] P. R. Struck and G. Burkard, Phys. Rev. B **82**, 125401 (2010).

12:51PM W28.00009 Sensory Organ Like Response of Zigzag Edge Graphene Nanoribbons[1] , VIJAY SHENOY, Indian Institute of Science Bangalore, SOMNATH BHOWMICK[2], Indian Institute of Science — Using a continuum Dirac theory, we study the density and spin response of zigzag edge terminated graphene ribbons subjected to edge potentials and Zeeman fields. Our analytical calculations of the density and spin responses of the closed system (fixed particle number) to the static edge fields, show a highly nonlinear Weber-Fechner type behavior where the response depends logarithmically on the edge potential. The dependence of the response on the size of the system (e.g. width of a nanoribbon) is also uncovered. Zigzag edge graphene nanoribbons, therefore, provide a realization of response of organs such as the eye and ear that obey Weber-Fechner law. We validate our analytical results with tight binding calculations. These results are crucial in understanding important effects of electron-electron interactions in graphene nanoribbons such as edge magnetism etc., and also suggest possibilities for device applications of graphene nanoribbons.
Reference: Somnath Bhowmick and Vijay B. Shenoy, *Physical Review B*, **82**. 155448 (2010)

[1]Work supported by DST, India through MONAMI and Ramanujan grants
[2]Currently at Rice University

1:03PM W28.00010 Transport Through Graphene Surface States , DOUGLAS MASON, ERIC HELLER, Harvard University — Of particular interest to models of transport through graphene has been the theoretical prediction of long-lived surface states on zigzag cuts. These states may have a strong influence on transport through finite graphene structures since, unlike infinite nanoribbon surface states, they can absorb and emit electrons traveling through the bulk of the structure. We will be presenting a novel approach to these surface states and postulate on their role in recent transport calculations.

1:15PM W28.00011 Quantum charge pumping in graphene nanoribbons[1] , TEJINDER KAUR, Ohio University, LILIANA ARRACHEA, Universidad de Buenos Aires, Argentina, NANCY SANDLER, Ohio University — The mechanism to generate DC currents in open-quantum systems by applying local de-phased time-dependent potentials is known as charge pumping. For graphene ribbons, pumping techniques provide an alternative route for current production that overcomes the role of contacts. We have analyzed the properties of zero-bias current through graphene nanoribbons using a tight-binding Hamiltonian description and the Keldysh formalism, which provides the proper description for these systems in the quantum non-equilibrium regime. After reviewing results for quantum pumping in a one-dimensional chain attached to two reservoirs, with two local single-harmonic potentials oscillating in time, we will introduce results for finite-width ribbons of square and graphene lattices. A discussion on the differences in transmission functions and DC currents between these two cases will be presented and the role of edge termination in graphene ribbons will be addressed.

[1]Supported by NSF-PIRE and DMR-MWN/CIAM

1:27PM W28.00012 Electronic properties of graphene nanoflakes: energy gap engineering , CARLOS RAMOS, EDUARDO CIFUENTES, ROMEO DE COSS, Cinvestav Unidad Merida, EDGAR MARTINEZ, Universidad Autonoma de Nuevo Leon — Graphene nanostructures show an energy gap resulting of the finite size, and are of current interest because of the potential applications in electronic devices. Thus, we discuss some recent progress in the synthesis of graphene nanoflakes obtained from the reaction of polyaromatic hydrocarbons. We are presenting ab-initio results for the electronic properties of graphene nanoflakes with a hexagonal-zigzag (HZ) structure and different effective radius (R). The calculations were performed using the Density Functional Theory as implemented in the pseudopotential-LCAO method. We find that the, Kohn-Sham gap decreases with size as R^{-1}, while the quasi-particle energy gap follow the $R^{-0.8}$ scaling rule. A formula to evaluate the energy gap of a HZ graphene nanoflake of arbitrary size is provided. This research was supported by Conacyt-México under Grant No. 83604.

1:39PM W28.00013 Electric and Magnetic Field Induced Insulating States in High Quality Bilayer Graphene pnp Junctions , LEI JING, JAIRO VELASCO, PHILIP KRATZ, Univ. of California, Riverside, GANG LIU, UCLA, WENZHONG BAO, MARC BOCKRAT, CHUN NING LAU, Univ. of California, Riverside — Band gap opening in bilayer graphene has generated significant interest in both technological application and fundamental research. By applying external electric and magnetic field, we observe an insulating state in our dual-gated bilayer graphene device. In addition, we also observe Quantum Hall plateaus with fractional values of e^2/h at large magnetic field, which arises from edge state equilibration at the interface of differentially doped regions, in agreement with theoretical predictions.

1:51PM W28.00014 Electron-Hole Asymmetry and Electron-Electron Interaction in Bilayer Graphene , K. ZOU, X. HONG, J. ZHU, Department of Physics, The Pennsylvania State University — We report precision measurements of the effective mass m^* in high-quality bilayer graphene samples using the temperature dependence of Shubnikov-de Haas oscillation. In the measured density range of $0.7\text{x}10^{12}/\text{cm}^2 < n < 4.1\text{x}10^{12}/\text{cm}^2$, both the hole mass $m^*_{\rm h}$ and the electron mass $m^*_{\rm e}$ increase with increasing n, with $m^*_{\rm h}$ being roughly 20-30% larger than $m^*_{\rm e}$ at the same density. We compare our results to tight-binding calculations and provide an accurate determination of several hopping parameters. The measured m^* is substantially suppressed compared to non- interacting values, demonstrating the importance of electron- electron interaction in bilayer graphene.

2:03PM W28.00015 Magneto-transport study of band structure of tri-layer graphene , RYUTA YAGI, SEIYA FUKADA, MIDOR SHIMOMURA, Hiroshima University — We have studied magneto-transport of high-quality tri-layer graphene samples. It has been observed Shubnikov-de Haas oscillations with two different frequencies that corresponded to two bands in tri-layer graphene. Detailed analysis of gate voltage dependence of the frequencies showed that sum of the carrier density for each band gave approximately the nominal carrier density tuned by the gate voltage. From temperature dependence of magnitude of the oscillation we have estimated cyclotron masses.

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W29 GQI: Symmetric Discrete Structures for Finite Dimensional Quantum Systems

C148

11:15AM W29.00001 Pairwise complementary observables and their mutually unbiased bases , BERGE ENGLERT, National University of Singapore — Pairs of complementary observables (PCO) characterize all quantum degrees of freedom and are central to a technical formulation of Bohr's principle of complementarity. A defining property of such pairs are their mutually unbiased bases (MUB) of eigenstates. MUB have found many applications for tasks in quantum information processing. Maximal sets of PCO and MUB are known, by explicit construction, for degrees of freedom that live in finite-dimensional Hilbert space whose dimension is a power of a prime; continuous sets of MUB are also known for most continuous degrees of freedom. I will review the situation and mention a couple of open problems.

11:51AM W29.00002 Quantum States as Probabilities from Symmetric Informationally Complete Measurements[1] , ÅSA ERICSSON, Institute Mittag-Leffler — If you pick d^2 symmetrically spread vectors in a d-dimensional Hilbert space, you get a symmetric informationally complete set of quantum states (or SIC for short). SICs have applications within quantum information science, such as to quantum state tomography and quantum cryptography, and are also of interest for foundational studies of quantum mechanics. In this talk I will review the representation of quantum states as probability distributions over the outcomes of a SIC measurement. Not all probability distributions correspond to quantum states, thus quantum state space is a restricted subset of all potentially available probabilities. We will explore how this restriction can be characterized. A recent publication (Fuchs and Schack, arXiv:0906.2187) advocates the SIC-representation and suggests that the Born rule rewritten in this language can be taken as a postulate for quantum mechanics. This motivates the introduction of so-called maximally consistent sets (Appleby, Ericsson, and Fuchs, arXiv:0910.2750); one such set is quantum state space.

[1]This work was supported in part by the U.S. Office of Naval Research (Grant No. N00014-09-1-0247).

12:27PM W29.00003 The Lie Algebraic Significance of Symmetric Informationally Complete Measurements , STEVEN FLAMMIA, Caltech — Examples of symmetric informationally complete positive operator valued measures (SIC-POVMs) have been constructed in every dimension less than 68. However, it remains an open question whether they exist in all finite dimensions. A SIC-POVM is usually thought of as a highly symmetric structure in quantum state space. However, its elements can equally well be regarded as a basis for the Lie algebra gl(d,C). We examine the resulting structure constants, which are calculated from the traces of the triple products of the SIC-POVM elements and which, it turns out, characterize the SIC-POVM up to unitary equivalence. We show that the structure constants have numerous remarkable properties. In particular we show that the existence of a SIC-POVM in dimension d is equivalent to the existence of a certain structure in the adjoint representation of gl(d,C). We hope that transforming the problem in this way, from a question about quantum state space to a question about Lie algebras, may help to make the existence problem tractable. This is joint work with M. Appleby and C. Fuchs.

1:03PM W29.00004 Experimental access to higher-dimensional discrete quantum systems, towards realizing SIC-POVM and MUB measurements, using integrated optics[1] , CHRISTOPH SCHAEFF, IQOQI — The aim of our work is to access and explore higher-dimensional photonic quantum systems. In terms of stability and complexity, normal bulk-optic setups greatly limit the capabilities of reaching higher-dimensional systems. However, the recent development in integrated photonic circuits has opened new possibilities [1]. Our approach is to use integrated photonic circuits on-chip, as well as in fiber, to reach photonic states of higher dimension. We are working toward a fully integrated realization of a multiport [2], a device which can apply any unitary transformation based on tunable internal parameters. Our first step is to realize a multiport in dimension four, implementing any unitary transformation on Qubits, Qutrits and Ququarts. Furthermore, we have built an integrated source using purely in-fiber components for creating higher-dimensional entangled photons. The combination of this source with the multiport yields a very general system applicable to a variety of experiments in higher dimensional Hilbert spaces. It is possible to realize different experimental setups by setting the device for different incoming entangled states, and subsequently applying unitary transformations. For example, this opens the possibility to observe new types of higher-order perfect correlations [3], or to realize full SIC-POVM measurements in higher dimensions.

[1] J.L.O'Brien, G.J.Pryde, A.G.White, T.C.Ralph and D.Branning, Nature Vol.426, pp264-267 (2003)
[2] M.Reck and A.Zeilinger, PRL Vol.73, No.1 (1994)
[3] M.Zukowski, A.Zeilinger and M.A.Horne, PRA Vol.55, No.1 (1997)

[1]The research has been supported by ERC Advanced Grant QIT4QAD and FWF SFB-grant F4007.

1:39PM W29.00005 Isotropic States in Discrete Phase Space , WILLIAM WOOTTERS, Williams College — An energy eigenstate of a harmonic oscillator is isotropic in phase space, in the sense that the state looks the same along any ray emanating from the origin. It is possible to extend this notion of "isotropic" to quantum systems with finite-dimensional state spaces—the rays are then rays in discrete phase space. In this talk I present examples of discrete isotropic states and discuss their properties. One can show that every isotropic state minimizes a specific information-theoretic measure of uncertainty with respect to a complete set of mutually unbiased bases. Numerical results on a certain class of isotropic state vectors suggest that their components, in any of those same mutually unbiased bases, exhibit a semicircular distribution when the dimension of the state space is large.

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W30 DCMP: Nanowires and Nanotubes: Optical Properties and Spectroscopy C147/154

11:15AM W30.00001 ABSTRACT WITHDRAWN –

11:27AM W30.00002 Low temperature electron transport spectroscopy of mechanically templated carbon nanotube quantum dots[1] , SAIFUL KHONDAKER, University of Central Florida, PAUL STOKES, UNIVERSITY OF CENTRAL FLORIDA TEAM — We report on the low temperature electronic transport measurements of mechanically templated carbon nanotube quantum dots (QDs). The devices were fabricated by precise dielectrophoretic placement of single walled carbon nanotubes (SWNTs) between 1 μm spaced Pd electrodes and over a local Al/Al_2O_3 bottom gate. The local gate defines the quantum dot due to the bending of SWNT at the edges of the gate, as well as controls its operation [1]. We performed detailed transport spectroscopy measurements of the templated SWNT QDs to determine how the tunnel barriers evolve with both the global back gate and local gate voltage. We will present models to explain the evolution of these devices as a function of local gate and back gate voltage. This study may allow for future size tunabiliy of SWNT QDs by further control over the tunnel barrier transparency and source, drain, and gate capacitance to fabricate room temperature single electron transistors.

[1] Paul Stokes and Saiful I. Khondaker, Appl. Phys. Lett. **92**, 262107 (2008).

[1]This work is supported by the U.S. National Science Foundation under Grant ECCS-0748091 (CAREER).

11:39AM W30.00003 Tunneling spectroscopy using carbon nanotubes quantum dots[1] , YANJING LI, NADYA MASON, University of Illinois — Tunneling spectroscopy is an important measurement technique, encompassing, for example, planar tunneling, scanning tunneling microscopy and superconducting tunnel probes. Here, we demonstrate that carbon nanotube quantum dots (QDs) can be used as tunneling probes. The sharp features in the density of states of the QDs in the Coulomb blockade regime can map out the density of states and the energy distribution function of the system to be studied. We present preliminary data showing tunneling from a carbon nanotube quantum dot into mesoscopic metal wires that have been driven out of equilibrium by a bias voltage. Previous measurements of these systems using superconducting probes [1-2] showed that the electron energy distribution functions and electron interactions can be determined. With the present measurements, the use of a QD instead of a superconductor allows us to probe at significantly higher temperatures and biases.

[1] H. Pothier, S. Gueron, Norman O. Birge, D. Esteve, and M. H. Devoret, Phys Rev Lett 79, 3490 (1997)
[2] Yung-fu Chen, Travis Dirks, Gassem Al-Zoubi, Norman O. Birge, and Nadya Mason, Phys Rev Lett 102, 036804 (2009)

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

11:51AM W30.00004 Photoconductivity Spectroscopy of Colloidal Lead Selenide Nanowires , RION GRAHAM, KA LEUNG, DONG YU, UC Davis — PbSe, with a large Bohr exciton radius of 46 nm, is ideally suited to study strong quantum confinement effects. Photoconductivity spectroscopy of single PbSe nanowire devices can remove the inhomogeneous broadening of ensemble measurements and allows for extraction of fine electronic structures in two dimensionally confined semiconductors. We have grown PbSe nanowires via a colloidal, oriented attachment mechanism, with diameters down to 6nm. Using a tunable wavelength laser, we have measured photoconductivity of single nanowire field effect transistors (FETs) as a function of excitation energy, temperature, and nanowire diameters.

12:03PM W30.00005 The optical properties of SnO_2 nano-wires by THz time-domain spectroscopy , DONGWOOK LEE, Nanyang Technological University, XINGQUAN ZOU, CHUANWEI CHENG, SARITHA K. NAIR, HONGJIN FAN, ELBERT E.M. CHIA — As feature seizes of devices are reduced below a hundred nanometers and chip frequencies reaches high GHz, a convenient method of characterizing thin films in the GHz to THz frequency range has been required. THz time-domain spectroscopy provides a non-destructive, non-contact, and high-sensitive tool to characterize thin films as well as nano-materials. The optical properties of SnO_2 nano-wires, which were grown on z-cut quartz, have been investigated by THz time-domain spectroscopy. The real and imaginary parts of the complex refractive index and optical conductivity are measured at THz frequency.

12:15PM W30.00006 Direct mapping of the exciton-polariton dispersion in tree-like ZnO micro-structures[1] , XIANGSHUN LU, Dept. of Physics, Univ. of Arkansas, HUAJUN ZHOU, Z. RYAN TIAN, Dept. of Chemistry and Biochemistry, MIN XIAO, Dept. of Physics, Univ. of Arkansas — We report a direct observation of branches of the exciton polaritons in tree-like ZnO micro-structures using second-harmonic generation (SHG) spectroscopy. Within the tunable range of a mode-locked Ti:Sapphire laser with pulse width of 100 femto-second, we are able to tune the second harmonic energy of the incident laser across the A, B and C excitons of ZnO. Under the resonant enhancement of the strong coupling between photons and excitons, we obtain for the first time the direct mapping of the branches of exciton-polariton dispersion at the room as well as liquid nitrogen temperatures. We also observed strong modulation of the polariton spectra by the whispering-gallery modes (WGMs) formed inside the tree-like micro-structure. The disappearance of the SHG in tree-like ZnO near/above the energy of the excitonic band gap indicates the much higher efficiency of energy conversion, comparing to the simple ZnO rod, and reveal the practical and important applications of the tree-like micro-structures in solar cell.

[1]We thank the partial funding support from NSF/MRSEC.

12:27PM W30.00007 Optical anisotropy of transparent multiwalled carbon nanotube sheets , JULIA BYKOVA, University of Texas at Dallas, Richardson, Texas, YAKOV LESNICHII, ALEKSEY ARSENIN, DMITRY FEDYANIN, Moscow Institute of Physics and Technology, Moscow, Russia, JONATHON SMITH, University of Texas at Dallas, Richardson, Texas, WILLIAM HOLMES, Solarno Inc., Irving, Texas, ANVAR ZAKHIDOV, University of Texas at Dallas, Richardson, Texas; Solarno Inc., Irving, Texas — Replace this text with your abstract body. The oriented carbon nanotube (CNT) sheets absorb polarized light anizotropically depending on its relative orientation to the incident light. Oriented aerogel of multi-walled carbon nanotubes (MWNT) created by dry-drawing of spinnable CNT forests has been shown to be a relatively good polarizer [1] even at high temperatures [2]. In this presentation it is shown how the qualitative factor of polarization (QFP) depends on the CVD synthesis conditions and CNT sheets process. The optimized QFP of MWNT sheet is found to be 2-3 times higher than reported before for CNT-based polarizers. Systematic characterization by UV-Vis spectroscopy, elipsometry combined with SEM showed how the polarization properties can be improved by annealing, stretching and electrical field, which enhance the anisotropy of MWCNT sheets. This work is supported by AFOSR grant FA 9550-09-10384 and AFRL/Rice grant via CONTACT consortium of Texas. [1] M. Zhang et al., Science, 309 (2005) 1215 [2] A. Aliev at al. Phys Let A, 372 (2008) 4938

12:39PM W30.00008 Synthesis and Optical Properties of Free Standing Titania Nanotubes Arrays for Photovoltaic and Photocatalytic Applications , DALMAU REIG-I-PLESSIS, MOHAMED ABD ELMOULA, EUGEN PANAITESCU, DONALD HEIMAN, LATIKA MENON, Northeastern University — Titanium oxide nanostructures, nanotubes arrays in particular, are key components for several emerging technologies, notably dye sensitized solar cells and supported gold nanoparticle catalysts. Free standing nanotube ordered arrays were produced by anodization of titanium foil in non-aqueous solutions. For optical measurement purposes the arrays were flaked off the titanium substrate. Flakes as large as several square centimeters, with a thickness of 30-50 μm were obtained, and coated either with N719 dye, or with gold nanoparticles (2-7nm). Both annealed (crystalline) and non-annealed (amorphous) samples were characterized by means of SEM and TEM imaging coupled with EDS and XRD spectroscopy. Subsequent optical measurements on gold decorated nanotubes offered insight on the gold-titania interaction, while measurements on both naked and dye coated tubes provided information on diffraction and thin film effects. These effects caused a significant wavelength dependent difference in the reflection spectrum depending on whether illumination was incident on the open or closed side of the tubes.

12:51PM W30.00009 Electro-Optic Effects in Colloidal Dispersion of Metal Nano-Rods with Nematic Ordering[1] , OLEG D. LAVRENTOVICH, Liquid Crystal Institute, Kent State University, ANDRII B. GOLOVIN, JIE XIANG, HEUNG-SHIK PARK, LUANA TORTORA, YURIY A. NASTISHIN, SERGIJ V. SHIYANOVSKII, Liquid Crystal Institute, Kent State University — In modern transformation optics, one explores metamaterials with properties that vary from point to point in space and time, suitable for applications in devices such as an "optical cloak" [1] and an "optical black hole" [2]. We propose an approach to construct spatially varying and switchable metamaterials that are based on colloidal dispersions of gold (Au) nano-rods (NRs) in dielectric fluids [3], in which dielectrophoretic forces, originating in the electric field gradients, create spatially varying configurations of aligned NRs. We quantify the electric field induced orientational order and concentration distribution of Au NRs and the describe the ensuing optical effects. We demonstrate that the gradient electric-field induces a nematic birefringent phase in the toluene dispersions of AuNR and determine how the refractive indices change in space. [1] W. Cai, U.K. Chettiar, A.V. Kildishev, V.M. Shalaev, Nature Phot. **1**, 224 (2007); [2] E.E. Narimanov, A.V. Kildishev, Appl. Phys. Lett. **94**, 041106 (2009); [3] A.B. Golovin, O.D. Lavrentovich, Appl. Phys. Lett. **95**, 254104 (2009).

[1]AFOSR FA9550-10-1-0527, DOE DE-FG02-06ER46331

1:03PM W30.00010 Measurement of carrier lifetimes in silicon vapor-liquid-solid wires , BRIAN BRYCE, Cornell University, MARK REUTER, BRENT WACASER , IBM Thomas J. Watson Research Center, SANDIP TIWARI, Cornell University — Minority carrier lifetimes are critically important to many semiconductor devices. For example, optimal photovoltaic design is almost completely dependent on knowledge of carrier lifetimes. We have extended traditional microwave photoconductance methods for use on aggregated films of nanowires. Using these methods we have measured the carrier lifetimes of both gold and aluminum catalyzed silicon vapor-liquid-solid wires in the 100-800 nm range. This approach allows for rapid characterization of wire quality prior to device design and fabrication.

1:15PM W30.00011 Exciton dynamics for single walled carbon nanotubes in the presence of a single ion , BENJAMIN TAYO, SLAVA ROTKIN, Lehigh University — We study the dynamics of excitons in single walled carbon nanotubes in the presence of a single ion placed on the surface of the tube. The scattering process is described in three main stages. First, we solve the Schrödinger equation in the tight binding approximation to calculate the quasiparticle wave functions and energies. Second, we use quasiparticle wave functions and energies in the Bethe-Salpeter equation to calculate exciton binding energies and wave functions. Finally, we use the exciton energies and wave functions to investigate the process of exciton-ion scattering. We model the potential of the single ion by that of a point charge. Our studies show exciton trapping in the presence of the ion.

1:27PM W30.00012 The emissivity of an incandescent carbon nanotube[1] , B.C. REGAN, SCOTT SINGER, MATTHEW MECKLENBURG, EDWARD WHITE, UCLA Department of Physics and Astronomy, and CNSI — A classical thermal emitter has physical dimensions large compared to the wavelength λ of the emitted light, and radiates power in proportion to its surface area. To explore the non-classical limit, we build tiny incandescent lamps with individual multi-walled carbon nanotubes as their filaments. We image a filament with atomic resolution in a transmission electron microscope, determining its length L and radius r. Separately we apply Joule heating to reach temperatures ~ 2000 K, where the nanotube radiates in the visible ($L \sim \lambda \gg r$), and collect the light with an optical microscope. Comparing the filament's brightness with its tiny physical dimensions, we find that a single carbon nanotube is surprisingly black.

[1]Supported by NSF CAREER award #0748880.

1:39PM W30.00013 Polarized Light Emission from a Single Hot Carbon Nanotube[1] , S.B. SINGER, MATTHEW MECKLENBURG, EDWARD WHITE, B.C. REGAN, UCLA Department of Physics and Astronomy, and CNSI — We fabricate nanoscale lamps, incandescent in the visible, which have a filament consisting of a single multiwall carbon nanotube. The radius r of the nanotube is much smaller than the wavelength λ of the emitted light, making it a very unusual thermal emitter. Transmission electron microscopy is used to determine the nanotube's axis as well as the parameters of the tube's geometry. We image both light polarizations on a CCD camera simultaneously and observe a degree of polarization between 70% and 85% along the tube's axis at visible wavelengths–highly polarized, yet less so than is expected for a conducting antenna. Furthermore, the polarization's variation with wavelength trends opposite to that predicted by classical models and analogy with graphene.

[1]Supported by NSF Career Award #0748880.

1:51PM W30.00014 Photoconductivity of complexes of chrysotile with tetra(4-sulfonatophenyl) porphyrins created via ionic self-assembly[1] , WESLEY CHU, WALTER SMITH, Haverford College, YE LU, A.T. JOHNSON, University of Pennsylvania, GIOVANNA DE LUCA, LUIGI SCOLARO, Università di Messina — Tetrakis(4-sulfonatophenyl) porphine (TPPS4) molecules form complexes with chrysotile nanotubes in a chloroform-methanol solvent; the self-assembly is driven by Coulombic attractions. The UV/vis absorption spectrum indicates J-aggregation. In AFM, the complexes appear as straight, long tubes when deposited onto oxidized silicon substrates. Preliminary experiments conducted in a dry nitrogen atmosphere (0.2% oxygen concentration) show that the aggregates are photoconductive. When illuminated for long periods at 428 nm, the photoconductivity grows slowly, and there is also a growth of persistent photoconductivity. These observations are similar to those for nanorods self-assembled from TPPS4 (without chrysotile),[2] though the current levels are much lower in the chrysotile complexes.

[1]This work is supported by NSF grant CHE-0616615.
[2]C. K. Riley et al., *J. Phys. Chem. C* **2010**, 114, 19227–19233.

2:03PM W30.00015 A confinement phase in carbon nanotubes as captured by the extended massive Schwinger model , TAKASHI OKA, HIDEO AOKI, The University of Tokyo — We propose that the strong-coupling excitons in carbon nanotubes with electric fluxes confined in one dimension can be a condensed-matter candidate for a confinement phenomenon. Namely, we show that the system, with the Coulomb interaction proportional to $|x|$, is in a confinement phase with many properties similar to QCD in 4D. Low-energy physics is described by the massive Schwinger model with multi-species fermions labelled by the band and valley indices. We propose two means to detect this. One is an optical measurement of the exciton spectrum, where the confinement phase should be hallmarked by an absence of continuous component in the exciton spectrum. The spectrum is actually calculated with the 't Hooft-Berknoff equation utilizing the light-front field theory, where the Gell-Mann-Oakes-Renner relation is shown to be satisfied by dark excitons. The second way is through the nonlinear transport, which is shown to be related to Coleman's "half-asymptotic" state. (arXiv:1007.5393)

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W31 GERA: Energy Production & Distribution, Nuclear, Hydrogen, Bio and Infrastructure C145

11:15AM W31.00001 Phonon dynamics of UO_2 at high temperature[1] , J.W.L. PANG, ORNL, A. CHERNATYNSKIY, U. Florida, B.C. LARSON, ORNL, S.R. PHILLPOT, U. Florida, W.J.L. BUYERS, Can. Inst. for Adv. Res. — Inelastic neutron scattering and numerical simulations are being used to investigate the fundamental aspects of phonons and thermal transport in UO2 as part of a DOE-EFRC "Center for Materials Science of Nuclear Fuel" project. Understanding thermal transport associated with nuclear fuel environments requires a correct accounting for a wide range of phonon scattering processes, including anharmonic phonon-phonon, phonon-fission product, and phonon-defect cluster. Reactor and spallation neutron measurements of phonon dispersion, phonon linewidths and density of states in UO_2 at room and high temperature are in progress for direct comparison with atomic potential lattice-dynamics simulations of phonon dispersion, phonon group velocity, phonon linewidth, and phonon density of states. Direct comparisons between experimental measurements and numerical simulations in UO_2 as a function of temperature will be presented.

[1]Research supported as part of the Center for Materials Science of Nuclear Fuel, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science

11:27AM W31.00002 An *Ab Initio* Study of α –Pu[1] , SARAH C. HERNANDEZ, ASOK K. RAY, University of Texas at Arlington — Hybrid density functionals, which replace a fraction of density functional theory exchange with exact Hartree-Fock exchange has been used to study the electronic, geometric, and magnetic properties of α – Pu. Different fractions of Hartree-Fock exchange have been used and the computations have been performed using the all-electron full-potential linearized augmented plane wave plus local orbitals basis method. Pu has been studied at the non-magnetic, ferromagnetic and anti-ferromagnetic configurations with spin-orbit coupling, orbital polarization, and *full* geometry optimizations. The variations of the optimized lattice constants, magnetic moments, bulk moduli, density of states, and the degree of $5f$ electron localization with the amount of Hartree – Fock exchange will be reported. Results will be compared with those of δ – Pu for which the performance of the hybrid functionals did *not* seem superior to that of the pure density functionals.[2]

[1]This work is partially supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525) and by the LSAMP-BD Program.
[2]R. Atta-Fynn and A. K. Ray, Europhys. Lett. 85, 27008 (2009).

11:39AM W31.00003 Electron Correlation and Tranport Properties in Nuclear Fuel Materials[1] , QUAN YIN, KRISTJAN HAULE, GABRIEL KOTLIAR, Rutgers University, SERGEY SAVRASOV, WARREN PICKETT, University of California, Davis — Using first principle LDA+DMFT method, we conduct a systematic study on the correlated electronic structures and transport properties of select actinide carbides, nitrides, and oxides, many of which are nuclear fuel materials. Our results capture the metal–insulator Mott transition within the studied systems, and the appearance of the Zhang-Rice state in uranium dioxide. More importantly, by understanding the physics underlying their transport properties, we suggest ways to improve the efficiency of currently used fuels.

[1]This work is supported by the DOE Nuclear Energy University Program, contract No. 00088708.

11:51AM W31.00004 Reaction Rate Measurement at the Californium User Facility (CUF) for unfolding the neutron spectrum[1] , MOHAMMAD HANNAN, RUBEN ORTEGA, The University of Texas- Pan American — Neutron Activation Analysis was used to determine Reaction Rate measurement of several activation detectors at the ORNL Californium User Facility (CUF). The irradiations were performed with 34 mg Cf^{252} neutron source strength.. Ten source capsules $>$ 34 mg were positioned concentrically around a sample cavity. We have determined absolute activity per atom of 9 detectors: Au^{197} (n,γ) Au^{198}, Al^{27}(n,α)Na^{24}, Al^{27}(n,p) Mg^{27}, Fe^{56}(n,p) Mn^{5}, Fe^{54}(n,p) Mn^{54}, In^{115} (n,γ)In^{116}, Ti^{46}(n,p)Sc^{46}, Ni^{60} (n,p) Co^{60}, Fe^{58}(n,γ) Fe^{59}. The errors are within 1.5-8% except Ni^{60} and Fe^{58} have errors of 46% and 32 %. These high errors may be attributed to the counting statistics. These reaction rate values will be used to unfold the neutron spectrum of the CUF using the MAXED 2000, a computer code for the de convolution of multi sphere neutron spectrometer data and the results are discussed.

[1]The authors acknowledge help, advise, and using facility at ORNL-CUF to Dr. Rodger martin and Mr. David C. Galsgow

12:03PM W31.00005 A first-principles investigation of III-V semiconductor-water interfaces for solar hydrogen production , BRANDON WOOD, TADASHI OGITSU, ERIC SCHWEGLER, LLNL — Photoelectrochemical devices promise sustainable hydrogen production using sunlight and water. Currently, the highest efficiency devices use III-V semiconductor photoelectrodes; however, stability of these materials under operating conditions remains an issue. In an effort to understand the chemical properties of the electrode-water interface, we have performed first-principles molecular dynamics simulations on model III-V surfaces in realistic aqueous environments. The structure, stability, and chemical activity of these surfaces are investigated, with the aim of understanding the reactive states precursory to photoexcitation and hydrogen evolution. Our results show that surface oxide nucleation is key to facilitating surface reactivity, and that the surface oxygen bonding arrangement is important for determining of the available pathways for water dissociation and corrosion. This points to the importance of III-V surface oxides as intermediates in the water-dissociation component of hydrogen evolution. Prepared by LLNL under Contract DE-AC52-07NA27344.

12:15PM W31.00006 Hydrogen Generation and Photoelectrochemical Effect of InGaN alloys , KRISHNA ARYAL, BED PANTHA, RAJENDRA DAHAL, JING LI, JINGYU LIN, HONGXING JIANG, Texas Tech University — Generation of hydrogen gas, a clean source of energy with the highest conversion efficiency, via water splitting, using renewable resources has attracted tremendous research work in recent years. For producing hydrogen gas, a promising method using semiconductor materials is direct photoelectrolysis by solar water splitting. $In_xGa_{1-x}N$ alloys grown by metal organic chemical vapor deposition (MOCVD) are very promising candidates for water splitting because of their direct band gap which can be tuned to the entire solar spectrum through band gap engineering. It was found that n-GaN has a higher photocurrent density (J_{ph}) at zero bias, while an InGaN alloy provides much higher hydrogen generation rate (R_H) with a small external bias. R_H of about 0.024 mL/min.cm^2 was obtained using an $In_{0.18}Ga_{0.82}N$ as working electrode. The characteristics of time dependent J_{ph} for a prolonged period of time (up to 7 days) showed higher chemical stability of the InGaN electrodes in aqueous solution of HBr.

12:27PM W31.00007 Sieving hydrogen based on its high compressibility , HANGYAN CHEN, DEYAN SUN, Department of Physics, East China Normal University, Shanghai, China, XINGAO GONG, Department of Physics, Fudan University, Shanghai, China, ZHIFENG LIU, Department of Chemistry and Center for Scientific Modeling and Computation, Chinese University of Hong Kong, Hong Kong, China — Based on carbon nanotube intramolecular junction and a C60, a molecular sieve for hydrogen is presented. The small interspace between C60 and junction provides a size changeable channel for the permselectivity of hydrogen while blocking Ne and Ar. The sieving mechanism is due to the high compressibility of hydrogen.

12:39PM W31.00008 ABSTRACT WITHDRAWN —

12:51PM W31.00009 Combining micro-structures and micro-algae to increase lipid production for bio-fuel , SAURABH VYAWAHARE, EMILLY ZHU, TROY MESTLER, ANDRÉ ESTÉVEZ-TORRES, ROBERT AUSTIN, Physics Department, Princeton University, Princeton NJ 08544 — 3rd generation bio-fuels like lipid producing micro-algae are a promising source of energy that could replace our dependence on petroleum. However, until there are improvements in algae oil yields, and a reduction in the energy needed for processing, algae bio-fuels are not economically competitive with petroleum. Here, we describe our work combining micro-fabricated devices with micro-algae *Neochloris oleoabundans*, a species first isolated on the sand dunes of Saudi Arabia. Inserting micro-algae of varying fitness into a landscape of micro-habitats allows us to evolve and select them based on a variety of conditions like specific gravity, starvation response and Nile Red fluorescence (which is a marker for lipid production). Hence, we can both estimate the production of lipids and generate conditions that allow the creation and isolation of algae which produce higher amounts of lipids, while discarding the rest. Finally, we can use micro-fabricated structures and flocculation to de-water these high lipid producing algae, reducing the need for expensive centrifugation and filtration.

1:03PM W31.00010 Structure and diffusion of furans and other cellulose-derived compounds in solvents via MD simulation , BROOKS RABIDEAU, AHMED ISMAIL, RWTH Aachen University, Aachen, Germany — There is now a large push towards the development of energy sources that are both environmentally friendly and sustainable; with the conversion of cellulose derived from biomass into biofuels being one promising route. In this conversion, a variety of intermediary compounds have been identified, which appear critical to successful expansion of the process to an industrial scale. Here we examine the structure and diffusion of these furans and acids derived from cellulose within ionic liquids via molecular dynamic simulation. Ionic liquids have shown the ability to dissolve cellulose with certain 'green' benefits over existing, conventional solvents. Specifically, we study the solvation properties of these chemicals by examining the pair correlation functions of solute with solvent, and by exploring the agglomeration and separation of these chemicals from the solvent as well as the hydrogen bonding between species. Additionally, we determine the diffusion constant of these compounds in ionic liquid and aqueous solvents.

1:15PM W31.00011 Molecular-dynamics study of proton transport near an ionomer-electrode interface[1] , PHILIP TAYLOR, ELSHAD ALLAHYAROV, Case Western Reserve University — Coarse-grained molecular-dynamics simulations have been used to study the behavior of an ionomer electrolyte in response to an induced current. We observe the changes in the distribution of charge concentration and local electrostatic field in the region near an electrode in contact with a Nafion-like ionomer. We have also analyzed how the morphology of the sulfonate clusters and the transport of water molecules depends on the current strength. In this study we insert protons at the electrode interface of the material and remove them at a plane some distance into the material. When a steady state is achieved we note the new charge distribution and average voltage difference between the faces of the simulation cell. We also note the change in distribution of water molecules within the material in response to the induced current of protons. We compare these results with those predicted by one-dimensional theoretical models.

[1]Work supported by DOE Grant DE-FG02-05ER46244

1:27PM W31.00012 Origin of colossal ionic conductivity in YSZ/STO multilayers , TIMOTHY PENNYCOOK, MARK OXLEY, Vanderbilt Univ., Oak Ridge National Laboratory, MATTHEW BECK, Vanderbilt Univ., JAVIER GARCIA-BARRIOCANAL, FLAVIO BRUNO, CARLOS LEON, JACOBO SANTAMARIA, Complutense Univ., Madrid, MARIA VARELA, Oak Ridge National Laboratory, STEPHEN PENNYCOOK, Oak Ridge National Laboratory, Vanderbilt Univ., SOKRATES PANTELIDES, Vanderbilt Univ., Oak Ridge National Laboratory — A colossal eight order of magnitude increase in the ionic conductivity of yttria- stabilized zirconia (YSZ) near room temperature was recently reported in YSZ/strontium titanate (STO) epitaxial heterostructures [1]. We present density functional theory results that explain the enhancement in terms of strain- and interface-induced disorder of the YSZ O-sublattice [2]. We further present experimental confirmation of O disorder using a combination of scanning transmission electron microscopy and electron energy loss spectroscopy. The O K-edge fine structure shows blurred-out features indicative of disorder [3]. Atomic-resolution elemental mapping clearly resolves the O sublattice in the STO but is blurred out in the YSZ, indicating disorder. This work is supported by DOE grant DE-FG02-09ER46554 and DOE Materials Sciences and Engineering Div. 1 J. Garcia-Barriocanal et al. Science 321, 676 (2008); 2 T.J. Pennycook et al., Phys. Rev. Lett. 104, 115901 (2010); 3 T.J. Pennycook et al., European Phys. J.

1:39PM W31.00013 Microscopic Understanding of Reactivity of Clinkers for Green Cement , ENGIN DURGUN, HEGOI MANZANO, ROLAND J. M. PELLENQ, JEFFREY C. GROSSMAN, Massachusetts Institute of Technology — Cement is the cause of up to 10 percent of global CO2 emissions, and yet, while it is one of the most common materials in use, we have remarkably little understanding of its microscopic properties. Toward this end, we use quantum mechanical simulations to examine the electronic properties and structure of cement crystals and to understand the surface reactivity of various clinker phases. Using these results, our aim is to clarify the mechanisms of cement dissolution, which is the initial stage of hydration and also one of the key processes that leads to the need for high temperature/energy manufacturing. As a first step we modeled the crystal structure of two major clinker phases, alite and belite and analyzed both electronic and mechanical properties. Next, we cleaved the clinker crystal in the simulation along different symmetry directions in order to obtain a prediction of the most stable surfaces. Dissolution occurs at the surface so accurate determination of the surface pattern is crucial. Using the computed surface energies, we can predict the full structure of the clinker nanocluster. This allows us to examine the interaction of water molecules with different nanocluster phases, in order to shed light on the dissolution mechanism and use this new understanding to predict possible novel routes for modifying and controlling the dissolution reactions.

1:51PM W31.00014 Comparison of Solar and Wind Power Output and Correlation with Real-Time Pricing[1] , KATHRYN E. HOEPFL, ALVIN D. COMPAAN, Dept. of Physics & Astronomy, University of Toledo, ANDREW SOLOCHA, Dept. of Finance, University of Toledo — This study presents a method that can be used to determine the least volatile power output of a wind and solar hybrid energy system in which wind and solar systems have the same peak power. Hourly data for wind and PV systems in Northwest Ohio are used to show that a combination of both types of sustainable energy sources produces a more stable power output and would be more valuable to the grid than either individually. This method could be used to determine the ideal ratio in any part of the country and should help convince electric utility companies to bring more renewable generation online. This study also looks at real-time market pricing and how each system (solar, wind, and hybrid) correlates with 2009 hourly pricing from the Midwest Interconnect.

[1]KEH acknowledges support from the NSF-REU grant PHY-1004649 to the Univ. of Toledo and Garland Energy Systems/Ohio Department of Development.

2:03PM W31.00015 Monte Carlo optimization of a matrix-based power-grid islanding algorithm , IBRAHIM ABOU HAMAD, PER ARNE RIKVOLD, Physics Department, Florida State University, SVETLANA V. POROSEVA, Mechanical Engineering Department, University of New Mexico — Spectral matrix methods are widely used for intelligent intentional islanding of power grids, the purposeful partitioning of a utility system to limit cascading disturbances. However, these methods may produce unbalanced islands of generators and loads when applied recursively. While some of the resulting islands have surplus generating capacity, others are deficient. We here implement a Monte Carlo simulated-annealing optimization procedure to load-balance the islands and increase their internal connectivity or modularity. After a matrix-based initial agglomeration of nearby loads and generators, Monte Carlo is used to redistribute loads among neighboring islands. The resulting network of islands is treated as a new network with the first-generation islands as the new nodes ("supergenerators" and "superloads"), and the same agglomeration and MC procedures are iteratively applied. We show here that combining matrix-based agglomeration and Monte Carlo methods results in well balanced, internally connected islands.

Thursday, March 24, 2011 11:15AM - 1:27PM –

Session W32 FIAP DCOMP: Focus Session: Frontiers in Computational Thermodynamics of Materials I C144

11:15AM W32.00001 Modeling the interactions of adsorbates with each other and with metal surfaces , JOHN KITCHIN, Carnegie Mellon University — The interactions of molecules with metallic surfaces are fundamental to the ability of metals to catalyze reactions. One often thinks of a metal like platinum as the catalyst, but under reaction conditions the reactivity of the metal surfaces is modified by the molecules that adsorb on them. We have used quantum chemical calculations in conjunction with cluster expansions to probe the adsorption behavior of atomic adsorbates such as C, N, O, and S on late transition metal surfaces such as Rh, Ir, Pd, Pt, Cu, Ag, and Au(111). There are remarkable similarities in the adsorption behavior of these adsorbates that can be interpreted in terms of a simple adsorbate-induced surface electronic structure modification mechanism that is common to all the adsorbates and surfaces. The variations between the adsorbates and metals are readily explained in terms of the size of the metal and adsorbate orbitals and the geometry dependent overlap of these orbitals. We have constructed a new Solid State Table of these orbital radii from the quantum chemical calculations that can be used in conjunction with a simple model to rapidly estimate the electronic structure of metal and alloy surfaces with adsorbates on them.

11:51AM W32.00002 An Automatic Symmetry-Leveraging Approach for Solving Incomplete Many-Atom Crystal Structures , BRYCE MEREDIG, CHRIS WOLVERTON, Northwestern University — We present a new first principles-based method, called a symmetry-leveraging genetic algorithm (SLGA), for fully and automatically solving large crystal structures when experimental diffraction studies do not identify all internal atomic positions. Such incomplete structural refinements may occur when crystals contain light atoms or when the characterization is performed under extreme conditions such as high pressure. We apply our method to solve the crystal structure of the promising hydrogen storage candidate magnesium imide (MgNH), which has remained a mystery for over 40 years. We also confirm *via* a fully automated procedure a recent specialized "by hand" prediction for the high-pressure phase of ammonia borane, NH_3BH_3. The MgNH prediction, which involves 36 atoms and a notoriously complex configuration space, to the best of our knowledge represents the largest-ever crystal structure solution derived from first-principles calculations without making simplifying assumptions about atom connectivity. The 32-atom NH_3BH_3 prediction is nearly as demanding. Our approach, which takes full advantage of existing experimental information to solve for structural unknowns, has great potential for completing thousands of partially determined crystal structures.

12:03PM W32.00003 Finite Temperature Lattice Vibrations and the Magnetic Structure of Fe and Ni[1] , G. MALCOLM STOCKS, Oak Ridge National Laboratory, YANG WANG, Pittsburgh SuperComputer Center, ROGER STOLLER, Oak Ridge National Lab., AURELIAN RUSANU, University of Tennessee, MARKUS EISENBACH, DONALD NICHOLSON, GERMAN SAMOLYUK, Oak Ridge National Lab. — Modern *ab initio* theories of the magnetic phase transition (Curie Temperature, T_C) of Fe and Ni based on the Disordered Local Moment (DLM) type models generally rely on (constrained) density functional theory calculations performed at 0K and assume that the atoms occupy their equilibrium lattice sites. Here we point out that finite temperature lattice vibrations can result in large fluctuations in the local moments associated with individual site beyond those already accounted for in these approaches. These conclusions are based on large cell ($\sim 10^4$ – atoms) *ab initio* calculations of the magnetic state of Fe and Ni based on the O[N] Locally Self-consistent Multiple Scattering (LSMS) method. Atom positions are obtained from freezes of individual time steps of molecular dynamics simulations based on classical interaction potentials. Calculations are performed for a range of temperatures up and beyond T_C that illustrate the extent of the moment fluctuations. We discuss the consequences of these findings for the adequacy of existing theories T_C.

[1]Work supported by the Center for Defect Physics in Structural Materials (CDP), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

12:15PM W32.00004 Combined Experimental and Theoretical Studies of Core-Shell Nanostructures in Al-Sc-Li Alloys , COLIN OPHUS, ABHAY GAUTAM, Lawrence Berkeley National Lab, EMMANUELLE MARQUIS, University of Michigan, VELIMIR RADMILOVICH, ULRICH DAHMEN, Lawrence Berkeley National Lab, MARK ASTA, University of California, Berkeley — We have used two aging treatments of Al-Li-Sc alloys to create highly monodisperse, coherent $L1_2$ structure core-shell precipitates. We perform detailed analyses of the compositional distributions in the precipitate structures with electron microscopy and atom probe tomography. By combining this information with first principles calculations and Monte Carlo simulations based on the cluster expansion formalism, we compute bulk and interfacial thermodynamic properties relevant to precipitate formation. We specifically focus on understanding how the presence of Li modifies the nucleation rate relative to that of pure Al3Sc precipitates.

12:27PM W32.00005 New structures in Pd-rich ordered alloys[1] , JACQUELINE CORBITT, GUS HART, Brigham Young University - Provo — An intriguing intermetallic structure with 8:1 stoichiometry was discovered in the 1950s in the Pt-Ti system. Since then, a handful of other Pt/Pd/Ni binary systems have been observed to exhibit this curious structure (e.g., Pt_8Zr, Pd_8Mo, Ni_8Nb, etc). This ordered structure can significantly increase the hardness of an alloy by forming precipitates. Recent calculations and experiments suggest that the 8:1 structure may form in about 20 previously unsuspected Pt/Pd binary systems. Using first-principles calculations, cluster expansion, Monte Carlo modeling, we have explored possible precipitate hardening (via the 8:1 structure) in Pd-Nb, Pd-Mg and Pd-Cu.

[1]Supported by NSF ACI Fellow Award DMR-0908753

12:39PM W32.00006 Pseudo-Random Number Generation for Brownian Dynamics and Dissipative Particle Dynamics Simulations on GPU Devices , CAROLYN PHILLIPS, JOSHUA ANDERSON, SHARON GLOTZER, University of Michigan — Brownian Dynamics (BD) and Dissipative Particle Dynamics (DPD) are implicit solvent methods commonly used in models of soft matter and biomolecular systems. The interaction of the numerous solvent particles with larger particles is coarse-grained as a Langevin thermostat is applied to individual particles or to particle pairs. The Langevin thermostat requires a pseudo-random number generator (PRNG) to generate the stochastic force applied to each particle or pair of neighboring particles during each time step. In a GPU parallel computing environment, small batches of random numbers must be generated over thousands of threads and millions of kernel calls. We introduce a PRNG scheme, in which a micro-stream of pseudorandom numbers is generated in each thread and kernel call. These high quality, statistically robust micro-streams are more computationally efficient than other PRNG schemes in memory-bound kernels, and uniquely enable the DPD simulation method . This scheme has been implemented in HOOMD-blue, a GPU-accelerated open-source general purpose molecular dynamics simulation package. By enabling BD and DPD to be performed in HOOMD-blue, a broad range of mesoscale coarse-grained simulations can now be accelerated in a massively parallel architecture.

12:51PM W32.00007 Efficient ab initio molecular dynamics using exact reweighting , VIDVUDS OZOLINS, University of California, Los Angeles, MARK ASTA, University of California, Berkeley — Density-functional theory (DFT) based *ab initio* molecular dynamics (AIMD) is a promising method for calculating high-temperature thermodynamic properties of solids and liquids. Nevertheless, computational expense associated with AIMD simulations has prevented general adoption of these methods. We show that substantial savings of computational effort can be realized by using less expensive (and less accurate) Hamiltonians to generate long MD trajectories and by recalculating statistically independent snapshots with high-accuracy DFT methods. A formally exact reweighting formula, based on the Jarzynski switching approach, is used to obtain thermal averages and thermodynamic properties in the high-accuracy DFT ensemble. If under-converged AIMD simulations with low energy cutoffs and coarse k-point meshes are used to generate trajectories, this approach can lead to savings of CPU time of a factor of 10 to 100, depending on the relevant correlations times. We also present extensions of the reweighting method to calculate impurity free energies and free energy barriers for interstitial diffusion. Robust methods for estimation of statistical errors based on random subsampling and variance extrapolation are discussed.

1:03PM W32.00008 Ab Initio Simulations of Hydrogen in Crystalline and Amorphous Metal Membranes , WILLIAM HUHN, MIKE WIDOM, Carnegie Mellon University — Solid metallic membranes are used to separate hydrogen from other gases for clean energy applications. In order to create cheaper, more effective membranes for hydrogen separation, it is desirable to model hydrogen transport through the membrane. Amorphous metal membranes in particular have potential for this type of application due to low expense and high theoretical hydrogen capacity. We computationally model hydrogen absorption and transport through materials in order to find materials that can be used to construct effective membranes for hydrogen capture. In this talk, we will obtain hydrogen binding sites and diffusion barriers in order to model the hydrogen diffusion through various nickel-based amorphous alloys and compare them to associated crystalline structures as well as elemental palladium, which is favored for this application despite its high expense. Ab initio methods (specifically the Vienna Ab Initio Simulation Package, VASP) are used to develop the hydrogen binding energy spectrum, from which thermodynamic models can be constructed. Kinetic Monte Carlo methods are used to model the hydrogen transport through the bulk, from which we can obtain the permeability.

1:15PM W32.00009 The enigmatic Ag-Pt phase diagram and yet another derivative structure algorithm , GUS L.W. HART, LANCE J. NELSON, RODNEY W. FORCADE, Brigham Young University — The Ag-Pt phase diagram as published in the most recent phase diagram compilations (Massalski, Pauling File) is entirely speculative below 1000° C. The phase diagrams and our calculations both suggest a stable $L1_1$ phase at 50 at.-% Pt. However, an experimental study published after the compilations supports a significantly different phase diagram. In this new phase diagram, the only stable phases at low temperatures are the elemental fcc Ag and Pt phases and one ordered phase at the unusual concentration of 53 ± 0.5 at.-% Pt. The experimental study shows that the homogeneity range for the ordered phase is narrow (almost like a line compound), and its X-ray data suggests that the unit cell of this phase contains 32 atoms with a stoichiometry of 15:17. We developed a new derivative structure enumeration algorithm specifically designed for large unit cells with known concentrations. This is necessary because our old algorithm enumerated all concentrations and was therefore limited to smaller unit cells. We have explored, via first-principles, the structural details of this enigmatic phase in the Ag-Pt phase diagram. I will discuss our first-principles results for Ag-Pt, and I will discuss the how the new algorithm is useful for large unit cells when partial structural information is known.

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W33 DCMP: Insulators and Dielectrics I C143/149

11:15AM W33.00001 An *Ab Initio* Study of $PuO_{2\pm0.25}$, $UO_{2\pm0.25}$, and $U_{0.5}Pu_{0.5}O_{2\pm0.25}$[1] , LI MA, ASOK RAY, University of Texas at Arlington — Hybrid density functional theory has been used to systematically study the electronic, geometric, and magnetic properties of strongly correlated materials $PuO_{2\pm x}$, $UO_{2\pm x}$, and $U_{0.5}Pu_{0.5}O_{2\pm x}$ with x=0.25. The calculations have been performed using the all-electron full-potential linearized augmented plane wave plus local orbitals basis (FP-L/APW+lo) method. Each compound has been studied at the ferromagnetic (FM) and anti-ferromagnetic (AFM) configurations with and without spin-orbit coupling (SOC) and *full* geometry optimizations. The optimized lattice constants, bulk moduli, and band gaps will be reported. Total energy calculations indicate that the ground states are AFM for all compounds studied here and the band gaps are typically higher than 1.0 eV, and characteristic of semiconductors. The total energy is lowered significantly and the band gaps increase with the inclusion of SOC. The chemical bonds between the actinide metals and oxygen atoms are primarily ionic in character.

[1]This work is partially supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525) and by the Department of Energy.

11:27AM W33.00002 Characterization of point defects in UO2 by positron annihilation spectroscopy: a first-principles study , MARC TORRENT, GERALD JOMARD, Commissariat a l Energie Atomique et Aux Energies Alternatives, Paris, France — abstract- Positron Annihilation Spectroscopy is a powerful experimental tool for probing defects in crystalline materials. The correct identification of defects with PAS requires the knowledge of accurate positron lifetimes for the various kinds of defects. That can be provided by numerical calculations in the framework of the Two-Component Density-Functional Theory. This method accurately treat on the same footing, the electrons and positron densities as well as the atomic structure. We have implemented this formalism within the Projector Augmented-Wave method in the ABINIT code, optimizing the electrons and positron densities self-consistently and calculating positron-induced forces accurately. That allows to properly determining the relaxed geometries of defects that trapped positron. We have applied the TC-DFT to various point defects in UO2. The use of the PAW method allows considering large super cells to simulate point defects, we have typically used cells that contain 32 UO2 unit formulas. We use the LDA+U framework in order to treat strong electronic correlations. This work is a first attempt to help for the interpretation of PAS experiments on UO2 but it seems really promising.-

11:39AM W33.00003 Effect of Dielectric Materials on the Topological Insulator Bi_2Se_3 Surface States , JIWON CHANG, LEONARD REGISTER, SANJAY BANERJEE, BHAGAWAN SAHU, Microelectronics Research Center, The University of Texas at Austin — We study the effects of crystalline dielectric materials on the electronic surface states of a strong topological band insulator (TI) Bi_2Se_3 using a density functional based electronic structure method [1]. We will discuss the sensitivity of Dirac point degeneracy and linear band dispersion of the TI with respect to different dielectric surface terminations as well as different relative atom positions of the dielectric and the TI. Both passivated and non-passivated substrate surfaces will be considered. Two representative dielectrics SiO_2 and boron nitride will be chosen to understand the physics of interplay of interface potential, linear band dispersion and the chemical environments of the TI surface states. Our findings have implications in interpreting experiments and designing novel nanoelectronics device concepts based on TIs.

[1] "Intrinsic and extrinsic perturbations on the surface states of topological insulator Bi_2Se_3," J. Chang, P. Jadaun, L. F. Register, S. K. Banerjee and B. Sahu (In preparation)

11:51AM W33.00004 First-Principles Investigation of Low Energy E' Center Precursors in Amorphous Silica , NATHAN ANDERSON, School of Materials Engineering, Purdue University, RAVI VEDULA, School of Electrical and Computer Engineering, Purdue University, PETER SCHULTZ, Sandia National Laboratories, RENEE VAN GINHOVEN, Pacific Northwest National Laboratory, ALEJANDRO STRACHAN, School of Materials Engineering, Purdue University — We show that oxygen vacancies are not necessary for the formation of E' centers in amorphous SiO2 and that a single O-deficiency can lead to two charge traps. Employing molecular dynamics with a reactive potential and density functional theory we generate an ensemble of stoichiometric and oxygen-deficient amorphous SiO2 atomic structures and identify low-energy network defects. Three-coordinated Si atoms appear in several low-energy defects both in stoichiometric and O-deficient samples where, in addition to the neutral oxygen vacancy, they appear as isolated defects. Various charge transition levels for each defect are also presented.

12:03PM W33.00005 Structure and energetics of ferroelectric domain walls in $LiNbO_3$ from atomic level simulations[1] , DONGHWA LEE, Lawrence Livermore National Laboratory, HAIXUAN XU, Oak Ridge National Laboratory, VOLKMAR DIEROLF, Lehigh University, VENKATRAMAN GOPALAN, Pennsylvania State University, SIMON PHILLPOT, University of Florida, UNIVERSITY OF FLORIDA TEAM, LEHIGH UNIVERSITY COLLABORATION, PENNSYLVANIA STATE UNIVERSITY COLLABORATION — Due to its unique ferroelectric and nonlinear optical properties, $LiNbO_3$ has a wide range of applications in optoelectronics and nonlinear optics. These unique properties of $LiNbO_3$ are, however, quite sensitive to point defects and ferroelectric domain walls. Therefore, detailed characterization of the ferroelectric domain walls and their interaction with the defects at atomistic scale is highly important The local structure and energetics of the ferroelectric domain walls in $LiNbO_3$ are examined using density functional theory (DFT) and atomistic-level simulation methods. The energetics and electric dipoles associated with the pertinent point defects and domain walls in $LiNbO_3$ are investigated in detail. In particular, the variation of polarization due to 180˚ ferroelectric domain walls, the coupling of defect-domain wall interactions and their effects on domain wall motion are discussed

[1]This work was supported by NSF under Materials World Network Grant Number DMR-0602986, DMR-0908718, and DMR-0820404.

12:15PM W33.00006 Study of Defects That Trap Excitons in Yttrium Aluminum Garnets Doped With Rare-Earth Elements[1] , FARIDA SELIM, CHRIS VARNERY, GARY COLLINS, DAVID MCKAY, SHERIF REDA, Washnigton State University — Excitons play a fundamental role in transporting energy in photonic materials. Understanding and controlling excitons dynamics through their interactions with activating impurities and lattice defects is key to improving scintillation and optical properties. Singles crystals of yttrium aluminum garnet (YAG) crystals doped with rare-earths were studied by positron annihilation, thermolunuinescence and optical spectroscopy. Evidence of defect complexes was found in the YAG structure. Positron lifetime measurements were performed to characterize those defects. Effects of dopants on the optical properties and lattice defects were investigated.

[1]NSF-DMR1006772

12:27PM W33.00007 Charge-Flow Regulation at Material Interfaces in Atomistic Models[1] , STEVEN VALONE, Los Alamos National Laboratory — An important class of materials problems of great interest consists of composites of metals and metal oxides. At sharp metal/metal oxide interfaces, the oxygen concentration is varying radically over short distances. For this reason, at the atomistic level, variable-charge atomistic models are required that control charge flow at these interfaces. Charge flow is controlled through chemical potential equalization among its constituents. Existing models of chemical potential, such as the Iczkowski-Margrave (IM) model, are linear in the charge as is appropriate for metals. Here a new, "fragment" model Hamiltonian is constructed at the atomistic level commensurate with the IM model, as opposed to the one-electron model Hamiltonians that underlie tight-binding and related methods. Essential properties of the fragment model Hamiltonian include an alternative charge dependence compared to the IM model, charge-flow regulation, absent in the IM model, preservation of a sense of covalent-ionic balance, and capture of important theoretical limits.

[1]Support from the Center for Materials at Irradiation and Mechanical Extremes, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number 2008LANL1026, is acknowledged.

12:39PM W33.00008 Infrared laser ablation of polystyrene from microseconds to picoseconds , RICHARD HAGLUND, SERGEY AVANESYAN, KENNETH SCHRIVER, Vanderbilt University, MALTE DUERING, BARRY LUTHER-DAVIES, Australian National University, HEE PARK, AppliFlex LLC, SINGARAVELU SENTHILRAJA, Old Dominion University, MICHAEL KLOPF, Jefferson National Acceleratory Facility, MICHAEL KELLEY, College of William and Mary — We describe experiments on both resonant and non-resonant infrared pulsed laser of polystyrene across time scales varying from microseconds to picoseconds for the purpose of determining the ways in which the rate of energy deposition changes the response of both the ablated material and the residual substrate. RIR-PLD has been shown to be a relatively low-temperature process leading to evaporation and deposition of intact molecules. We compare the characteristics of ablation craters and ablation plumes deposited by Nd:YAG and Er:YAG lasers, picosecond and nanosecond optical parametric oscillators, and two different infrared free-electron lasers with differing pulse profiles. The films were characterized by profilometry, digital optical microscopy, scanning electron microscopy, and Fourier-transform infrared spectroscopy. Based on the experiments and computational modeling, we discuss the constraints on laser parameters that produce non-destructive ablation by resonant infrared excitation.

12:51PM W33.00009 The effect of substrate temperature on the structure and morphology of titanium nitride compounds grown by DC magnetron sputtering , MOHAMMAD R. HANTEHZADEH, REZA BAVADI, Plasma Physics Research Center, Science and Research branch, Islamic Azad University — The TiN thin films were deposited on p-type silicon (100) substrates using reactive planar DC magnetron sputtering system. The target was 99.99% pure Ti. The reactive sputter gas was a mixture of Ar (99.999%) and N_2 (99.999%) with the ratio Ar (97%) and N_2(3%) by volume. Structural characterization of the coating was done using X-ray diffraction (XRD). The surface roughness of the coating was determined using an Atomic Force Microscope (AFM). The reflectivity of thin films was investigated by a spectrophotometer system. The X-ray diffraction measurements showed that by increasing the substrate temperature during the growth, change in crystalline structure will occur. The crystallite size of the films determined by Scherer's equation, and the crystallite size measured by AFM also increased by increasing the substrate growth temperature. The surface reflectivity measurements indicate that by increasing the substrate growth temperature, the optical properties of the films changes. The change in optical properties and crystalline structure of the films indicate that substrate growth temperature plays an important role in structure and morphology of the grown layers.

1:03PM W33.00010 Growth of Erbium doped Yttrium oxide thin films by atomic layer deposition , NICHOLAS BECKER, THOMAS PROSLIER, J. KLUG, J. ELAM, Argonne National Laboratory, T. SANAMYAN, M. DUBINCKII, J. GIROLAMI, M. PELLIN, Argonne National Laboratory — Er-doped Yttrium oxide (Er^{3+}:Y_2O_3) has gained recent attention for its possible use in optoelectronic devices. Here we report the use of atomic layer deposition (ALD) to synthesize thin films of Yttrium oxide with various doping levels of Erbium ions (Er^{3+}) using different chemistries. ALD uses self-limiting surface reactions to deposit highly conformal thin films over large areas and substrates of arbitrary shape. This allows for the uniform layered doping of Yttrium oxide with Er^{3+}. The spatial separation of the Erbium ions can be controlled using organometallic precursors with varying ligand sizes. The doping concentration (volume ratio of Er^{3+} sites to Y^{3+} sites) is controlled by the ratio of the precursor pulses. We comprehensively studied ALD-grown films of Er^{3+}:Y_2O_3 obtained from the Erbium precursors Er(MCp)$_3$ and Er(BA)$_3$ and the Yttrium precursors Y(MCp)$_3$ and Y(Cp)$_3$ using either water or hydrogen peroxide as an oxygen source. Detailed description of the studied optical and spectroscopic properties, stoichiometry, and physical characteristics of these films will be presented.

1:15PM W33.00011 Atomic Layer Deposition of AlOx for Metal-AlOx-Metal Trilayers and Resonators , A. KOZEN, L. HENN-LECORDIER, X. CHEN, M. SCHROEDER, University of Maryland, C. MUSGRAVE, University of Colorado, G. RUBLOFF, University of Maryland — The dielectric layer in conventional Josephson junction qubits is fabricated by thermal oxidation of aluminum. These dielectrics suffer from high loss tangents thought to be due to defect-related quantum two level systems. Our collaborators have identified the -OH rotor associated with hydroxyl species in the AlOx as a prime defect candidate. We demonstrate the fabrication of the AlOx dielectric in MIM structures using atomic layer deposition (ALD) from trimethylaluminum and both H2O and D2O precursors. ALD enables precise control of film growth at the atomic scale, while comparison of D2O vs H2O as the oxidation precursor should reveal the role of this defect in the loss tangent. We have developed the D2O based ALD process, observed similar kinetics and properties for D2O and H2O based ALD for AlOx, and characterized the materials by SIMS, XPS, and electrical measurements of MIM capacitor structures. Correlation between room temperature electrical measurements and low temperature resonator performance will be discussed.

1:27PM W33.00012 Improvements of Defect Analysis by Space-Charge Wave Spectroscopy[1] , KAY-MICHAEL VOIT, University of Osnabrueck, BURKHARD HILLING, HEINZ-JÜRGEN SCHMIDT, MIRCO IMLAU — We report on our recent advancements in space-charge wave spectroscopy, which can be used to investigate defect structures in classical high-resistive semiconductors and insulators. It permits to estimate the effective trap concentrations as well as the effective donor density N_{eff} and the product $\mu\tau$ of electron mobility and life-time in the conduction band. We present a novel method of space-charge wave excitation, using a superposition of a running and a static sinusoidal illumination pattern. Thus we acquire – in contrast to the former oscillating pattern – a distinct direction of movement. The proposed new technique can be regarded as an effective amelioration, as the theoretical analysis is no longer limited by numerous presumptions like low modulation depth or small oscillation amplitudes. It not only overcomes these limits of the experimental configuration improving accuracy of SCW spectroscopy, but it also provides additional information, such as the sign of the charge carriers.

[1]Financial support by the DFG within the graduate college 695 "Nonlinearities of Optical Materials" and the project IM 37/5-1 is gratefully acknowledged.

1:39PM W33.00013 First-principles studies of Ce and Eu doped inorganic scintillator gamma ray detectors[1] , ANDREW CANNING, ANURAG CHAUDHRY, Lawrence Berkeley National Laboratory, UC Davis, ROSTYSLAV BOUTCHKO, STEPHEN DERENZO, Lawrence Berkeley National Laboratory — We have performed DFT based band structure calculations for new Ce and Eu doped wide band gap inorganic materials to determine their potential as candidates for gamma ray scintillator detectors. These calculations are based on determining the 4f ground state level of the Ce and Eu relative to the valence band of the host as well as the position of the Ce and Eu 5d excited state relative to the conduction band of the host. Host hole and electron traps as well as STEs (self trapped excitons) can also limit the transfer of energy from the host to the Ce or Eu site and therefore limit the light output. We also present calculations for host hole traps and STEs to compare the energies to the Ce and Eu excited states.

[1]The work was supported by the U.S. Department of Homeland Security and carried out at the Lawrence Berkeley National Laboratory under U.S. Department of Energy Contract No. DE-AC02- 05CH11231

1:51PM W33.00014 Novel Approaches in Energy Conversion by Molecular Charge Transfer from Diamond Surfaces[1] , FRANZ A.M. KOECK, Arizona State University, JEFF SHARP, Marlow Industries, Inc, ROBERT J. NEMANICH, Arizona State University — Vacuum thermionic energy conversion is based on electron transfer from a hot emitter across a vacuum gap to the collector. Our approach for an efficient emitter utilizes nanostructured, negative electron affinity doped diamond films. With a low effective work function of less than 1.3 eV thermionic emission commences at 260 C and observes the law of Richardson – Dushman with a significant emission current $>$ 5 mA at 500 C. Pairing this emitter with a similar collector results in a potential across the gap and introduction of an ohmic load establishes a current indicative of energy conversion. Utilizing ionization processes of gaseous species at the emitter surface can enhance inter-electrode charge transfer and increase output power. In the ionization process an electron is trapped in an occupied molecular orbital establishing a negative ion state. The electron affinity and negative ion binding energy determines stability of the transient negative species, and we present results for H2 and CH4. As these species are introduced in the inter-electrode gap an increase in output power is observed with a concurrent shift of maximum output power to lower load resistance.

[1]This research is supported by the Office of Naval Research.

2:03PM W33.00015 Diamond Based Electron Emitters for Photon Enhanced Thermionic Energy Conversion[1] , TIANYIN SUN, FRANZ A. KOECK, ROBERT J. NEMANICH, Arizona State University — Energy conversion cells utilize either direct photon illumination or indirect thermal energy for electron excitation. Nitrogen-doped, hydrogen terminated nanocrystalline diamond films display a negative electron affinity and have shown low temperature thermionic emission which can be employed for energy conversion in a vacuum thermionic emission cell. However, the low work function of such films suggests that the current could be enhanced through visible light illumination to induce photoelectron emission. We present measurements of the spectrum of emitted electrons from N-doped diamond films for light illumination between 600 and 340nm, while the film is heated from ambient to 500C. Features due to thermionic and photo-emission are identified, and a complex interaction is observed between the two processes at various temperatures and illumination wavelengths. The results indicate the potential application of diamond emitters as combined thermal and photon energy converters, and we present a new approach to enhance the performance of diamond-film energy converters.

[1]This research is supported through the Office of Naval Research.

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W34 DMP: Focus Session: Optical Properties of Nanocrystals C141

11:15AM W34.00001 Evolution of CdSe/ZnS Quantum Dot Ensembles Under Prolonged Excitation[1] , GEORGIY SHCHERBATYUK, RICHARD INMAN, SAYANTANI GHOSH, University of California, Merced — We study the spectral evolution of self-assembled ensembles of CdSe/ZnS core/shell quantum dots (QDs) under photo-excitation in ambient conditions. We use spatially-resolved photoluminescence (PL) scanning microscopy in conjunction with spectrally-resolved time-resolved spectroscopy to measure variations in spectral intensity, emission wavelength and recombination lifetimes. Our results indicate that the spectral intensity of the ensemble undergoes both photo-induced brightening and darkening, and these rates have a complicated dependence on the concentration of the QD samples. They initially decrease with decreasing concentration but are greatly enhanced in the dilute limit. The photo-exposure also causes a rapid spectral red-shift followed by a slow blue-shift. The recombination lifetimes increase with the red-shift for all concentrations but do not correlate to the blue-shift in a straightforward manner in different samples. We conclude the possible explanation of this behavior is the inter-play of photo-induced surface trap discharging and preferential photo-oxidation of the smaller QDs in the ensemble.

[1]This work was supported by NSF DMR.

11:27AM W34.00002 Photoluminescence spectroscopy and lifetime measurements from self assembled semiconducting quantum dot- metal nanoparticle hybrid arrays , M. HARIDAS, J.K. BASU, Indian Institute of Science — We demonstrate how the emission properties of a hybrid array consisting of semiconducting quantum dot (QD) and metal nanoparticles (NP) can be controlled by varying the density and distance between QD and NP independently. Our hybrid system consists of chemically synthesized cadmium selenide quantum dots (CdSe QDs) and polymer capped gold nanoparticles (Au NP) embedded in a block copolymer matrix having the topology of cylinders oriented perpendicular to the substrate. We have prepared hybrid arrays with two different densities of CdSe QDs (ρ_{QD}) each having same Au NP densities (ρ_{Au}). The photoluminescence measurements (PL) from such hybrid system shows enhancement in emission with increase in ρ_{Au}, compared to the CdSe QD film and the enhancement factor is lower for hybrid films with high ρ_{QD}. The lifetime measurement shows double exponent PL decay with systematic reduction in exciton lifetime for hybrid arrays with respect to ρ_{Au}. The film with high ρ_{QD} shows larger reduction in lifetime. Similarly, the amplitudes of the two relaxations switch over with increase in ρ_{Au}. It is clear that the shorter time becomes the dominant relaxation mode with increasing ρ_{Au}. Observed phenomena have been explained in terms of exciton plasmon interaction.

11:39AM W34.00003 Manipulating coupling between a single semiconductor quantum dot and single gold nanoparticle[1] , FARBOD SHAFIEI, DANIEL RATCHFORD, SUENNE KIM, XIAOQIN LI, Department of Physics, University of Texas at Austin, STEPHEN GRAY, Chemistry Division and Center for Nanoscale Materials, Argonne National Laboratory — We report the manipulation of coupling in a simple model system, a single semiconductor quantum dot (QD) near a single metallic nanoparticle, and study the resulting changes in QD photoluminescence (PL) dynamics. We used atomic force microscopy nanomanipulation to controllably push a Au NP proximal to a CdSe/ZnS QD. We observed gradual and reversible changes in the QD PL lifetime and blinking dynamics. In some cases, the total lifetime reduced from 30 ns to well below 1 ns. This decrease is accompanied by the disappearance of blinking behavior as the nonradiative energy transfer from QD to the Au NP becomes the dominant decay channel. In comparison to previous studies, our experiments report changes in the PL dynamics of the same QD, therefore, eliminating the ambiguity of variable properties of individual QDs.

[1]Support: NSF, ONR, Welch Foundation, AFOSR, and the Alfred P. Sloan Foundation

11:51AM W34.00004 Carbon Nanotube CdSe Nanoparticle Hybrid Materials: Synthesis and Optical Properties , AUSTIN AKEY, CHENGUANG LU, IRVING P. HERMAN, Columbia University — Carbon nanotubes present remarkable opportunities as a base for construction of advanced nanomaterials with uniques properties. We report novel heterostructures composed of single-walled carbon nanotubes and monodisperse cadmium selenide nanoparticles (3.5 to 6 nm in diameter). The optical properties of the hybrid material differ significantly from those of the unbound nanoparticles and nanotubes, pointing to the existence of strong electronic/optical interaction effects between the two. Specific differences in absorption/emission behavior and the photoluminescence Stokes shift in the nanoparticles will be presented, along with experiments exploring the underlying mechanisms of this interaction. We believe this system exhibits "hot" excitation-transfer behavior from the nanoparticles to the nanotubes, which makes it of great interest for photovoltaic applications. This work is primarily supported by the Nanoscale Science and Engineering Center at Columbia University, which is supported by the Nanoscale Science and Engineering Initiative of the NSF under Award Number CHE-0641523.

12:03PM W34.00005 Enhanced Optical Absorption of Glancing Angle Deposited Semiconducting Nanostructures for Photovoltaic Solar Cell Applications , HILAL IS, MEHMET CANSIZOGLU, Department of Applied Science, University of Arkansas at Little Rock, Little Rock, AR, 72204, MIRIA FINCKENOR, NASA Marshall Space Flight Center, AL 35812, TANSEL KARABACAK, Department of Applied Science, University of Arkansas at Little Rock, Little Rock, AR, 72204 — Semiconducting nanostructures with controlled geometries can provide enhanced optical absorption and effective collection of photo-charges for high efficiency photovoltaic solar cells and photoconductive devices. Glancing angle deposition (GLAD) provides a unique capability of producing nanostructured arrays of various materials with controlled shapes, size, and separation. In this study, as a model system, we fabricated arrays of semiconducting indium sulfide nanostructures by GLAD in the shapes of springs, screws, rods, and zigzags. We show that GLAD nanostructures have significantly lower reflectance and higher optical absorption compared to conventional flat thin films. In addition, we observed a superior photoconductivity (PC) response of about 80% for nanorod array samples, which is believed to be mainly due to their high optical absorption. On the other hand, PC response was less than 1% for conventional thin films of indium sulfide.

12:15PM W34.00006 In-Situ Studies of Photoluminescence Quenching in Single Crystal Quantum Dot Sensitized Solar Cells , DOUGLAS SHEPHERD, Department of Physics, Colorado State University, YONG-QI LIANG, School of Energy Resources, University of Wyoming, JUSTIN SAMBUR, Department of Chemistry, Colorado State University, BRUCE PARKINSON, School of Energy Resources, University of Wyoming, MARTIN GELFAND, Department of Physics, Colorado State University, ALAN VAN ORDEN, Department of Chemistry, Colorado State University — Single crystal quantum dot sensitized solar cells (QDSSC) are a promising photovoltaic system in which collection of multiple charge carriers per photon has recently been reported.[1] Utilizing time-correlated single photon counting we have studied both the fluorescence intensity and fluorescence decay time from CdSe quantum dots coupled to both single crystal TiO_2 and ZnO substrates through short and long chain ligands. We find that for all configurations the fluorescence decay time is quenched compared to unbound quantum dots in solution, while the photovoltaic properties of the system strongly depend on the chain-length of the ligand. These results suggest there exist interactions between either the individual quantum dots or the quantum dots and substrate that may compete with the charge injection process in QDSSCs.

[1]Justin B. Sambur, Thomas Novet, B.A. Parkinson, *Science* **330** (6000) 63-66

12:27PM W34.00007 Particle Morphology and Interfacial Energy Transfer in CdSe/CdS Nanocrystals , NICHOLAS BORYS, MANFRED WALTER, University of Utah, JING HUANG, DMITRI TALAPIN, University of Chicago, JOHN LUPTON, University of Utah — CdSe/CdS core-shell nanocrystal heterostructures are unique systems to study nanoscale energy migration. We perform single-particle excitation spectroscopy at low temperatures by monitoring both the luminescence intensity and energy of the core as a function of optical excitation energy in three different heterostructure shapes: spherical particles, rods, and tetrapods. In the tetrapod and rod structures, the shapes of the PLE spectra fall into one of two classes while the spherical particles all exhibit one universal form, which we attribute to the general shape and quantum confinement symmetry of the CdS shell. We confirm this assignment by correlated single particle SEM and PLE measurements. By resolving the core emission energy as a function of excitation energy, we identify two distinct exciton species in the tetrapods indicating the presence of a barrier that prevents charge transfer across the heterostructure interface [1].

[1] Borys et al., Science (in press)

12:39PM W34.00008 Copper-doped core-shell ZnSe/CdSe nanocrystals with efficient and widely tunable photoluminescence , RANJANI VISWANATHA, SERGIO BROVELLI, VICTOR I. KLIMOV, Chemistry Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545 — We report synthesis and spectroscopic studies of Cu-doped ZnSe/CdSe nanocrystals (NCs) with a wide range of shell thicknesses. Incorporation of copper ions into the NCs introduces an atomic-like state within the NC band gap. This results in a three-level system in which emission occurs due to the transition coupling the NC lowest-energy conduction-band level to the localized hole state associated with the Cu ions. Cu is incorporated into the NC core while the shell remains nominally undoped, which allows us to manipulate the shell thickness (and thus emission color) without affecting the overall level of NC doping. We demonstrate a wide-range spectral tunability of photoluminescence (PL) (from 3.1 eV to 1.25 eV), and "giant" Stokes shifts ($\sim$ 0.8 eV), which reduce emission losses due to reabsorption. We show that hole trapping at the Cu sites occurs primarily from the top of the valence band (i.e., no hot-hole transfer processes are detected) and that the main nonradiative mechanism is electron trapping at surface defects, which can be suppressed at cryogenic temperatures, resulting in PL quantum yields of $\sim$40%. High intrinsic emission efficiencies, wide-spectral tunability, and a large Stokes shift make these novel NCs attractive candidates for radiation detection, light-emitting diodes, and lasers.

12:51PM W34.00009 Breakdown of Volume Scaling in Auger Recombination in CdSe/CdS Heteronanocrystals: The Role of the Core-Shell Interface , SERGIO BROVELLI, FLORENCIO GARCÍA-SANTAMARÍA, RANJANI VISWANATHA, HAN HTOON, SCOTT CROOKER, VICTOR I. KLIMOV — Spatial confinement of electronic excitations in semiconductor nanocrystals (NCs) results in a significant enhancement in nonradiative Auger recombination (AR) of multiexcitons, which is detrimental to promising NC lasing applications. In standard NCs, AR times scale linearly with NC volume. We investigate multiexciton dynamics in NCs composed of CdSe cores and CdS shells of tunable thickness. Thicker shells dramatically reduce AR, particularly during initial shell growth, which cannot be explained by traditional volume scaling alone. Rather, low-temperature fluorescence-line-narrowing studies strongly suggest that suppressed AR derives primarily from the formation of an alloy layer at the CdSe/CdS interface, and a corresponding "smoothing" of the confinement potential (CP). These findings support the recent theory, which predicts that the change from abrupt to smoothly-varying CPs reduces the high-spatial-frequency Fourier components of the exciton wave function, thereby minimizing overlap with the high-energy states involved in nonradiative Auger decay. Our results highlight the importance of NC interfacial structure in the AR process in zero-dimensional NCs and provide general guidelines for the design of new nanostructures with suppressed AR for future lasing applications.

1:03PM W34.00010 Complete suppression of Blinking and convergence to a single emissive state in giant nanocrystal quantum dots , ANTON MALKO, SIDDHARTH SAMPAT, The University of Texas at Dallas, Department of Physics, YOUNG-SHIN PARK, JAVIER VELA, YOUNGFEN CHEN, JENNIFER HOLLINGSWORTH, VICTOR KLIMOV, HAN HTOON, Los Alamos National Laboratory, Chemistry Division and Center for Integrated Nanotechnologies — We report a systematic study of photoluminescence (PL) emission intensities and lifetimes of individual core-shell CdSe/CdS "giant" nanocrystal quantum dots (gNQDs) as a function of the shell thickness. We observed a complete suppression of blinking for gNQDs overcoated with more than 16 monolayers (ML) of CdS shell. An analysis of the photon emission statistics reveals a highly super-Poissonian distribution for thin shell (4-12 ML) gNQDs and near perfect Poissonian distribution for non-blinking, thick-shell gNQDs. Measurements of PL decay rates as a function of PL intensity show that while PL lifetimes vary continuously with PL intensity for thin-shell gNQDs, only one PL decay constant is observed for the thicker shell gNQDs. This result clearly indicates that while the thin-shell gNQDs possess continuous distribution of emission states, PL of the non-blinking, thick-shell gNQDs originates from a single emissive state.

1:15PM W34.00011 A comparative study of carrier multiplication in PbS and PbSe nanocrystals[1] , JOHN STEWART, LAZARO PADILHA, DOH LEE, BISHNU KHANAL, JEFFREY PIETRYGA, VICTOR KLIMOV, Los Alamos National Laboratory — In this talk I will present our recent studies of carrier multiplication (CM) in PbS and PbSe nanocrystals (NCs). CM is a process in which absorption of a single photon produces multiple excitons. In our experiments, we evaluate its efficiency based on the amplitude of the Auger decay signature of multiexcitons in carrier dynamics recorded using both transient absorption and time-resolved photoluminescence. In the case of PbSe NCs, we have measured the CM quantum efficiencies and Auger lifetimes for a large range of NC sizes, including very large particles with a band gap around 0.5 eV. Using excitation at 3.1eV we observe that the quantum efficiency is low for small NCs and increases monotonically toward the bulk value for larger dots. Despite many apparent similarities in the band structure of PbSe and PbS NCs, our preliminary studies of PbS nanoparticles hint at a quite different spectral behavior of quantum efficiencies compared to PbSe NCs. In particular, while the quantum efficiencies are similar for smaller NCs, we see discrepancies for the larger NCs for which the energy gap approaches the bulk limit. We discuss these discrepancies in the context of our comparative studies of intraband relaxation and Auger recombination in these two types of the NCs.

[1]Center for Advanced Solar Photophysics

1:27PM W34.00012 Carrier recombination pathways in Copper Indium Sulfide (CIS) nanocrystals , ANSHU PANDEY, LIANG LI, JEFFREY M. PIETRYGA, VICTOR I. KLIMOV — Ternary and Quaternary compounds are rapidly gaining interest because of potential applications in areas such as thin-film photovoltaics and light-emitting diodes. We will discuss carrier dynamics in Copper Indium Sulfide (CIS) nanocrystals (NCs), one of the better studied members of the ternary-quaternary family. While as-prepared CIS NCs exhibit photoluminescence (PL) quantum yields less than 10%, overgrowth with a few monolayers of CdS or ZnS increases PL quantum efficiency to more than 80%. We investigated the reasons for this dramatic improvement in efficiency through time-resolved PL and transient absorption measurements. Our results suggest that while electrons in CIS NCs remain delocalized, the holes are rapidly localized due to trapping at defects. PL emission arises through the radiative recombination of a delocalized electron with a hole at the interior defect site (radiative decay center). We also observe surface defects that serve primarily as centers for nonradiative recombination. Overcoating of CIS NCs with CdS or ZnS eliminates surface traps and results in a long single-exponential PL decay that appears to be unique among visible-emitting NCs.

1:39PM W34.00013 Nonradiative Energy Transfer in Assemblies of Nanostructures with Mixed Dimensionality , PEDRO LUDWIG HERNANDEZ-MARTINEZ[1], HILMI VOLKAN DEMIR[2], Department of Physics, Department of Electrical and Electronics Engineering, UNAM, Bilkent University, Ankara 06800, Turkey — We study the exciton-exciton interaction and nonradiative energy transfer in nanostructure assemblies with mixed dimensionality. We investigate possible combinations in terms of dimensionality for these nanostructures, and analyze the resulting nonradiative energy transfer rates as a function of dimensionality. Depending on the direction of the energy transfer, arrangements of such nanostructures have potential applications in both photovoltaics [1] and light generation [2].

[1] J. Sambur, et al., "Multiple Exciton Collection in a Sensitized Photovoltaic System", Science 330, 63 (2010).
[2] R. Yan, et al., "Nanowire Photonics," Nature Photonics, 3, 569-576 (2009).

[1]UNAM - National Nanotechnology Research Center and Institute of Material Science and Nanotechnology, Bilkent University

[2]Physics and Applied Physics Division, School of Physical and Mathematical Sciences, Microelectronics Division, School of Electrical and Electronics Engineering, Nanyang Technological University, Singapore 639798, Singapore

1:51PM W34.00014 Charge and Shape Effects on the Carrier Dynamics of 25 Atom Au Nanoclusters , MATTHEW SFEIR, Brookhaven National Laboratory, HUIFENG QIAN, RONGCHAO JIN, Carnegie Mellon University — We study a series of semiconducting gold clusters that exhibit strong quantum confinement effects on their optical properties. In contrast to larger metallic nanoparticles, the surface plasmon resonance disappears a large optical gap ($>$ 1.3 eV) is formed. Recent synthetic advances have permitted the study of truly monodisperse clusters with precise control on the atomic scale. Using femtosecond and nanosecond transient absorption spectroscopy, we have investigated the excited state relaxation dynamics of spherical and prolate 25 atom isomers. We have determined that these particles exhibit long excited state lifetimes and that the carrier dynamics that are strongly influenced by the charge state and the physical arrangement of the atoms.

2:03PM W34.00015 Transparent Conducting Metallic Film for Applications in Photovoltaics and Optoelectronic Devices , TRILOCHAN PAUDEL, PIOTR PATOKA, WEN-CHEN CHEN, MICHAEL GIERSIG, WILLIE PADILLA, ZHIFENG REN, KRIS KEMPA — Oxides such as Indium-Tin Oxide (ITO) known as transparent conducting oxide (TCO) have been used for a long time in most of the thin film solar cell fabrications. It simultaneously works as an electrically conducting and optically transparent electrode. However, the electrical conductivity and optical transparency are not good enough. Here, we discuss our experimental and simulated results on nanostructured metallic films as a possible alternative replacement to TCO. This structure may possibly outperform the conventional ITO for applications in photovoltaics and optoelectronic devices such as LEDs.

Thursday, March 24, 2011 11:15AM - 2:15PM –
Session W35 DCMP: Topological Insulators: Superconductivity C140

11:15AM W35.00001 New forms of superconductivity and magnetism in a doped topological insulator , L. ANDREW WRAY, Lawrence Berkeley National Lab, SUYANG XU, Princeton University, HSIN LIN, Northeastern University, M. ZAHID HASAN, Princeton University — Topological insulators achieve a phase of matter characterized by the quantum topology of electron kinetics rather than by broken symmetries. The topological insulator state gives rise to spin-helical surface states that dramatically alter the surface physics and allow new phenomena in the presence of purturbations such as superconductivity and magnetism. We have used angle resolved photoemission spectroscopy to map electron dynamics at the surface of a topological insulator in the presence of magnetic surface ions and with doping compositions that superconduct. Our measurements establish that bulk Cu-doped $Cu_{0.12}Bi_2Se_3$ realizes a new form of superconductivity (Wray et al, Nat. Phys. 6, 855 (2010)) and is likely to host localized non-Abelian Majorana fermions on the crystal surface. We observe that surface-deposited ions lead to the formation of new topoligically-derived surface Dirac bands, and our data suggest that magnetic moments of deposited Fe undergo a phase transition to align along the out-of-plane axis (arXiv:1009.6216).

11:27AM W35.00002 Coupling superconductors to topological insulators , MENNO VELDHORST, MARCEL HOEK, MARIEKE SNELDER, Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, the Netherlands, XIAOLIN WANG, Institute for Superconducting and Electronic Materials, University of Wollongong, Wollongong, NSW, Australia, HANS HILGENKAMP, ALEXANDER BRINKMAN, Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, the Netherlands — The recent discovery of the topological insulators sparked an enormous attention. The experimental investigation of topological insulators with surface sensitive spectroscopic techniques evidently exposed the helical Dirac fermions living at the surface of a bulk insulator. In transport experiments, intrinsic bulk conduction challenges the observation of the topological surface states. We have observed electrical transport through the surface states of Bi_2Te3 by utilizing the electrical field effect and by utilizing intrinsically transparant interfaces to metallic electrodes. Of particular interest is coupling topogical insulators to superconductors, where at the interface the elusive Majorana fermion is predicted to recide. We fabricated superconductor – topological insulator – superconductor Nb-Bi_2Te_3-Nb junctions and observed a supercurrent over a length scale of more than a micrometer. Shapiro steps appear under microwave irradiation. The supercurrent is found to be surprisingly robust in large magnetic fields.

11:39AM W35.00003 Stability of surface Majorana modes in superconducting doped topological insulators , ASHVIN VISHWANATH, PAVAN HOSUR, POUYAN GHAEMI, ROGER MONG, University of California at Berkeley — In recent years, several model condensed matter systems have been predicted to harbor Majorana fermion zero modes. One such system is the surface of a strong topological insulator with proximity-induced superconductivity. A vortex in this surface superconductor was shown to host a topologically protected Majorana mode. Since then, bulk superconductivity has been induced in several strong topological insulators via doping or application of pressure. Here, we address the question of whether a vortex in these superconductors will trap Majorana zero modes at the surface. Viewed as a 1D system, the vortex can be characterized by a Z_2 topological invariant which denotes the presence or absence of a Majorana mode at its end. For weak pairing, we find that, the transition point between the two topological phases is determined by a Fermi surface property in the normal state. Hence, the phase transition can be achieved by simply varying the Fermi level. At the transition, the vortex supports gapless Majorana excitations along its length. Using this criterion, we discuss whether surface Majorana modes exist in the experimentally established superconductors $Cu_x Bi_2Se_3$, p-doped $TlBiTe_2$ and $Pd_x Bi_2Te_3$. Interestingly, the Fermi surface criterion also allows superconducting vortices in systems with non-topological band structures to be associated with surface Majorana modes.

11:51AM W35.00004 Surface Spectral Function in the Superconducting State of a Topological Insulator[1] , TING-KUO LEE, LEI HAO, Academia Sinica, Taiwan — We discuss the surface spectral function of superconductors realized from a topological insulator, such as the copper-intercalated Bi_2Se_3. These functions are calculated by projecting bulk states to the surface for two different models proposed previously for the topological insulator. Dependence of the surface spectra on the symmetry of the bulk pairing order parameter will be discussed with particular emphasis on the odd-parity pairing. Exotic spectra like an Andreev bound state connected to the topological surface states will be presented.

[1]We wish to acknowledge the support of NSC under Grant No. 98-2112-M-001-017-MY3.

12:03PM W35.00005 Superconductivity in Topological Parent Compound Induced via Pressure[1] , C.Q. JIN, Institute of Physics, CAS, China, J.L. ZHANG, S.J. ZHANG, H.M. GONG, W. ZHANG, P.P. KONG, J. ZHU, R.Z. YU, L.X. YANG, S.M. FENG, Q.Q. LIU, X.C. WANG, R.C. YU, Institute of Physics, Chinese Academy of Sciences, China, W.G. YANG, L. WANG, HPSync, APS, ANL, USA, S.C. ZHANG, Department of Physics, Stanford University, USA, X. DAI, Z. FANG, Institute of Physics, Chinese Academy of Sciences, China — We report successful observation of pressure induced superconductivity in topological compound of Bi_2Te_3 single crystal induced via pressure [1]. The combined high pressure structure investigations with first-principles calculations indicated that the superconductivity occurs at the ambient phase of topologically nontrivial. The results suggest topological superconductivity can be realized in the parent state of Bi_2Te_3 topological material. Ref: [1] J. L. Zhang et al., "Pressure induced superconductivity in the parent compound of Bi_2Te_3" (submitted)..

[1]This work is supported by NSF & MOST of China through research projects.

12:15PM W35.00006 Detecting Majorana Bound States , COLIN BENJAMIN, Univ. of Georgia, Athens, GA, USA, JIANNIS PACHOS, Univ. of Leeds, UK — We propose a set of interferometric methods on how to detect Majorana bound states induced by a topological insulator. The existence of these states can be easily determined by the conductance oscillations as function of magnetic flux and/or electric voltage. We study the system in the presence and absence of Majorana bound states and observe strikingly different behaviors. Importantly, we show that the presence of coupled Majorana bound states can induce a persistent current in absence of any external magnetic field.

12:27PM W35.00007 Chain of Majorana States from Superconducting Dirac Fermions at a Magnetic DomainWall , TITUS NEUPERT, Condensed Matter Theory Group, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland, SHIGEKI ONODA, AKIRA FURUSAKI, Condensed Matter Theory Laboratory, RIKEN, Wako, Saitama 351-0198, Japan — We study theoretically a strongly type-II s-wave superconducting state of two-dimensional Dirac fermions in proximity to a ferromagnet having in-plane magnetization. It is shown that a magnetic domain wall can host a chain of equally spaced vortices in the superconducting order parameter, each of which binds a Majorana-fermion state. The overlap integral of neighboring Majorana states is sensitive to the position of the chemical potential of the Dirac fermions. Thermal transport and scanning tunneling microscopy experiments to probe the Majorana fermions are discussed.

12:39PM W35.00008 Global Properties of 3D Topological Insulator Surface/Superconductor Junctions , MATTHEW GILBERT, Department of Electrical and Computer Engineering, University of Illinois, 1406 W. Green St., Urbana IL 61801, TAYLOR HUGHES, CHING-KAI CHIU, Department of Physics, University of Illinois, 1110 West Green St., Urbana IL 61801, ANDREI BERNEVIG, Department of Physics, Princeton University, Princeton, NJ 08544 — The ability to precisely find and manipulate non-Abelian anyons[1] has long been sought after as a potential means for the realization of robust quantum information processing. The simplest of these particles, Majorana fermions, have been predicted to exist in a new class of materials commonly referred to as topological insulators[2] when they are coupled with s-wave superconducting contacts.[3] This proposal is the focus of intense experimental research whose aim is to prove the existence of Majorana fermions trapped at the surface of topological insulators paired with superconductors. We will present our initial theoretical investigations into the surface properties of 3D topological insulator/superconductor junctions.

[1]A. Kitaev, *Ann. Phys (N.Y.)* **303**, 2 (2003).
[2]B. A. Bernevig and S. C. Zhang, *Phys. Rev. Lett.* **96**, 106802 (2006).
[3]L. Fu and C. L. Kane, *Phys. Rev. Lett.* **100**, 096407 (2008).

12:51PM W35.00009 Order parameter and triplet correlations near a superconductor-topological insulator interface , MAHMOUD LABABIDI, ERHAI ZHAO, George Mason University — At the interface between a 3D topological band insulator and an s- wave superconductor forms a remarkable 2D superconductor that can host Majorana fermions at vortex cores. Going beyond the original work of Fu and Kane [Phys. Rev. Lett. 100, 096407 (2008)], we present a microscopic theory for the proximity effect near the TI-S interface. We compute the superconducting order parameter as a function of the distance away from the interface by self-consistently solving the Bogoliubov-de Gennes equation. We discuss the suppression of the order parameter by the topological insulator. Moreover, we show that triplet superconducting correlations of $p_x \pm ip_y$ orbital symmetry are induced near the interface by the spin-orbit coupling inside the topological insulator.

1:03PM W35.00010 Superconductivity and Majorana fermion creation at the quantum spin Hall insulator edge , ANNICA M. BLACK-SCHAFFER, NORDITA — We focus on properties related to Majorana fermion creation in a self-consistent study of a microscopic interface between a quantum spin Hall insulator (QSHI) and a superconductor (SC). For a spin-singlet s-wave SC we show that large odd-in-momentum, or p-wave, order parameters exist for all doping levels of the QSHI and that they can be related to different spinless Cooper pair amplitudes. This result demonstrates that it is natural that the Majorana mode at a SC-ferromagnet (SF) interface survives even at zero doping. Despite the induced p-wave order parameters, the induced superconducting gap in the QSHI always retains its s-wave character, thus validating the commonly used effective model for superconductivity in a topological insulator. We also self-consistently model an SFS Josephson junction along the QSHI edge and report on Majorana mode occurrence in the junction, the current-phase relation, and novel odd-frequency spin-triplet correlations.

1:15PM W35.00011 Measurements of Electrical Noise at the Interface between Bi2Se3 and a Superconductor , J.S. LEE, D.M. ZHANG, A.R. RICHARDELLA, NITIN SAMARTH, Physics Dept., Penn State University, University Park PA 16802 — The narrow band gap semiconductor Bi_2Se_3 is a promising candidate for exploring exotic quantum states that might arise at the interface between topological insulators and superconductors (Phys. Rev. Lett. **100**, 096407 (2008)). Motivated by proposed approaches for detecting such states (Phys. Rev. B **79**, R161408 (2009)), we have embarked on measurements of electrical noise in mesoscopic Bi_2Se_3 devices with superconducting electrodes. Present measurements focus on CVD-grown Bi_2Se_3 nanoribbons which show proximity-induced superconductivity below ~ 5 K when contacted by (dirty) W electrodes. The measurements are carried out using a balanced bridge technique over a temperature range of $0.5\mathrm{K} \leq \mathrm{T} \leq 40$ K and in magnetic fields up to 80 kOe. We observe 1/f noise over a wide range of temperature and discuss the variation in noise spectral density across the normal-superconductor transition as well as its dependence upon excitation current and magnetic field. We will also describe extensions of these studies to mesoscopic devices lithographically patterned from thin films of Bi_2Se_3 grown by molecular beam epitaxy. Supported by NSF and ONR.

1:27PM W35.00012 Study of the interface of superconductor and topological insulator , DONG QIAN, XIAOMEI WANG, CHUNLEI GAO, CANHUA LIU, JINFENG JIA, Shanghai Jiao Tong University — State-of-art Molecular beam epitaxy (MBE) has been carried out to grow high quality topological insulator (TI) films on some BCS s-wave superconductor (SC) substrates. The growth dynamics and the electronics structures of the SC/TI interface were studied using high energy reflected electron diffraction and ultralow-temperature scanning tunneling microscopy (STM). Electronic structure, superconducting gap, vortex dynamics would be reported in this presentation. The superconducting state of the topological insulator due to approximate effect and the formation of Majorana Fermion would be discussed.

1:39PM W35.00013 Self-consistent study at the superconductor-3D topological insulator interface , XIAOTING ZHOU, CHEN FANG, JIANGPING HU, Purdue University — We perform a theoretical study of the interface between a 3D topological insulator (TI) and an s-wave conventional superconductor (both in normal and superconducting state) using the BdG self-consistent formulation. The robustness of the TI surface state when in contact with a metal is discussed and the topological superconductivity on the interface induced by the proximity effect is studied in detail. We find that in general a mixed singlet and triplet pairing can be observed on the interface as the spin-orbit coupling breaks the SU(2) symmetry in TI. The Majorana edge states of such a mixed pairing 2D topological superconductor are also studied.

1:51PM W35.00014 Proximity induced superconductivity in Bi_2Se_3 nanoribbons , D.M. ZHANG, J. WANG, J.S. LEE, H.R. GUTIERREZ, M.H.W. CHAN, N. SAMARTH, Physics Dept., Penn State University, University Park PA 16802 — Proposals for possible realizations of Majorana fermions in condensed matter provide a strong motivation for interfacing superconductors with topological insulators (PRL **100**, 096407 (2008)). We describe experiments that accomplish an important first step in this context: the realization of proximity-induced superconductivity in a candidate topological insulator. We have measured the bias-dependent differential conductance in Bi_2Se_3 nanoribbons contacted with superconducting electrodes over a temperature range 0.5 K $\leq T \leq$ 6 K in magnetic fields up to 8 T. We observe signatures of both proximity-induced superconductivity and incoherent multiple Andreev reflections in these mesoscale devices. In addition, we find periodic magneto- resistance oscillations for magnetic field perpendicular to both the nanoribbon axis and the superconducting contacts. The temperature- and field-dependence of the magneto-resistance oscillation amplitude and period are suggestive of dissipative vortex dynamics in the vicinity of the contacts. Supported by NSF-MRSEC, NSF-NNIN and ONR.

2:03PM W35.00015 Majorana Fermions in a Spin Ladder System , WADE DEGOTTARDI, SMITHA VISHVESHWARA, University of Illinois at Urbana-Champaign, DITPIMAN SEN, Centre for High Energy Physics, Indian Institute of Science, KITAEV LADDER COLLABORATION — We consider a two-legged spin chain version of Kitaev's honeycomb model. Like its parent, this model supports Z_2 vortices at every plaquette. The topological phase of the system is sensitive to, *inter alia*, the spatial pattern of these vortices. The topological phases are gapped in the bulk but possess isolated zero energy Majorana modes at each end. The existence of such Majorana modes can be inferred from a new topological invariant. We show that there is an intimate relation between the existence of Majorana modes and the spontaneous breaking of the global Z_2 symmetry.

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W36 DMP: Focus Session: Graphene Structure, Dopants, and Defects: Graphene Oxide and Fluoride C142

11:15AM W36.00001 Properties of Dilute Fluorinated Graphene , XIA HONG, The Pennsylvania State University — I will discuss our recent studies on dilute fluorinated graphene (DFG). Fluorine adatoms are covalently added to a graphene sheet using a controlled and reversible approach to create a dilute coverage on the order of $10^{12}/\text{cm}^2$, as determined by scanning tunneling microscopy studies. These adatoms are atomically sharp defects, interact strongly with the electronic states of graphene and drastically modify the transport properties of pristine graphene. This unusual 2D system exhibits several remarkable properties. Mid-gap state scattering dominates conduction at high temperature, the magnitude of which is determined by the adatom density and is correlated with Raman spectra. The temperature-dependent conductivity of the DFG sample follows weak localization at high carrier density and variable-range hopping at low carrier density. The transition is strongly correlated with the fluorine adatom density. In the variable-range hopping regime, DFG samples exhibit very large, negative magnetoresistance, which shows unusual staircase-like field dependence at low temperature. In the weak localization regime, we observe anomalous phase breaking behavior. I will discuss possible origins of these observations in the context of magnetism and localization. (In collaboration with S.-H. Cheng, C. Herding, and J. Zhu.)

11:51AM W36.00002 Electronic and structural properties of fluorinated graphene[1] , CHAD E. JUNKERMEIER, STEFAN C. BADESCU[2], THOMAS L. REINECKE, NRL, Washington, DC — Experiments have shown that the electronic structure of graphene can be tailored from that of a semimetal to that of a wide bandgap semiconductor through adsorption of fluorene. This makes fluorinated graphene C_xF ($x \geq 1$) attractive for electronics applications. Here we present first-principle calculations that reveal the dependence of C_xF electronic structure on the degree of fluorination in the range $1 \leq x \leq 8$. We present a systematic analysis of bandgap opening and p-doping, as well as of adsorption energies, lattice constants, bulk modulus and surface corrugation for single-face and two-face functionalization. We rationalize these with a band-interpolation scheme in terms of localized orbitals that clarify the C-C, C-F and F-F bonding. We discuss the relevance of tunable Young modulus for nanomechanical resonators.

[1]This work was supported in part by ONR.

[2]Currently at AFRL, Dayton, Ohio

12:03PM W36.00003 Patterning nanoroads and quantum dots on fluorinated graphene , MORGANA RIBAS, Rice University, ABHISHEK SINGH, Indian Institute of Science and Rice University, PAVEL SOROKIN, BORIS YAKOBSON, Rice University — Graphene nanoroads [1] and quantum dots [2] patterned on functionalized graphene combine metallic and semiconducting properties on a same mechanically intact sheet. Using density functional methods we investigate different stoichiometric phases of fluorinated graphene and find that the complete "2D-teflon" CF phase is thermodynamically more stable. The formation of fluorinated graphene favors the nucleation of aromatic "magic" clusters, but unlike hydrogenated graphene [3] it does not have a nucleation barrier. The CF is an insulator and turns out to be a perfect matrix-host for patterning nanoroads and quantum dots of pristine graphene. Depending upon the edge orientation and width the electronic and magnetic properties of the nanoroads can be tuned. The HOMO-LUMO energy gaps are size dependent and show a typical confinement of Dirac fermions. Furthermore, we study the effect of different coverage of F on graphene (CF and C_4F) on the band gaps, and show their suitability to host quantum dots of graphene with unique electronic properties. References: [1] Singh, A. K.; Yakobson, B. I., Nano Lett. 2009, 9 (4), 1540.[2] Singh, A. K.; Penev, E. S.; Yakobson, B. I., ACS Nano 2010, 4 (6), 3510. [3] Lin, Y.; Ding, F.; Yakobson, B. I., Phys. Rev. B 2008, 78 (4), 041402.

12:15PM W36.00004 Anomalous Phase Breaking in Dilute Fluorinated Graphene , XIA HONG, SHIH-HO CHENG, JUN ZHU, Department of Physics, The Pennsylvania State University — Quantum interference induced weak localization and phase breaking measurements are sensitive tools to probe the existence of magnetic impurities in mesoscopic systems. In this work, we study the low-field magnetoresistance of dilute fluorinated graphene (DFG), with a fluorine adatom density of $\sim 10^{12}/\text{cm}^2$. In the DFG samples, the phase breaking time τ_ϕ follows T^{-1} at high temperature and saturates at $T \sim 10$ K. The former is consistent with electron-electron interaction. The latter cannot be accounted for by conventional theories based on sample size and charge inhomogeneity. We show the dependence of the saturated τ_ϕ on the carrier density and fluorine coverage and discuss the effects of spin-flip scattering and localization in phase breaking. Our observations point to the presence of adatom induced local magnetic moments in dilute fluorinated graphene.

12:27PM W36.00005 Functionalization of exfoliated graphene by grafting aryl groups , HANG ZHANG, ELENA BEKYAROVA, ZENG ZHAO, WENZHONG BAO, JHAO-WUN HUANG, MIKHAIL ITKIS, SANDIP NIYOGI, XIAOLIU CHI, HUAZHOU WEI, FENGLIN WANG, ROBERT HADDON, CHUN NING LAU — We studied the transport properties of aryl functionalized exfoliated graphene. For the functionalization the graphene devices were immersed in a solution of diazonium salt. The attachment of aryl free radical to the basal carbon atoms changes the hybridization of the graphitic atoms from sp2 to sp3 thereby modifying the lattice's electronic structure. We observe that this opens a Coulomb gap at low temperatures and transport measurements indicate a variable range hopping mechanism. In suspended graphene, which allows for functionalization on both sides, we observe a large transport gap.

12:39PM W36.00006 Field emission from atomically thin edges of reduced graphene oxide , HISATO YAMAGUCHI, Rutgers Univeristy, KATSUHISA MURAKAMI, Osaka University, GOKI EDA, Imperial College London, TAKESHI FUJITA, Tohoku University, JULIEN BOISSE, Rutgers University, PENGFEI GUAN, Tohoku University, FUJIO WAKAYA, Osaka University, KYEONGJAE CHO, YVES CHABAL, University of Texas at Dallas, MINGWEI CHEN, Tohoku University, MIKIO TAKAI, Osaka University, MANISH CHHOWALLA, Rutgers University — Point sources show the best electron emission properties due to local field enhancement at the tip. A drawback of tip emitters is that they must be positioned sufficiently apart to achieve field enhancement, limiting the number of emission sites and therefore the overall current. In contrast, we report ultra-low threshold voltage emission of multiple electron beams from atomically thin edges of individual reduced graphene oxide (rGO) sheets. The emission sites observed by field emission (FEM) and field ion (FIM) microscopies are atomically spaced along the edge. FEM measurements indicate evidence for interference, suggesting that the emitted electron beams are coherent. Based on our spectroscopy, high-resolution transmission electron microscopy and theory results, field emission is attributed to the aggregation of oxygen groups in the form of cyclic edge ethers. Such closely spaced electron beams from rGO offer prospects for novel applications and understanding the physics of linear electron sources.

12:51PM W36.00007 Electronic structure of graphite oxide , HAE KYUNG JEONG, Daegu University, CHEOLSOO YANG, Samsung Electronics, BONG SOO KIM, KI-JEONG KIM, Pohang Accelerator Laboratory (PAL) — We have investigated the electronic structure of graphite oxide by photoelectron spectroscopy at the Pohang Accelerator Laboratory, Korea. The typical sp^2 hybridization states found in graphite were also seen in graphite oxide. However, the π state disappeared near the Fermi level because of bonding between the π and oxygen-related states originating from graphite oxide, indicating electron transfer from graphite to oxygen and resulting in a downward shift of the highest occupied molecular orbital (HOMO) state to higher binding energies. The band gap opening increased to about 1.8 eV, and additional oxygen-related peaks were observed at 8.5 and 27 eV.

This research was supported by the Basic Science Program through the National Research Foundation of Korea (NRF), funded by the Ministry of Education, Science and Technology (2010-0004592), and partly by the MEST (2009-0087138). Experiments at the PLS were supported in part by POSTECH and MEST.

1:03PM W36.00008 Computational Studies for Reduced Graphene Oxide in Alcohol- and Hydrogen-Rich Environments , RAMIN ABOLFATH, CHENG GONG, MUGE ACIK, YVES CHABAL, KYEONGJAE CHO, University of Texas at Dallas — We employ *ab-initio* molecular dynamic simulations to analyze the chemical reaction mechanisms for the oxygen removal process of graphene oxide upon annealing in the presence of water molecules and compare various thermal pathways in alcohol- and hydrogen-rich environments. Our first principles calculation shows damage-repair mechanisms of sp^2-C bonds in the etch holes of reduced graphene oxide and formation of dangling and/or sp^3-C bonds. The initial oxygen-abstraction results in the propagation of broken bonds and multi-site sp^2-C bond damage driven by the cascade of chemical reactions. The interplay between the environmentally induced damages and self-repair mechanisms of sp^2-C bonds determines the quality of the sheets after chemical treatments in alcohols or with hydrogen-rich environment. Water molecules form C=O and C-H bonds in the etch holes. We show that the alcohol- and hydrogen-rich environment provide an efficient transformation of C=O to the C-O bonds, and the removal of oxygen that is rarely observed with alcohol-rich environment alone.

1:15PM W36.00009 Electron Phonon Coupling Mechanism in Thermally Reduced Graphene , MUGE ACIK, GEUNSIK LEE, CECILIA MATTEVI, MANISH CHHOWALLA, KYEONGJAE CHO, YVES J. CHABAL, THE UNIVERSITY OF TEXAS AT DALLAS COLLABORATION, RUTGERS UNIVERSITY COLLABORATION — Infrared absorption of atomic and molecular vibrations in solids can be affected by electronic contributions through non-adiabatic interactions, such as the Fano effect. Typically, the IR absorption lineshapes are modified or IR forbidden modes are detectable as a modulation of the electronic absorption. In contrast to such known phenomena, we report here the observation of a giant IR absorption band in reduced graphene oxide (GO), arising from the coupling of electronic states to the asymmetric stretch mode of a yet unreported structure [1], consisting of oxygen atoms aggregated at edges of defects. DFT calculations show that free electrons are induced by the displacement of the oxygen atoms, leading to a strong IR absorption that is in-phase with the phonon mode. This new phenomenon is only possible when all other oxygen-containing chemical species including hydroxyl, carboxyl, epoxide and ketonic functional groups are removed from the region adjacent to the edges, i.e. clean graphene patches are present. *The authors acknowledge funding from the NRI SWAN program and Texas Instruments. [1] Acik, M.; Lee, G.; Mattevi, C.; Chhowalla, M.; Cho, K.; Chabal, Y. J. *Nature Materials.* **9,** 840-845 (2010)

1:27PM W36.00010 Grain-boundary unzipping by oxidation in polycrystalline graphene[1] , SIMONE ALEXANDRE, UFMG-Brazil, ALINE LUCIO, UFLA-Brazil, RICARDO NUNES, UFMG-Brazil — The need for large-scale production of graphene will inevitably lead to synthesis of the polycrystalline material [1,2]. Understanding the chemical, mechanical, and electronic properties of grain boundaries in graphene polycrystals will be crucial for the development of graphene-based electronics. Oxidation of this material has been suggested to lead to graphene ribbons, by the oxygen-driven unzipping mechanism [3]. A cooperative-strain mechanism, based on the formation of epoxy groups along lines of parallel bonds in the hexagons of graphene's honeycomb lattice, was proposed to explain the unzipping effect in bulk graphene [3] In this work we employ *ab initio* calculations to study the oxidation of polycrystalline graphene by chemisorption of oxygen at the grain boundaries. Our results indicate that oxygen tends to segregate at the boundaries, and that the unzipping mechanism is also operative along the grain boundaries, despite the lack of the parallel bonds due to the presence of fivefold and sevenfold carbon rings along the boundary core.

[1] J. Cervenka et al., PRB 79, 195429 (2009).
[2] J. da Silva-Araújo and R. W. Nunes, PRB 81, 073408 (2010).
[3] J-L. Li *et al.*, PRL 96, 176101 (2006).

[1]We acknowledge support from the Brazilian agencies: CNPq, Fapemig, and INCT-Materiais de Carbono.

1:39PM W36.00011 Influence of Gate Voltage on the diffusion of Oxygen on Graphene , ALEJANDRO SUAREZ, Department of Physics, The Pennsylvania State University, LJUBISA RADOVIC, Department of Energy and Mineral Engineering, The Pennsylvania State University, EZRA BAR-ZIV, Ben-Gurion University of the Negev, Beer-Sheva, Israel, JORGE SOFO, Department of Physics, The Pennsylvania State University — We calculate the surface diffusion of Oxygen on Graphene using Density Functional Theory. We find the activation energy for diffusion to be 0.71 eV. Charging the graphene plane causes the diffusion barrier to change substantially. Electron doping graphene lowers the diffusion barrier, resulting in activation energies as low as 0.15 eV for a carrier concentration of 7.6x10^{13} cm^{-2}. This barrier reduction yields diffusion coefficients reaching over nine orders of magnitude lower than that of diffusion on neutral graphene. After study of the change in charge density distribution and local density of states, this effect is explained by a mixture of bond weakening under the equilibrium state and bond strengthening during the transition state. With this large fluctuation in diffusivity, patterning of oxidized regions in graphene may be achieved through variation of the gate voltage.

1:51PM W36.00012 Coulomb blockade and hopping conduction in graphene quantum dots array , DAEHA JOUNG, LEI ZHAI, SAIFUL KHONDAKER, Nanoscience Technology Center, Department of Physics, Department of Chemistry, University of Central Florida, Orlando, Florida 32826 — We show from the low temperature electron transport measurements that the transport properties of chemically reduced graphene oxide (RGO) sheets can be explained as a sequential tunneling of charges through a two dimensional polydispersed array of graphene quantum dots (GQD), where graphene domains act like QDs while oxidized domains behave like tunnel barriers between QDs. As the temperature is decreased to lower than 15 K, a complete suppression of current (I) below a threshold voltage (V_t) was observed due to Coulomb blockade (CB) of charges through GQD array. For $V >$ V_t, the current follows a scaling behavior, I $\propto [(V - V_t)/V_t]^{\alpha}$ with α ~ 2.8, implying a quasi 2D GQD array. Temperature dependent current – gate voltage ($I - V_g$) curves show reproducible Coulomb oscillations due to a single electron tunneling through GQD array that washes out between 70 and 120 K corresponding to charging energies of 6.2 $\sim$ 10 meV giving estimated GQD sizes of 5 - 8 nm. Temperature dependent resistance data show Efros-Shklovskii variable range hopping (ES VRH) arising from CB, structural and size induced disorder.

2:03PM W36.00013 Ink jet printed graphene oxide (GO) coplanar waveguide (CPW) structures for measurement of microwave propagation in GO , KATE DUNCAN, STCD CERDEC, EDWIN BARRY, MARK GRIEP, WMRD ARL, JOHHNY DANIEL, DEREK MORRIS, STCD CERDEC, SHASHI KARNA, WMRD ARL — Chemically reduced graphene (CGR) has been successfully inkjet printed using a commercially available printer. The CGR with sheet sizes below 200 nm were dispersed in a mixture of water and ethanol. Coplanar waveguide (CPW) structures were deposited on CGR and plastic substrates, scattering (S) parameters were measured in order to extract material parameter for incorporation into simulation tools. Measurements and modeling of microwave propagation in graphene shall be presented.

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W37 DMP: Focus Session: Graphene: Growth, Characterization, and Devices: Quantum Hall Effect C146

11:15AM W37.00001 A study of the quantum Hall effect in CVD graphene synthesized on Cu , TIAN SHEN, Department of Physics, Purdue University, West Lafayette, IN, 47907 / PML, NIST, Gaithersburg, MD, 20899, WEI WU, Center for Advanced Materials, and ECE, University of Houston, Houston, Texas, 77204, HELIN CAO, YONG CHEN, Department of Physics, Purdue University, West Lafayette, IN, 47907, DAVID NEWELL, CURT RICHTER, PML, NIST, Gaithersburg, MD, 20899, QINGKAI YU, Center for Advanced Materials, and ECE, University of Houston, Houston, Texas, 77204 — Graphene films grown by Chemical Vapor Deposition (CVD) have provided a viable way to large area, low cost graphene-based electronics. Graphene CVD grown on Cu was transferred to SiO2/Si substrates and Hall-bar devices with sizes as large as 150 μm were fabricated, exhibiting carrier mobility of $\sim$3000cm^2/Vs. At low temperatures, the half integer quantum-Hall effect (QHE) and Shubnikov-de Haas (SdH) oscillations confirmed the single layer quality of the transferred graphene films. Systematic measurements in the quantum Hall region such as the DC/AC current dependence, temperature dependence, and AC frequency dependence were carried out, and their impact on the breakdown of the QHE was investigated. From weak localization peak fitting, the phase coherence length of the CVD graphene is determined to be $\sim$3μm at 1.6K.

11:27AM W37.00002 Strain-induced pseudo-magnetic fields and charging effects on CVD-grown graphene , R.T.-P. WU, M.-L. TEAGUE, N.-C. YEH, Dept. of Physics, Caltech, Pasadena, CA 91125, S. YEOM, B.L. STANDLEY, D.A. BOYD, M.W. BOCKRATH, Dept. of Applied Physics, Caltech, Pasadena, CA 91125 — Atomically resolved imaging and spectroscopic characteristics of chemical vapor deposition (CVD) grown graphene on Cu are studied using scanning tunneling microscopy and spectroscopy. CVD-grown graphene remaining on Cu exhibits large ripples and appears strongly strained. Different regions show different lattice structures and electronic density of states (DOS). Ridges appear along the boundaries of different lattice structures, which reveal excess charging effects. The large, non-uniform strain induces pseudo-magnetic fields up to $\sim$50 Tesla, yielding integer and fractional quantum Hall effects (IQHE and FQHE) as quantized conductance peaks in the DOS. For CVD-grown graphene transferred from Cu to SiO_2, the average strain and the resulting charging effects and pseudo-magnetic fields are much reduced. Fourier transformation of the local DOS of strained samples as well as data on the effects of real magnetic fields versus pseudo-magnetic fields will be presented. This work was jointly supported by NSF and NRI.

11:39AM W37.00003 Transport phenomena of suspended graphene in the quantum Hall regime , HSIN-YING CHIU, CHING-TZU CHEN, DAVID DIVINCENZO, PHAEDON AVOURIS, IBM Thomas J. Watson Research Center — Towards the goal of making qubits in graphene, it is important to develop graphene quantum point contact for quantum-gate operations. Klein tunneling effect implies that confining charge carriers in graphene using external potential is challenging. Hence, we resort to electric-field controlled band gap opening for charge confinement. We have successfully fabricated high quality suspended few-layer graphene devices with local electrostatic gates. In this talk, we present our observation of voltage-controlled band gap opening and anomalous quantum Hall features upon applying vertical electrical filed, revealing rich physics of symmetry breaking in the few-layer graphene system.

11:51AM W37.00004 Measurement of the 1/3 Fractional Quantum Hall Effect Energy Gap in Multi-terminal Suspended Graphene Devices , FERESHTE GHAHARI KERMANI, YUE ZHAO, PAUL CADDEN-ZIMANSKY, Columbia University, KIRILL BOLOTIN, Vanderbilt University, PHILIP KIM, Columbia University — In recent investigations of transport properties in two-terminal high mobility suspended graphene devices, a quantized conductance corresponding to the 1/3 FQHE state has been observed. However, due to the inherent mixing between longitudinal and transverse resistivities in this two-terminal measurement, quantitative characterization of the observed FQHE states such as the FQHE energy gap is difficult. In this talk, we present the measurement of multi-terminal IQHE and FQHE states in ultraclean suspended graphene samples in low density regime. The energy gap of the 1/3 FQHE, measured by its temperature-dependent activation, is found to be much larger than the corresponding state found in the 2DEGs of high-quality GaAs heterostructures, indicating that stronger e-e interactions are present in graphene.

12:03PM W37.00005 Symmetry breaking of zero energy landau level in monolayer graphene , YUE ZHAO, Physics Department, Columbia University, PAUL CADDEN-ZIMANSKY, FERESHTE GHAHARI, PHILIP KIM — We experimentally study the nature of the symmetry breaking of the zero energy landau level (LL) in monolayer graphene using Corbino geometry and Hall bar geometry devices. At high magnetic fields, in the absence of the edge state channel connection in Corbino devices, we observe a gap opening in $\nu = 0$ QH state whose gap is independent of in-plane magnetic field. In Hall-bar geometry devices where edge state connection is allowed, we observe similar QH Insulator behavior independent of the in-plane magnetic field, indicating that the observed insulating behavior at the charge neutrality point of monolayer graphene at high magnetic field is originated from the degeneracy lifting of the zero LL via the valley pseudospin polarization rather spin polarization.

12:15PM W37.00006 Fractional quantum Hall effect in graphene on boron nitride , CORY DEAN, Columbia University, Electrical Engineering & Mechanical Engineering, ANDREA YOUNG, PAUL CADDEN-ZIMANSKY, Columbia University, Department of Physics, LEI WANG, Columbia University, Electrical Engineering, HECHEN REN, Columbia University, Department of Physics, KENJI WATANABE, Advanced Materials Laboratory, National Institute for Materials Science, Japan, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, PHILIP KIM, Columbia University, Department of Physics, JAMES HONE, Columbia University, Mechanical Engineering, KEN SHEPARD, Columbia University, Electrical Engineering — Graphene is a remarkable 2D material exhibiting many unique and surprising many-body effects resulting from strong electron interactions. A continuing challenge remains the fabrication of ultra-high mobility devices that allow the intrinsic character of graphene to be fully explored. In my talk I will discuss our recent advancements in fabricating very-high quality graphene devices on boron nitride. Magnetoresistance measurements under very large applied fields will be presented including our recent observation of the fractional quantum Hall effect in multi-terminal devices over a broad range of carrier densities.

12:27PM W37.00007 Transport on gated C-face epitaxial graphene , CLAIRE BERGER, CNRS-Institut Neel, Grenoble and Georgia Tech, School of Physics, Atlanta — We present transport and electronic properties on single layer and multilayered epitaxial graphene layers grown on 4H-SiC-(000-1) (C-face) by the Confinement Controlled Sublimation method [1]. Single layers present all the characteristics of isolated graphene layers. In particular quantum Hall effect plateaus develop at half-integer values, concomitant with vanishing longitudinal resistivity. High mobility up to μ=14,000 cm^2/V.s at 300 K is achieved despite contamination and substrate steps. Multilayered epitaxial graphene (MEG) on the C-face consists of non-graphitic rotationally stacked graphene layers, exhibiting the band structure of a single graphene layer [2]. Transport in MEG presents also graphene characteristics. In some cases transport anomalies are observed indicating a much richer picture.

[1] R. Ming et al. Materials Science and Engineering – Reports (submitted)
[2] M. Sprinkle et al, Phys. Rev. Lett. 103, 226803 (2009).

1:03PM W37.00008 Quantum Hall Effect of Hybrid Monolayer-bilayer Graphene Structures: Observation of Broken electron-hole Symmetry , YONG P. CHEN, JIFA TIAN, ISAAC CHILDRES, HELIN CAO, Department of Physics, Purdue University — Quantum Hall Effect (QHE) in both monolayer (1L) and bilayer (2L) graphene has been well studied in the past few years. Little attention has been paid to the magneto-transport across the 1L ∼2L graphene interface. Here, we present the magnetotransport measurements of several exfoliated graphene quasi-Hall bar devices which consist of partly 1L and partly 2L graphene. We focused on the Hall resistance (R_{xy}) across the interface between 1L and 2L graphene when the carrier types and densities are changed using a back gate voltage. We observed that when the carrier type is p type (hole), R_{xy} typically shows QHE of bilayer graphene with filling factor of 4N, N being integers. When the carrier type is changed into n type (electron), the corresponding R_{xy} typically shows QHE of single layer graphene with filling factor of 4(N+1/2), N being integers. We discuss possible explanations for the observed broken electron-hole symmetry in such hybrid structures.

1:15PM W37.00009 Multi-terminal transport property on hybrid structure of monolayer and bilayer graphene , YONGJIN JIANG, Zhejiang Normal University, JIANGPING HU, Purdue University — We study the transport properties of Hybrid structures formed by monolayer and bilayer graphene. The energy spectrum and edge states of various junctions in strong magnetic field are analyzed. The transport properties are affected by the mixing effect of interfaces and the scattering between edge states, and display many novel features in multi-terminal measurements, Our results explains recent experimental results on such hybrid structure systems.

1:27PM W37.00010 Electric field induced transition between spin to valley polarized ν=0 quantum Hall state in dual-gated graphene bilayers[1] , KAYOUNG LEE, SEYOUNG KIM, BABAK FALLAHAZAD, EMANUEL TUTUC, The University of Texas at Austin — Graphene bilayers in Bernal stacking exhibit a transverse electric field dependent energy gap, thanks to the on-site electron energy asymmetry between the two layers. In a perpendicular magnetic field, the applied transverse electric field (E) will induce a quantum Hall state (QHS) at the charge neutrality point (filling factor ν=0) marked by a insulating behavior of the longitudinal resistance (ρ_{xx}), and a plateau in the Hall conductivity. Using dual-gated graphene bilayers, we investigate here the E-field dependence of the ν=0 QHS in high perpendicular magnetic fields (B), up to 30T. The temperature dependence of ρ_{xx} measured at ν=0 shows an insulating behavior, which is strongest in the vicinity of E=0 as well as at large E-fields. At a fixed B-field, as a function of the applied E-field the ν=0 QHS undergoes a transition, marked by a ρ_{xx}minimum, as well as a temperature independent ρ_{xx} at a finite E-field value. This observation can be explained by a transition from a spin polarized ν=0 QHS at small E-fields, to a valley (layer) polarized ν=0 QHS at large E-fields. The E-field value at which the transition occurs follows a linear dependence on the applied perpendicular magnetic field, with a slope of ∼18 mV/nm·T.

[1]We thank NRI and NSF for support.

1:39PM W37.00011 Giant Spin-Hall Effect and Nonlocal Transport in Graphene , DMITRY ABANIN, Princeton, K.S. NOVOSELOV, A.K. GEIM, Manchester, L.S. LEVITOV, MIT — Graphene provides a unique opportunity to explore quantum-relativistic phenomena in a condensed matter laboratory. Interesting phenomena associated with the parity anomaly, including quantum Hall effect in the absence of magnetic field and quantum spin-Hall effect in quantizing magnetic fields, have been theoretically proposed, but could not be observed so far largely due to disorder and density inhonogeneity. We show that weak magnetic field induces large bulk non-quantized spin-Hall effect in graphene. The effect occurs due to Zeeman spin splitting which generates the imbalance of the Hall resistivities of the two spin species. The spin-Hall effect is robust in the presence of disorder and interactions. It will manifest itself in large nonlocal transport mediated by long-lived spin currents, as well as in spin injection and spin accumulation experiments. The effect peaks at the Dirac point, and can serve as a hallmark of the relativistic character of carriers in graphene and other Dirac materials.

1:51PM W37.00012 Quantum Hall effect and Landau level crossing in trilayer graphene , THITI TAYCHATANAPAT, Department of Physics, Harvard University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, PABLO JARILLO-HERRERO, Department of Physics, MIT — We report the experimental observation of quantum Hall effect in Bernal stacked trilayer graphene (TLG) on hexagonal boron nitride substrate. The mobility of our TLG reaches 110,000 $cm^2/V{\cdot}s$ allowing us to observe the Shubnikov-de Haas oscillation at a magnetic field as low as 300 mT and broken- symmetry states at high magnetic field. In addition, the unique band structure of Bernal stacked TLG which consists of monolayer-like and bilayer-like subbands at low energy allows us to observe the Landau level crossing between these two subbands. The positions of these crossings in magnetic field and filling factors enable us to estimate relevant Slonczewski-Weiss-McClure parameters.

2:03PM W37.00013 Suspended graphene electromechanics in quantum Hall regime , VIBHOR SINGH, GANESH SUBRAMANIAN, BUSHRA IRFAN, HARI SOLANKI, MANDAR DESHMUKH, Tata Institute, Mumbai, India — There has been a keen interest in the NEMS community in probing the coupling between charge and mechanical degrees in NEMS resonators. These experiments show that electron transport and mechanical motion of the resonator influence each other. Motivated by this, we have probed the electron transport in the ultra clean graphene devices in quantum Hall regime at low temperature while it is mechanically perturbed. There can be several mechanisms that can lead to the resistance change due to mechanical vibrations like, by strain due to deformation of the flake, redistribution of the carrier density etc, electron scattering within the flake due to changes in the energy landscape. In our study we find that upon mechanical vibrations the resistance of the device changes. We try to understand these changes caused by the non-linear dependence of resistance on carrier density.

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W38 DMP DPOLY: Focus Session: Organic Electronics and Photonics – Charge transport A130/131

11:15AM W38.00001 Charge Transport in Functionalized Fluorinated Pentacenes , OANA JURCHESCU, DANIEL DAVID, CLAIRE MCLELLAN, Wake Forest University, BALAJI PURUSHOTHAMAN, University of Kentucky, SHUBIN LIU, University of North Carolina, VEACESLAV COROPCEANU, Georgia Institute of Technology, JOHN ANTHONY, University of Kentucky, LAURIE MCNEIL, University of North Carolina — We report on charge transport in fluorinated functionalized pentacenes and discuss the effect of trialkylsilyl and the number of fluorine atoms. We show that modifications in the chemical composition influence the molecular packing, crystal formation and electrical properties, allowing us to measure mobilities from 10^{-5} to 1.7 cm^2/Vs. The mobilities correlate with the packing, demonstrating that tuning the solid-state order to induce pi-stacking improves electrical properties. By combining Raman measurements with theoretical calculations predicting the vibrational spectrum, we explore the vibrational modes of the crystals, providing information about the intermolecular coupling and electron-phonon interactions governing charge transport. We calculate the intermolecular electronic couplings and band structures by using density functional theory, and study the effect of fluorination and trialkylsilyl substitution on crystal packing and the electronic properties.

11:27AM W38.00002 Semicrystalline high performance poly (thienothiophene) thin films: crystallites and defects , CHENCHEN WANG, Applied Physics, Stanford University, JAVIER DACUÑA, Electrical Engineering, Stanford Univerisity, BJÖRN BRÄUER, Stanford Institute of Materials and Energy Science, DAN DARANCIANG, Department of Chemistry, Stanford Univerisity, ALBERTO SALLEO, Material science and engineering, Stanford Univerisity — Effects of liquid crystalline temperature annealing and surface treatment on Poly(2,5-bis(3-alkylthiophen-2-yl)thieno[3,2-b]thiophenes) (PBTTT) thin films were studied. Time resolved terahertz spectroscopy (TRTS), which measures the local carrier mobility, suggests that the mobility improvement of annealed PBTTT on octadecyltrichlorosilane (OTS), compared with as cast film, is mainly due to superior local carrier mobility. Scanning transmission x-ray microscopy (STXM), which measures the in-plane molecular orientation with 30nm spatial resolution, shows similar domain size of annealed films on both OTS and SiO_2, and implies that the higher mobility of film on OTS cannot be accounted for by domain size. These results are also supported by the mobility edge model, which extracts trap density and quasi-free carrier mobility in crystallites from transistor characterization. Annealing film on OTS improves mobility in crystallites, but has little effects of reducing trap density. The modeling shows great elimination of interface trap density of film on OTS, compared with film on SiO_2, which might be the main reason for its higher mobility.

11:39AM W38.00003 First-principles study of polythiophene and polyselenophene crystals for organic electronics[1] , TAKAO TSUMURAYA, JUNG-HWAN SONG, A.J. FREEMAN, Northwestern University — Semiconducting polymers, like regioregular poly(3-hexylthiophene)/poly(3-hexylselenophene) (rr-P3HT/rr-P3HS) are currently the most widely studied materials in a variety of applications for polymer based bulk-heterojunction (BHJ) solar cells and organic field-effect transistors (OFET). [1,2] For both applications, the performance of devices has been attributed to thin film structures of rr-P3HT/rr-P3HS on substrates. To understand their mechanisms, the crystal structure has been extensively investigated by using various experimental techniques. However the crystal structure has yet to be unambiguously characterized. Here, we proposed several possible structures and investigated their stabilities from first-principles density functional calculations based on the all-electron FLAPW method. [3] We found that two base-centered monoclinic structures belonging to space group $A2$ are in the degenerate lowest energy structures. The electronic and transport properties are also discussed. Lastly, we report on the differences in electronic and crystal structure between rr-P3HT and rr-P3HS.
[1] G. Li *et al.*, Nature Mater. **4**, 864 (2005).
[2] H. Sirringhaus *et al.*, Nature **401**, 685 (1999).
[3] E. Wimmer *et al.*, Phys. Rev. B **24**, 864 (1981).

[1]Supported by ANSER, a DoE EFRC (DE-SC0001059).

11:51AM W38.00004 Analysis of Metallic Conduction at the Interface of TTF and TCNQ Crystals[1] , VIKTOR ATALLA, Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, MINA YOON, ORNL, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin — Organic materials are promising candidates for a next generation of electronic devices, since they offer a variety of new intriguing electronic phenomena while being environmentally friendly, low cost, and mechanically flexible. Here we study the donor/acceptor interface of TTF and TCNQ organic molecular crystals which was found to exhibit metallic conduction whereas the individual crystals are large band-gap semiconductors. Using density functional theory (DFT) we first compare the performance of different exchange-correlation (XC) functionals for TTF and TCNQ dimers. All employed XC functionals consistently give electron transfer from TTF to TCNQ and the van der Waals (vdW) corrected molecular binding distances are within ≈ 0.1 Å of the MP2 value, indicating that within DFT the system can be qualitatively described by semilocal functionals. We construct interfaces between the two types of crystals and calculate their electronic structures. On a PBE + vdW level we find indications for metallic conduction at the interface, due to metallic bands that are exclusively induced from the interface layers of TTF and TCNQ molecules.

[1]Sponsored by the Max Planck Society and the DOE, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

12:03PM W38.00005 Charge Trapping in Organic Thin-Film Transistors , CLAIRE MCLELLAN, JACK OWEN, Wake Forest University, MARSHA GRIMMINGER, JOHN ANTHONY, University of Kentucky, OANA JURCHESCU[1] — Charge trapping in the bulk of the organic semiconductors and at interface with the gate dielectric and/or contacts is one of the determining factors governing charge transport in organic thin-film transistors (OTFTs). We explore the current-voltage characteristics in different charge density regimes and extract the field-effect mobility. The dependence of mobility on gate/drain voltage give us valuable insight into the mechanism of charge transport and the relevance of trapping states. We perform measurements on devices fabricated using different methods, such as spin-coating, drop-casting or spray-coating, on a silicon gate electrode, silicon dioxide gate dielectric, and gold source and drain contacts. We demonstrate that the performance of OTFTs is strongly dependent on processing details. We show that even when using the same processing method, we are able to systematically tune the charge trapping states by chemically modifying the contact and dielectric surfaces with self-assembly monolayers.

[1]Wake Forest University

12:15PM W38.00006 Organic electrical double layer transistors gated with ionic liquids[1] , WEI XIE, C. DANIEL FRISBIE, Department of Chemical Engineering and Materials Science, University of Minnesota — Transport in organic semiconductors gated with several types of ionic liquids has been systematically studied at charge densities larger than 10^{13} cm^{-2}. We observe a pronounced maximum in channel conductance for both p-type and n-type organic single crystals which is attributed to carrier localization at the semiconductor-electrolyte interface. Carrier mobility, as well as charge density and dielectric capacitance are determined through displacement current measurement and capacitance-voltage measurement. By using a larger-sized and spherical anion, tris(pentafluoroethyl)trifluorophosphate (FAP), effective carrier mobility in rubrene can be enhanced substantially up to 3.2 cm^{2}V^{-1}s^{-1}. Efforts have been made to maximize the charge density in rubrene single crystals, and at low temperature when higher gate bias can be applied, charge density can more than double the amount of that at room temperature, reaching 8*10^{13} cm^{-2} holes (0.4 holes per rubrene molecule).

[1]NSF MRSEC program at the University of Minnesota

12:27PM W38.00007 Hopping transport in electrolyte-gated P3HT organic field effect transistors[1] , SHUN WANG, MINGJING HA, MICHAEL MANNO, C. DANIEL FRISBIE, C. LEIGHTON, Department of Chemical Engineering and Material Science, University of Minneosta — Using ion-gel-gated poly (3-hexylthiophene) (P3HT), we successfully fabricated p-type organic field effect transistors (OFET) with on/off ratios of 10^5 and mobility of the order of 1 cm^2/V s at room temperature. We studied charge transport in the electrochemically doped P3HT as a function of gate voltage, temperature, magnetic field, film thickness, and roughness. Carrier concentrations were obtained from both gate charging current and Hall effect measurements. The resistance vs. temperature (down to 5K for large gate voltages) characteristics indicate 2D hopping transport. Large positive magnetoresistance at temperatures lower than 50 K was observed, but with anomalously low anisotropy due to high roughness.

[1]Work supported by NSF MRSEC.

12:39PM W38.00008 Charge transport and velocity distribution in ambipolar organic thin film Transistors based on a diketopyrrolopyrrole-benzothiadiazole copolymer , TAE-JUN HA, The University of Texas at Austin, PRASHANT SONAR, SAMARENDRA PRATAP SINGH, Institute of Materials Research and Engineering(A*STAR), ANANTH DODABALAPUR, The University of Texas at Austin — There have been reports of charge transport mechanisms in organic thin film transistors (OTFTs) focusing on steady-state characteristics but these measurements provide limited information. Time-resolved measurements can provide additional information in understanding transport mechanisms but existing reports have focused on unipolar organic characteristics. No previous reports on ambipolar organic devices have involved entire velocity distribution and charge transport mechanisms. Recently, we have fabricated ambipolar OTFTs based on a diketopyrrolopyrrole-benzothiadiazole copolymer (PDPP-TBT) with a field-effect mobility of more than 0.2 cm^2 $V^{-}1$ $s^{-}1$. Velocity distributions are measured by performing specialized dynamic measurements while keeping the RC-time constant of the measurement circuit small. This yields a distribution in arrival times of charge carriers from source to drain which can be converted to velocity distributions. We will also describe dynamic transport measurements on high-k-dielectric PDPP-TBT OTFTs.

12:51PM W38.00009 Organic field effect transistor fabricated by directly grown poly (3 hexylthiophene) crystalline nanowires on solution processed carbon nanotube aligned array electrodes , BIDDUT SARKER, Nanoscience Technology Center, Department of Physics, University of Central Florida, Orlando, FL 32826, JIANHUA LIU, LEI ZHAI, Nanoscience Technology Center, Department of Chemistry, University of Central Florida, Orlando, FL 32826, SAIFUL KHONDAKER, Nanoscience Technology Center, Department of Physics, and School of Electrical Engineering and Computer Science, University of Central Florida — We demonstrate convenient and highly reproducible approach to fabricate organic field effect transistors (OFETs) using the direct growth of crystalline P3HT nanowires on aligned array SWNT interdigitated electrodes. Compared to the OFETs with metal electrodes, the OFETs with SWNT electrodes show high mobility and high current on-off ratio with a maximum of 0.13 cm^2/Vs and 3.1×10^5, respectively. The improved device characteristics are also demonstrated by the absence of short channel effect which is dominant in gold electrode OFETs. Such remarkable improvement of the device performance as high mobility, high current on-off ratio, absence of short channel effect and better charge carrier injection can be attributed to the improved contact via strong $\pi-\pi$ interaction SWNT electrodes with the crystalline P3HT nanowires as well as the improved morphology of P3HT due to one dimensional crystalline structure. .

1:03PM W38.00010 Interfacial Width Measurements of Dielectric/P(NDI2OD-T2) Using Resonant Soft X-ray Reflectivity[1] , HONGPING YAN, ZIRAN GU, ELIOT GANN, BRIAN COLLINS, NC State Univ., SUFAL SWARAJ, SOLEIL, CHENG WANG, Advanced Light Source, TORBEN SCHUETTFORT, CHRIS MCNEILL, Univ. of Cambridge, HARALD ADE, NC State Univ. — Interfaces between a conjugated polymer and a dielectric play a critical role in organic thin-film transistors, yet it's difficult to measure. Resonant Soft X-ray Reflectivity (R-SoXR) is a unique and relatively simple method to investigate such interfaces. By tuning the soft X-ray energies, we are able to selectively and quantitatively characterize the interfacial width and thicknesses of the films. In an effort to relate performance to interface structure, we have used R-SoXR to investigate polystyrene (PS) or poly(methyl methacrylate) (PMMA) as the top layer and poly{[N,N9-bis(2-octyldodecyl)-naphtha-lene-1,4,5,8-bis(dicarboximide)-2,6-diyl]-alt-5, 59-(2,29-bithiophene)} (P(NDI2OD-T2)) as bottom layer supported on a Si substrate. We found that the device with PS as dielectric has a higher threshold voltage, which correlates to the increased interfacial trapping due to increased interfacial roughness. The extension of R-SoXR to the energy of fluorine K absorption edge is also demonstrated.

[1]NSF DMR-0906457, DOE DE-FG02-98ER45737

1:15PM W38.00011 Temperature Induced Structure Evolution of Regioregular Poly (3-hexylthiophene) in Dilute Solution and its Influence on Thin Film Morphology , CHARLES HAN, YE HUANG, HE CHENG, Joint Laboratory of Polymer Science and Materials, ICCAS, Beijing, China, JOINT LABORATORY OF POLYMER SCIENCE AND MATERIALS, ICCAS, BEIJING, CHINA TEAM — The structure evolution of regioregular Poly (3-hexylthiophene) (P3HT) in THF dilute solution, and its influence on thin film morphology were studied. A thermal treatment at high temperature effectively re-disperses P3HT micro-sized aggregates, and introduces two modes in DLS measurements. The structures of these 2 modes are identified, and the two structures of P3HT in dilute solution can greatly influence the morphology on subsequent thin films produced. Since the P3HT structures are carried into the film morphology, proper understanding and control of the structures in solution are important and can enhance electronic and opto-physical properties of the final devices.

1:27PM W38.00012 Effect of Cooling Rate on Microstructure and Charge Transport in Semiconducting Polymer Thin Films[1] , EVAN KANG, EUNSEONG KIM, KAIST, CENTER FOR SUPERSOLID AND QUANTUM MATTER RESEARCH TEAM — Thermal annealing of polymer thin films often enhances charge carrier mobility which can be attributed to self-healing of the film morphology. We have investigated the effect of cooling rate following the annealing treatment on the thin film microstructure and the charge transport properties using a high performance semiconducting polymer, poly(2,5-bis(3-alkylthiophen-2-yl)thieno[3,2-b]thiophene) (PBTTT). The cooling rate plays a key role in determining the microstructure and performance of polymer thin films. Differential scanning calorimeter measurement shows that fast cooling suppresses the crystallization process. The microstructure of thin films is investigated by using 2D X-ray diffraction and atomic force microscopy. Slow cooling results in well-connected large domains with enhanced three dimensional ordering whereas fast cooling leads to misalignment of small domains with relatively rough surface. Transport characteristics at various temperatures show increase in the charge carrier mobility and decrease in the activation energy when the cooling rate is slowed. This change in the mobility and activation energy becomes saturated with cooling rate below 15 $^\circ$C/min.

[1]E. S. H. K. and E. K. gratefully acknowledge financial support from the National Research Foundation of Korea through the Creative Research Initiatives (CSQR).

1:39PM W38.00013 Exponential behavior of the Ohmic transport in organic films , CORNELIU COLESNIUC, Department of Physics and Center for Advanced Nanotechnology, University of California San Diego, La Jolla, California 92093 , RUDRO BISWAS, Department of Physics, Harvard University, Cambridge, Massachusetts 02138, SAMUEL HEVIA, Facultad de Física, Universidad Católica de Chile, Casilla 306, Santiago, Chile 6904411, ALEXANDER BALATSKY, Theoretical Division and Center for Integrated Nano-Technologies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, IVAN SCHULLER, Department of Physics and Center for Advanced Nanotechnology, University of California San Diego, La Jolla, California 92093 — An exponential dependence of conductance on thickness and temperature was found in the low voltage, Ohmic regime of copper (CuPc) and cobalt (CoPc) phthalocyanine, sandwiched between palladium and gold electrodes, unlike ever claimed in organic materials. A comparison with conventional models fails to explain all the data with a single set of parameters. On the other hand, a model which incorporates tunneling between localized states with thermally-induced overlap agrees with the data, and decouples the contributions to conductance from the electrode-film interface and the bulk of the film. Work supported by AFOSR, DOE and the UCOP program on carbon nanostructures.

1:51PM W38.00014 Atomistic Molecular Dynamics Simulation of the Surface Properties of P3HT Films[1]

, YENENEH YIMER, SIMA MOFAKHAM, ALI DHINOJWALA, MESFIN TSIGE, Department of Polymer Science, University of Akron — In recent years P3HT has attracted much interest mainly because of its potential applications in solar cells, light emitting diodes and field effect transistors. The performance of these devices is strongly dependent on the structural packing, morphology and interfacial properties of the P3HT. In order to improve the devices efficiency, understanding the structural and dynamical properties of P3HT at the atomic level is important. Most studies on P3HT have mainly focused on understanding its bulk properties. However, the orientation of P3HT chains at the polymer/air interface has not been well investigated. Using molecular dynamics simulations we have studied the interfacial properties of free-standing P3HT films. The simulation results show that at the air/polymer interface the alkane side groups of the P3HT chains orient mainly to the interface in qualitatively good agreement with SFG experimental results. The surface tension of P3HT in its melt state shows strong dependence on temperature and chain length and is directly related to the roughness of the P3HT surface.

[1]This work is supported by the NSF (DMR0847580)

2:03PM W38.00015 Switching or triggering by light organic materials in the 100 nm size range

, VINA FARAMARZI, JEAN FRANCOIS DAYEN, BERNARD DOUDIN, IPCMS/CNRS/UDS, DMONS TEAM — We investigate optoelectronic fabrication and characterization of organic electronics devices in the 100 nm range. This intermediate size has advantages in simplicity of device fabrication and robustness of observed properties. For this aim high aspect ratio lateral electrodes separated by a sub 100nm gap were produced by means of simple optical lithography techniques [1]. The electrical measurements set-up is integrated with an inverted optical microscope, allowing simultaneous optical and electrical measurements followed by temperature and magnetic field studies. We demonstrate that electrical contacts are suitable for a wide range of current measurements going from 10^{-13} to 10^{-2} A. This versatility makes the nanotrench design compatible for studying a broad variety of nanoparticles and molecular systems. Electrical transport properties of different devices are presented, e.g molecular switches, Iron based spin-transition nanoparticles, Conductive molecular chains and 2D nanoparticle networks. The promising reproducible results reveal novel intrinsic transport properties and confirm the high interest and reliability of this approach for further studies in the field of molecular electronics and spin dependent transport in molecular structures.
[1] J-F Dayen, V Faramarzi et al, *Nanotechnology* **21**(33), 335303 (2010)

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W39 DBP: Experimental Techniques in Biophysics A124/127

11:15AM W39.00001 ABSTRACT WITHDRAWN –

11:27AM W39.00002 Spatially resolved absorption spectroscopy of bio - assemblies on a micron scale

, SILKI ARORA, Department of Physics and College of Optics, University of Central Florida, JENNIFER MAUSER, DEBOPAM CHAKRABARTI, Burnett School of Biomedical Sciences, University of Central Florida, ALFONS SCHULTE, Department of Physics and College of Optics, University of Central Florida — We have developed a novel approach to measure optical absorption spectra with spatial resolution at the micron scale. The setup employs a confocal microscope with a broadband white light excitation beam in transmission geometry. An aperture controls the amount of illuminating light and localizes the area of excitation. The setup is employed to measure the absorption spectrum of single red blood cells ($\sim$ 7 microns diameter) under solution conditions. The spatial resolution in the lateral direction is found to be better than three microns. Through measurements of the transmitted intensity in met- myoglobin and calcein dye nanoliter solutions at fixed path lengths, we establish that the absorbance varies linearly with concentration over the range from 0.1 to 2 mM. Our instrument enables measurements of spatial variations in the optical density of small samples and may find application in monitoring biological assemblies at the single cell level.

11:39AM W39.00003 Stochastic super resolution imaging by diffusive probes

, THOMAS DORN, JOHN EWALT, FRANCISCO MARQUEZ, GEORGE SHUBEITA, UT-Austin, Physics — Optical microscopy is a powerful tool for the imaging of cells and bio-materials, however the resolution is limited by diffraction and thus objects closer than a few hundred nanometers cannot be individually resolved. We report a novel stochastic super-resolution technique which relies on diffusing probes in which the resolution is determined by probe size and Forster radius of energy transfer. By recording a time-series of images similar to other super-resolution techniques, the centers of bright spots can be determined with sub-pixel accuracy by fitting to the point spread function. The centroids can then be used to reconstruct a super-resolution image.

11:51AM W39.00004 Near-field Approaches to Subcellular Tissue Abalation

, DEEPA RAGHU, George Washington University, JOAN HOFFMANN, Applied Physics Laboratory, BENJAMIN GAMARI, University of Massachusetts, ANDREW GOMELLA, MARK REEVES, George Washington University — We report on the development of a near-field approach to MALDI (Matrix-assisted laser desorption and Ionization). In this technique analytes embedded in an energy- absorbing matrix are ablated from the surface of a sample. In the infrared region, the matrix can be water by exciting the 3-micron vibrational mode of the water molecule. We use a 3-micron wavelength lasers, coupled with a near-field scanning microscope to ablate material from cells of different membrane stiffness. We have been able to reproducibly ablate features as small as 1 micron in diameter in cell and have characterized the power-dependence of the ablation process. We will review our findings and describe demonstrations of tissue modification by this approach at length scales smaller than a single cell. This approach has the potential to allow the identification and mapping of proteins expressed in intact cells and tissues, which is of great interest as protein expression connects genomic information with the functioning of an organism.

12:03PM W39.00005 Rotational Diffusion of Plasmon-Resonant Gold Nanorods for Depth-Resolved Microrheology Using Optical Coherence Tomography[1]

, AMY OLDENBURG, RAGHAV CHHETRI, University of North Carolina at Chapel Hill, KRYSTIAN KOZEK, AARON JOHNSTON-PECK, JOSEPH TRACY, North Carolina State University — The ability to perform microrheology in optically thick samples would enable analysis of bulk tissues. Optical coherence tomography (OCT) provides imaging several mean free scattering path lengths into tissue. In this study we report the use of plasmon-resonant gold nanorods as microrheological sensors in OCT. Nanorods exhibit a longitudinal mode that is excited when they are oriented parallel to the polarization of the incident light, which is favorable for passive microrheology using polarized light to monitor their rotational diffusion. We demonstrate measurements of the rotational diffusion of unconfined, colloidal gold nanorods using polarization-sensitive OCT, and validate the Stokes-Einstein relationship for the nanorods in simple fluids of varying viscosity. We then show that OCT provides depth-resolved imaging of fluid viscosity through measurements of the rotational diffusion rate of the nanorods.

[1]We acknowledge support from the Carolina Cancer Center for Nanotechnology Excellence (C-CCNE NIH (NCI) #U54CA119343).

12:15PM W39.00006 Monte-Carlo Study of Binding Kinetics in Surface Plasmon Resonance Systems , MATTHEW RAUM, UWE TÄUBER, Virginia Tech, Department of Physics, KIMBERLY FORSTEN-WILLIAMS, Virginia Tech, Department of Chemical Engineering — Surface plasmon resonance (SPR) has become a standard tool for studying ligand-receptor binding reactions in real-time. Ideally the data obtained with this technique allows measurement of kinetic reaction rates (rather than merely the equilibrium constant for the reaction). In typical experimental configurations one species is immobilized near the active surface while its binding partner is initially suspended in solution, flowing across the active surface. It is generally appreciated that reaction rates observed in SPR experiments are affected by mass transport if the time scales for reaction and transport in the system are comparable. The issue of ensuing effective reaction rates has been treated through different approaches in the literature. The goal of this research is a quantitative study of how faithfully intrinsic binding rates can be measured in SPR devices. We employ a lattice Monte Carlo method to simulate SPR experiments in order to test the efficacy of common SPR analytical techniques. We point out where existing analytical techniques succeed or fail in measuring binding and dissociation rates, and investigate the influence of secondary parameters in the system (such as the flow rate) on experimental data.

12:27PM W39.00007 Fluorescence Correlation Spectroscopy of Tryptophan-containing Proteins in Sugar Solutions using Two Photon Excitation[1] , DAVID SIDEBOTTOM, NATHAN HOLMAN, YULI WANG, MICHAEL NICHOLS, Creighton University — Simple sugars are often incorporated in cryopreserving media to aid in the preservation of biomaterials and functional proteins. However, the mechanism by which sugars provide protection is still openly debated. As part of a project to investigate the behavior of proteins in sugar solutions, we are developing Fluorescence Correlation Spectroscopy (FCS), using a novel two photon excitation at 532 nm, as a selective probe of protein dynamics for tryptophan-containing proteins. Our goal is to monitor possible alterations in the protein's hydrodynamic radius caused by preferential binding of sugars to its surface.

[1]This work is supported by a grant from National Institute of Biomedical Imaging and Bioengineering (R01EB009644)

12:39PM W39.00008 Continuous Nano-Particle Transport in a Standing Wave Optical Line Trap , VASSILI DEMERGIS, ERNST-LUDWIG FLORIN, The University of Texas at Austin — Since the introduction of the single beam optical trap (SBT) by Ashkin et. al. in 1986, trapping and manipulation of micron-sized particles by optical forces has become instrumental in many areas of research. However, controlled transport of large numbers of particles is difficult using a SBT. Here we introduce a technique for controlled transport that we call an Optical Capillary (OC), named for its ability to strongly confine and continuously transport nanometer-sized particles. The OC, generated by an optical standing wave pattern, is especially strong along the optical axis due to the compensation of the axial scattering force. We utilize the lateral scattering forces to control the transport of particles along a line perpendicular to the optical axis. The measured velocity profiles of single particles in the OC agree with our model predictions.

12:51PM W39.00009 Laser- based Insect Tracker (LIT) , LEONARDO MESQUITA, SHIVA SINHA, ROB DE RUYTER VAN STEVENINCK, Indiana University Bloomington, Dep. of Physics — Insects are excellent model systems for studying learning and behavior, and the potential for genetic manipulation makes the fruitfly especially attractive. Many aspects of fruitfly behavior have been studied through video based tracking methods. However, to our knowledge no current system incorporates signals for behavioral conditioning in freely moving flies. We introduce a non-video based method that enables tracking of single insects over large volumes (>8000cm3) at high spatial (<1mm) and temporal (<1ms) resolution for extended periods (>1 hour). The system uses a set of moveable mirrors that steer a tracking laser beam. Tracking is based on feedback from a four-quadrant sensor, sampling the beam after it bounces back from a retro reflector. Through the same mirrors we couple a high speed camera for flight dynamics analysis and an IR laser for aversive heat conditioning. Such heat shocks, combined with visual stimuli projected on a screen surrounding the flight arena, enable studies of learning and memory. By sampling the long term statistics of behavior, the system augments quantitative studies of behavioral phenotypes. Preliminary results of such studies will be presented.

1:03PM W39.00010 Power dependent study of kinetics of TRF2 recruitment in cells due to DNA damage caused by ultrafast near-IR Laser , MANAS BHALERAO, UT Arlington, NAZMUL HUDA, DAVID GILLEY, IUPUI, SAMARENDRA MOHANTY, UT Arlington — Ultrafast laser microbeam is finding widespread applications in eliciting highly localized damage to cellular components allowing study of in-situ repair machinery. While the high peak power density that exists in ultrafast laser can cause various types of DNA damage including double strand breaks (DSB), tuning the power of these laser microbeams may cause specific type of DNA damage. Here, we report wavelength and dose dependent parametric study of kinetics of TRF2 recruitment in cells due to DNA damage caused by ultrafast near-IR Laser. A tunable Ti: Sapphire laser beam was coupled via laser port of an inverted microscope. Spot and line laser micro-irradiation pattern in nuclear sites of HT1080 cells expressing YFP-tagged TRF2 was achieved by piezo-scanning mechanism. The recruitment of TRF2-YFP was found to depend highly on the peak irradiance of the near-IR laser microbeam, the required threshold irradiance being much higher than that observed for DSB. Further, recruitment kinetics revealed that the time constant for TRF2 recruitment depends on the laser irradiance parameters. The time required for TRF2 recruitment was found to decrease with increased peak irradiance. We will present these results and also elucidate on physical mechanism of DNA damage caused by ultrafast laser microbeam.

1:15PM W39.00011 Background Elimination and Noise Reduction by Mechanical Modulation Raman Spectroscopy , KATHLEEN HINKO, CHIEZE IBENECHE, ANDREA KEIDEL, TOBIAS BARTSCH, ERNST-LUDWIG FLORIN, University of Texas at Austin — Raman spectroscopy is widely used by biophysicists for the molecular identification of cellular substructures. However, there are high levels of background and noise associated with Raman spectra from other molecules in the microscopic detection volume. We present two methods of mechanical modulation for background subtraction and noise reduction in a Raman microscope: (1) a three-axis stage modulation for fixed objects and (2) a separate optical trap modulation for objects in solution. With our technique, we completely eliminate the background in our spectra and improve the signal-to-noise ratio by two orders of magnitude. We applied this technique to lipid vesicles and fission yeast cells in solution. Additionally, we obtained mechanical modulation Raman spectra of fission yeast in three dimensions and observed spatial differences in the molecular composition for different metabolic states of a single yeast cell.

1:27PM W39.00012 Ultraweak bioluminescence dynamics and singlet oxygen correlations during injury repair in sweet potato , MARIUS HOSSU, LUN MA, WEI CHEN, UT Arlington — Ultraweak bioluminescence at the level of hundreds of photons per second per square centimeter after cutting injury of sweet potato was investigated. A small emission peak immediate after cutting and a later and higher peak were observed. Selective singlet oxygen inhibitors and sensors have been use to study the contribution of singlet oxygen during the curing process, demonstrating increased presence of singlet oxygen during and after the late bioemission peak. It was confirmed that singlet oxygen has direct contribution to ultraweak bioluminescence but also induces the formation of other exited luminescent species that are responsible for the recorded bioluminescence.

1:39PM W39.00013 Obtaining optical properties using Representative Layer Theory[1] , NEEMA RAZAVI, BRAIN YUST, DHIRAJ SARDAR, University of Texas San Antonio — Reliable and minimally invasive methods for diagnosis of toxicity and onset of disease are important for advances in clinical practices. This is commonly achieved through the optical properties, such as a change in the absorption or scattering strength of the diseased tissue. Thus, being able to quantitatively characterize these changes is important to advancements in medical diagnostic methods. By adapting the Representative Layer Theory to the integrating sphere technique, very thin biological samples may be optically characterized, yielding a quick and easy method for monitoring optical changes as a function of disease progression. Samples, consisting of cells, dyes, and nanoparticles of known concentrations were optically characterized at multiple wavelengths. Optical properties obtained by the Representative Layer Theory are compared to those obtained through other methods, such as Kubelka-Munk and Inverse Adding Doubling which are known to have sample thickness limitations.

[1]This work is also supported in part by National Science Foundation PREM Grant No. DMR - 0934218 and UTSA Collaborative Research Seed Grant Program (CRSGP).

1:51PM W39.00014 An *in vitro* approach to understanding intracellular motor-based cargo transport , RAFAEL LONGORIA CASASA, University of Texas at Austin, Physics Department, HAYLEY MANNING, GEORGE SHUBEITA, University of Texas at Austin, Physics Department — Microtubule-based molecular motors are responsible for the long range transport of intracellular cargoes. Most cargoes move bidirectionally yet reach their destination in the cell. The mechanism by which the seemingly random bidirectional motion of cargoes is regulated by the cell to produce directed transport remains unclear. Two distinct models have been proposed: coordination via a tug-of-war, the dynamics of which depend only on the properties of the motors; and coordination via non-motor proteins. However, no direct evidence for either one has been found yet. We present an experimental method that can address the different predictions of these models. We reconstitute *in vitro* transport of endogenous motor-driven lipid droplets purified from *Drosophila* embryos. Global transport dynamics are observed under varied medium conditions by DIC microscopy. Combined with stall force measurements using an optical trap, these investigations relate the global dynamics to local changes in force production of the motors which give us a direct handle to differentiate between the different models of transport.

2:03PM W39.00015 Nonlinear optical microscopy in biology: Combining second-harmonic generation and two-photon fluorescence imaging , KOEN CLAYS, University of Leuven, Belgium — Optical microscopy has been since long a truly enabling visualization technique in the biological and biomedical sciences. Linear optical microscopy relies on simple linear optical effects. Nonlinear optical microscopy relies on the nonlinear optical properties of endogenous or exogenous chromophores to produce a better image. Two-photon fluorescence (TPF), a third-order nonlinear optical effect and observed at the focal spot only due to the quadratic intensity dependence, results in inherently higher resolution than possible for one-photon fluorescence, observed over the complete Rayleigh range. Second-harmonic generation (SHG) is a second-order nonlinear optical effect only observed for non-centrosymmetric arrangements of non-centrosymmetric chromophores. While this does put a restriction on the chromophores that can be used, it also results in structural information about symmetry when used in combination with TPF. TPF, being a third-order nonlinear process, is not restricted by any symmetry consideration. We will review the molecular design criteria for exogenous probes for combined SHG and TPF nonlinear microscopy, provide examples of optimized chromophores and show microscopy images demonstrating the use of such chromophores in nonlinear microscopy.

Thursday, March 24, 2011 11:15AM - 2:03PM –

Session W40 DPOLY: Polymer Blends A122/123

11:15AM W40.00001 Entanglement Dynamics in Miscible Polyisoprene / Poly(p-*tert*-butyl styrene) Blends , HIROSHI WATANABE, Kyoto University — Viscoelastic and dielectric behavior was examined for well entangled, miscible blends of high-M *cis*-polyisoprene (PI) and poly(p-*tert*-butyl styrene) (PtBS). The dielectric data of the blends, reflecting the global motion of the PI chains having the type-A dipoles, indicated that PI and PtBS were the fast and slow components therein. At high temperatures T, the blends exhibited two-step entanglement plateau. The high frequency (ω) plateau height was well described by a simple mixing rule of the entanglement length based on the number fraction of the Kuhn segments. At low T, the blend exhibited the Rouse-like power-law behavior of storage and loss moduli, $G' = G'' \sim \omega^{0.5}$, in the range of ω where the high-ω plateau was supposed to emerge. This lack of the high-ω plateau was attributed to retardation of the Rouse equilibration of the PI chain over the entanglement length due to the hindrance from the slow PtBS chains: The PI and PtBS chains were equilibrated cooperatively, and the retardation due to PtBS shortened the plateau for PI to a width not resolved experimentally. A simple model for this cooperative equilibration formulated on the basis of the dielectric data described the viscoelastic data surprisingly well.

11:27AM W40.00002 Local Relaxation Behavior and Dynamic Fragility in Hydrogen Bonded Polymer Blends[1] , JAMES RUNT, Penn State University, KEVIN MASSER, Penn State Univerity, HANQING ZHAO, PAUL PAINTER, Penn State University — The dynamics of intermolecularly hydrogen bonded polymer blends of poly(p-(hexafluoro-2-hydroxyl-2-propyl)styrene) with poly(vinyl acetate), poly(ethylene[30]-co-vinyl acetate[70]) and poly(ethylene[55]-co-vinyl acetate[45]) are investigated by broadband dielectric relaxation spectroscopy and Fourier transform infrared spectroscopy. Each blend component exhibits a glassy state (beta) relaxation, and these relaxations are affected by the formation of intermolecular associations. The glassy state behavior of the blends can be modeled using the Painter-Coleman association model. All blends exhibit a single Tg and a single dielectric segmental (alpha) relaxation, indicative of strong segmental-level coupling. The fragility of the glass-formers depends on the volume fraction of intermolecularly associated segments, and the association model predicts which compositions have the highest fragilities. A relaxation related to the breaking and reforming of hydrogen bonds is observed at temperatures above the alpha process, and its temperature dependence varies systematically with ethylene content.

[1]Supported by NSF-DMR Polymers Program

11:39AM W40.00003 Partial Miscibility in Copolymer Blends[1] , ELIZABETH CLARK, JANE LIPSON, Dartmouth College — Copolymers can be used to affect the miscibility of otherwise immiscible polymer blends by acting as compatibilizers. To better understand the energetics of these types of systems, we use a simple lattice model to study phase separation in binary copolymer/homopolymer blends. We focus on a copolymer that contains both A and B type monomers and a homopolymer that contains purely A type monomer. An example of a system that we are investigating is polyethylene mixed with either random or alternating poly(ethylene-co-propylene). The sequence effect on miscibility as the copolymer microstructure is varied from random to alternating is investigated as well.

[1]The support of GAANN is gratefully acknowledged.

11:51AM W40.00004 ABSTRACT WITHDRAWN –

12:03PM W40.00005 Properties of polystyrene/poly(dimethyl siloxane) blends partially compatibilized with star polymers containing a gamma-cyclodextrin core and polystyrene arms , C. MAURICE BALIK, North Carolina State University, BRAD J. BUSCHE, Pacific Northwest National Lab, ALAN E. TONELLI, North Carolina State University — Cyclodextrins (CDs) are cyclic starch molecules having a hollow central cavity which can be threaded by a polymer to form an inclusion compound. This characteristic is exploited in a new type of compatibilizer: a star polymer with a gamma-CD (g-CD) core and polystyrene (PS) arms (CD-star). Spun-cast thin films of PS containing up 20 weight percent poly(dimethyl siloxane) (PDMS) are compatibilized by CD-star. The mechanism of compatibilization involves threading of the CD core by PDMS and solubilization of the resulting slip-ring graft copolymer via the PS star arms. Thin spun-cast films of these blends exhibit a a nanoscale level of mixing and remain well-mixed after annealing at 125 C for three days. In contrast, thicker solution-cast films of these blends exhibit larger-scale phase separation since the film solidification process occurs over a period of days rather than seconds. This allows some of the PDMS to de-thread from the CD-star and phase separate. However, DSC, DMA and PDMS leaching data show that PS and PDMS remain partially compatibilized in the solution-cast films.

12:15PM W40.00006 Crystallization in the Binary Blends of Crystalline-Amorphous Diblock Copolymers Bearing Chemically Different Crystalline Block[1] , CHE-YI CHU, HSIN-LUNG CHEN, BHANU NANDAN, Department of Chemical Engineering, National Tsing Hua University, Hsin-Chu 30013, Taiwan., MING-SIAO HSIAO, Material and Chemical Research Laboratories, Industrial Technology Research Institute, Hsin-Chu 300, Taiwan. — The crystallization behavior of a series of lamellae-forming blends of a shorter PS-b-PEO (SEO) and a longer PS-b-PLLA (SLLA) has been studied. In SLLA-rich blends, the junction point constraint coupled with the poor chain mobility at low T_c ($\leq$45 °C) hampered the formal crystallization of PLLA. In this case, a local demixing between a fraction of PEO and PLLA chains took place, yielding the PLLA crystalline domains in which the PLLA crystalline stems were intervened by the PEO chains. This crystalline species gave rise to a relatively broad peak at 2θ= 15.92° in the WAXS profile and displayed a much lower melting point of ca. 100 °C compared to that of the typical α-form crystal of PLLA. It was suggested that the inserted PEO chains served as the molecular defects which induced an expansion of the a-axis and b-axis of the α-form PLLA unit cell and lowered the crystal melting point due to introduction of defect free energy.

[1]We gratefully acknowledge financial support from the National Science Council Taiwan under Contract NSC 95-2221-E-007-083.

12:27PM W40.00007 ABSTRACT WITHDRAWN –

12:39PM W40.00008 Effect of Organoclays on Immiscible Polymer Blends , MAI HA, RAMANAN KRISHNAMOORTI, University of Houston — The effect of adding organoclays on the phase behavior, rheological properties and bulk mechanical properties of immiscible polymer blends of polystyrene (PS) and poly(methyl methacrylate) (PMMA) is investigated. Traditional organoclays, prepared using alkyl ammonium chains, display a preference to segregate to the PS phase for high PS volume fraction blends where the PS forms the continuous matrix. On the other hand, for blends with low PS volume fractions, the organoclay segregates to the interface between the PS and PMMA domains and leads to a decrease in the domain size that does not change much with organoclay concentration variations from 0.1 to 2 wt %. Linear dynamic rheological data of these samples show significant increase in the low-frequency modulus of the blends with added organoclay. A thermodynamic model for estimating the interfacial modulus is proposed and the results agree well with the interfacial modulus calculated by Palierne's emulsion model. The toughness of the blends increases at low concentrations of added organoclays with the optimal improvements observed for less than 0.5 wt % added organoclay.

12:51PM W40.00009 Characterization of the Early Stages of Phase Separation in PS/PVME Blends Using Fluorescence , ANNIKA KRIISA, SUNG PARK, CONNIE ROTH, Dept of Physics, Emory University — Controlling the early stages of phase separation in polymer blends provides a potentially easy route towards obtaining interconnected nanostructured domains. We present results of thermally induced phase separation in polystyrene (PS) / poly(vinylmethylether) (PVME) blends using different fluorophores covalently attached to the PS component. Fluorescence identifies the phase separation temperature Tc at earlier stages then the more traditional method of light scattering. At Tc, a large increase in fluorescence intensity is observed due to a strong reduction in the fluorescence quenching caused by the intimate presence of the more polar PVME component. We discuss the spectral red shifts of pyrene associated with the dissolution of the weak hydrogen bonding in this blend and the change in polarity of the local environment during phase separation.

1:03PM W40.00010 Non-Isothermal Crystallization of PET/PLA Blends[1] , HUIPENG CHEN, Texas Tech University, MAREK PYDA, Rzeszow University of Technology, PEGGY CEBE, Tufts University — Binary blends of poly(ethylene terephthalate) with poly(lactic acid), PET/PLA, were studied by differential scanning calorimetry. The solution cast blends were miscible in the melt over the entire composition range. We report the non-isothermal crystallization of: a.) PET, with and without presence of PLA crystals, and b.) PLA, with and without presence of PET crystals. PET can crystallize in all blends, regardless of whether PLA is amorphous or crystalline, and crystallinity of PET decreases as PLA content increases. PLA crystallization is strongly affected by the mobility of the PET. When PET is wholly amorphous, PLA can crystallize weakly even in 70/30 blends. When PET is crystalline, PLA cannot crystallize when its own content is below 0.90. The different behaviors may be related to the tendency of each polymer to form constrained chains, i.e., to form rigid amorphous fraction, RAF. PET is capable of forming a large amount of RAF, whereas relatively smaller amount of RAF forms in PLA. Like the crystals, rigid amorphous fraction of one component may inhibit growth of crystals of the other blend partner.

[1]Supported by the National Science Foundation, Polymers Program of the Division of Materials Research under DMR-0602473 and the MRI Program under DMR-0520655.

1:15PM W40.00011 Critical Micelle Concentrations for Different Micelle Shape in Diblock Copolymer/Homopolymer Blends , JIAJIA ZHOU, AN-CHANG SHI, McMaster University — Diblock copolymers (AB) blended with homopolymers (A) may self-assemble into lamellar, cylindrical and spherical micelles. The critical micelle concentrations for different micelle shape are determined using self-consistent field theory. The effect of varying copolymer block asymmetry, homopolymer molecular weight and monomer-monomer interaction are considered.

1:27PM W40.00012 Ordered Materials via Additive Driven Assembly and Reaction using Surfactant-Based Templates , MICHAEL R. BEAULIEU[1], VIKRAM K. DAGA[2], ALAN J. LESSER, JAMES J. WATKINS, University of Massachusetts Amherst — We recently reported (1) the ordering behavior of Pluronic surfactant melts through the addition of aromatic additives with hydrogen bond donating groups, which exhibit selective interactions with the polyethylene oxide (PEO) block. The ordered blends had domain sizes ranging from 12 to 16 nm at additive loadings up to 80%.The goal of this work is to utilize condensation chemistries based on the functionality of similar additives, to yield ordered composite materials that could be used for applications involving membranes or dielectric materials. The structure of the blends and composites are determined by small angle x-ray scattering, which indicates that the ordered structure is preserved following reaction of the additives. Differential scanning calorimetry indicates that an increase in additive loading causes a decrease in the melting temperature and enthalpy of melting of the PEO, which demonstrates that the interaction between the PEO segments and the additive is strong. (1) Daga, V.K., Watkins, J. J. Macromolecules, ASAP.

[1]Polymer Science and Engineering Department
[2]Chemical Engineering Department

1:39PM W40.00013 Interfacial Structure and Dynamics of the liquid/liquid interface between Polydimethylsiloxane and Polystyrene[1] , MESFIN TSIGE, University of Akron — Many important phenomena in biology, chemistry and in various fields involve processes that occur at the interface between two immiscible liquids. A molecular level understanding of such interfaces is crucial for insight into the complex dynamics that are observed at such interfaces. In this study, atomistic molecular dynamics simulations were performed to study the structural and dynamical properties of the liquid/liquid interface between two immiscible polymers, polydimethylsiloxane (PDMS) and polystyrene (PS). A series of simulations is carried out to examine the temperature and molecular weight dependence of the orientation of molecules at and away from the interface, intermolecular correlation at the interface, interfacial tension and interfacial thickness. The results from these detailed simulations will be presented.

[1]This work is supported by the NSF (DMR0847580).

1:51PM W40.00014 Effect of linear contaminants on the dynamics and rheology of ring polymer melts , JONATHAN HALVERSON, Max Planck Institute for Polymer Research, GARY GREST, Sandia National Laboratories, KURT KREMER, Max Planck Institute for Polymer Research — Understanding the behavior of ring polymer melts remains a challenge. Early experimental efforts to characterize the rheological behavior of pure ring polymer melts have led to controversial results most likely because the samples were contaminated with linear chains. Recent studies found that stress relaxation follows a simple power law with no sign of a plateau. To further investigate these systems we have conducted molecular dynamics simulations for a semiflexible bead-spring model for chain lengths up to 14 entanglement lengths. The structure, dynamics and rheology of these systems are investigated for different concentrations of linear chains. We find that the viscosity of a ring melt increases dramatically when trace quantities of linear contaminants are present. The rings are found to swell slightly and diffuse more slowly with increasing linear concentration while the linear chains mostly behave as if in a pure linear melt. We use the concept of threading, analogous to thread passing through the eye of a needle, to explain the response of the ring melts to linear contaminants.

Thursday, March 24, 2011 11:15AM - 2:03PM –

Session W41 DCP: Focus Session: Electronic Structure and Applications to Energy Conversion I A115/117

11:15AM W41.00001 Tuning the electronic structure of II-VI semiconductors and nanostructures for energy applications , SHENYUAN YANG, Molecular Foundry, Lawrence Berkeley National Laboratory — Using first-principles calculations within density functional theory (DFT), we study the impacts of quantum confinement, strain, and surface ligand passivation on the electronic structure of typical II-VI wurtzite semiconductors and nanostructures. In CdSe/CdTe core/shell nanowires, large anisotropic strains develop due to the large lattice mismatch. These strains result in significant reductions in band gap in the CdSe core with increasing CdTe shell thickness, by amounts comparable to that expected from reduced quantum confinement [1]. The response of band gaps of wurtzite compounds to anisotropic strain is further shown to be large and highly non-linear, and system-dependent [2]. In addition, we also explore the effects of chemisorbed ligand on the electronic structure of CdSe surfaces. Substantial shifts in band edge energies are predicted due to the induced dipole at the CdSe-ligand interface and the intrinsic dipole of the ligand [3]. Our studies suggest well-defined routes to control both the band gaps and band edge energies of nanomaterials for light-harvesting applications.

[1] S. Yang, D. Prendergast, and J. B. Neaton, Nano Lett. 10, 3156 (2010).
[2] S. Yang, D. Prendergast, and J. B. Neaton, Appl. Phys. Lett., in press (2011).
[3] S. Yang, D. Prendergast, and J. B. Neaton, in preparation (2011).

11:51AM W41.00002 TR-2PPE Studies of Ultrafast Charge Separation at Organic Photovoltaic Interfaces , S.W. ROBEY, G.J. DUTTON, NIST, W. JIN, J.E. REUTT-ROBEY, University of MD — Dissociation of excitons in organic photovoltaic (OPV) devices occurs exclusively at interfaces between donor and acceptor molecular materials. To help understand critical charge separation processes, we have performed time-resolved two-photon photoemission (TR-2PPE) studies of sub-picosecond exciton dynamics at well-characterized organic donor-acceptor interfaces. Interfaces between phthalocyanines and C_{60} were engineered using organic MBE and characterized using STM, STS, and UPS. Ultrafast TR-2PPE measurements were performed on CuPc\$C_{60}$ structures by pumping the lowest optical $\pi \rightarrow \pi^*$ transitions (Q-band) to generate CuPc singlet (S_1) excitons and probing this population with a time-delayed UV pulse. For thick films, CuPc S_1 decay is dominated by vibrational relaxation (several 100's femtoseconds) and singlet-to-triplet conversion ($\sim$ 1 picosecond). Directly at the interface, however, charge transfer to C_{60} dominates decay of S_1 exciton, ($\sim$ 100 femtoseconds) . We also find evidence for important recombination routes from the charge separated state back to lower-lying CuPc T_1 triplet excitons. To test the impact of intersystem crossing to triplet levels, we have performed analogous investigations for H_2Pc\$C_{60}$ interfaces. Results for this interface will be compared and contrasted with the CuPc\$C_{60}$ case.

12:03PM W41.00003 Near- and Far-Field Effects on Excited States at Organic Semiconductor and Metal Interfaces , OLIVER MONTI, MARY STEELE, NAHID ILYAS, LEAH KELLY, University of Arizona — We present an investigation of the evolution of excited states at the interface of the dipolar organic semiconductor vanadyl naphthalocyanine on highly oriented pyrolytic graphite. Using two-photon photoemission we observe several excited states at sub-monolayer to few-monolayer coverages. Excited states of this organic semiconductor are progressively stabilized with coverage, an effect that is somewhat mirrored in the image state manifold as well. These findings can be understood in the context of a simple electrostatic model that considers how molecular levels and vacuum level are influenced differentially by the the strong electrostatic fields present at the interface with dipolar molecules: While the vacuum level rises continuously with coverage, the molecular states are significantly depolarized as a function of electric fields in the near-field regime. This indicates that the interfacial excited state electronic structure is strongly sensitive to long-range intermolecular interactions mediated by the surface, with direct implications for energy level alignment and charge transfer dynamics at the interface. Interfacial electrostatic fields may therefore be used to manipulate in a concrete fashion interfacial charge transfer processes such as photoinduced interfacial electron transfer.

12:15PM W41.00004 Time-domain ab initio studies of excitation dynamics in semiconductor quantum dots , OLEG PREZHDO, University of Rochester — Solar energy applications require understanding of dynamical response of novel materials on nanometer scale. Our state-of-the-art non-adiabatic molecular dynamics techniques, implemented within time-dependent density functional theory, allow us to model such response at the atomic level and in real time. The talk will focus on single and multiple exciton generation, relaxation, annihilation and dephasing in semiconductor quantum dots.

References:
[1] O. V. Prezhdo, "Multiple excitons and electron-phonon bottleneck in semiconductor quantum dots: Insights from ab initio studies", *Chem. Phys. Lett. – Frontier Article*, **460**, 1 (2008)
[2] O. V. Prezhdo "Photoinduced dynamics in semiconductor quantum-dots: insights from time-domain ab initio studies", *Acc. Chem. Res.*, **42**, 2005 (2009)
[3] A. B. Madrid, H.-D. Kim, O. V. Prezhdo, "Phonon-induced dephasing of excitons in silicon quantum dots: multiple exciton generation, fission and luminescence", *ACS-Nano*, **3**, 2487 (2009)
[4] C. M. Isborn, O. V. Prezhdo, "Quantum dot charging quenches multiple exciton generation: first-principles calculations on small PbSe clusters", *J. Phys. Chem. C,* **113**, 12617 (2009)
[5] S. V. Kilina, D. S. Kilin, O. V. Prezhdo, "Breaking the phonon bottleneck in PbSe and CdSe quantum dots: time-domain density functional theory of charge carrier relaxation", *ACS-Nano*, **3**, 93 (2009).
[6] S. A. Fischer, A. B. Madrid, C. M. Isborn, O. V. Prezhdo, "Multiple exciton generation in small Si clusters: A high-level, ab initio study", *J. Phys. Chem. Lett.,* **1**, 232 (2010).

12:51PM W41.00005 Hole Localization in Molecular Crystals From Hybrid Density Functional Theory[1] , NA SAI, PAUL F. BARBARA, University of Texas at Austin, KEVIN LEUNG, Sandia National Laboratory — Charge trapping in organic solids and interfaces plays an important role in organic photovoltaic efficiencies. Experimental confirmation of intrinsic charge trapping at the atomic scale and the tools to directly probe the trap energy landscape, however, remain lacking. We use first principles computational methods to examine hole trapping in organic molecular crystals. We present a computational scheme based on the tuning of the fraction of exact exchange in hybrid density functional theory to eliminate the many-electron self-interaction error [1]. With small organic molecules, we show that this scheme gives accurate descriptions of ionization and dimer dissociation. We demonstrate that the excess hole in perfect molecular crystals can form self-trapped hole polarons. The predicted absolute ionization potentials of both localized and delocalized holes are consistent with experimental values.

[1] N. Sai, P. Barbara, and K. Leung (submitted).

[1]The work is supported by Energy Frontier Research Center funded by the U.S. DOE Office of Basic Energy Sci ences under Award number DE-SC0001091. KL is also supported by the DOE under Contract DE-AC04-94AL85000.

1:03PM W41.00006 Linear Dichroism and Photoluminescence Microscopy Imaging of Grain Boundaries in Crystalline Metal-Free Phthalocyanine Thin Films[1] , ZHENWEN PAN, CODY LAMARCHE, ISHVIENE COUR, NAVEEN RAWAT, LANE MANNING, RANDALL HEADRICK, MADALINA FURIS, PHYSICS DEPT. AND MATERIAL SCIENCE PROGRAM, UNIVERSITY OF VERMONT, BURLINGTON, VT 05405 TEAM — We employed a combination of linear dichroism and photoluminescence microscopy with spatial resolution of 5μm to study the excitonic properties of solution-processed metal-free phthalocyanine (H2Pc) crystalline thin films with millimeter-sized grains. We observe a highly-localized, sharp, monomer-like emission at the high angle grain boundaries, in contrast to samples with more uniform grain orientation where no such feature has been observed. The energy difference between the grain boundary luminescence and the HOMO-LUMO singlet exciton recombination of the crystalline H2Pc is measured to be 160meV. Our systematic survey of grain boundaries indicates this localized state is never present at low angle boundaries where the π-orbital overlap between adjacent grains is significant. It supports recent results which associated a decrease in carrier mobility with the presence of large angle boundaries in similar crystalline pentacene films.

[1]This project is supported by DMR- 0722451; DMR-0348354; DMR- 0821268.

1:15PM W41.00007 Theories and applications for characterizing electronic coupling factors , CHAO-PING HSU, Academia Sinica — The transport of charges and excitation energy are two processes of fundamental importance in many biological and material systems. One of the fundamental parameters in the transport rates is the electronic coupling, which is essentially an off-diagonal Hamiltonian matrix element between the initial and final diabatic states. We have developed ways to define the diabatic states and calculate the coupling factors, including those for electron transfer (ET) and excitation energy transfer (EET). The fundamental method development and applications will be discussed. For characterizing TEET, the Fragment Spin Difference (FSD) was developed and it can be to calculate the TEET coupling over a general class of systems. TEET in bacterial light-harvesting complex LH2 and the peridinin chlorophyll-a protein (PCP) of dinoflagellates were calculated and analyzed. Our results are in good agreement with experimental results and it offers limits to the photoprotection models. Therefore, with the FSD scheme, it is possible to quantify and analyze the electronic couplings in TEET processes in large systems, and to derive insights and limits of theoretical models.

1:51PM W41.00008 Ab initio calculation of optical spectra of solvated molecules: GW+BSE method for liquid environments , JEEHYE LEE, TOMAS ARIAS, Cornell University — Electronic excitations for solvated systems have drawn a great interest in the energy community because they provide a possibility to engineer photoexcitation processes. Time-dependent DFT (TDDFT) and the hybrid QM/MM approach successfully calculate the solvent shift in excitation energies (solvatochromic shift) for confined systems, but are well known to work best for small systems and Frenkel excitons. Here we present a new modification of the GW and Bethe-Salpeter equation (GW+BSE) methods which allows treatment of solvated systems beyond the TDDFT level by including the frequency-dependent polarizability of the solvent at the diagrammatic level. In this initial work, we present the solvatochromic and ionization potential shifts for a series of molecules in aqueous solution.

Thursday, March 24, 2011 11:15AM - 2:15PM –
Session W42 DPOLY: Focus Session: Polymer Brushes A302/303

11:15AM W42.00001 Responsive Grafted Polymer Layers: the role of pH, temperature and surface geometry , IGAL SZLEIFER, Northwestern University — The competition between chemical equilibrium, e.g. protonation, and physical interactions determines the molecular organization and functionality in biological and synthetic systems. Charge regulation by displacement of acid-base equilibrium induced by changes in the local environment provides for a feedback mechanism that controls the balance between electrostatic, van der Waals, steric interactions and molecular organization. What are the mechanisms that determine the interplay between all these different factors? In this talk I will describe a molecular theory to address this question. In particular, the theory will be used to study the structural and thermodynamic properties of end-grafted polyacids with hydrophobic backbones. The molecular theory explicitly includes the size, shape, conformations, charge and charge distribution of all the molecular species in the system and incorporates excluded volume, van der Walls and electrostatic interactions coupled with acid-base equilibrium. On planar surfaces, the theory predicts the formation of surface micelles with morphologies that depend upon the bulk pH, solution ionic strength, temperature and surface coverage. The self assembled aggregates, present domains of varying local pH that is very different from that of the bulk solution. We show that a qualitatively new form of local organization arises that is only found when there is explicit coupling between charge regulation and physical interactions. The different morphologies can be manipulated by changing the bulk solution conditions and they provide for local domains with controlled charge and pH with large gradients with a characteristic size of a few nanometers. Following this we will discuss how ion conductivity in nanopores functionalized with polybases changes as a function of solution pH. The predictions of the theory are in quantitative agreement with experiments and they provide a physical explanation of the interplay between molecular organization and charge in the nanopore. The last part of the talk will be devoted to a new system in which we show how to use the theory under non-equilibrium conditions to study the flux of ions in finite nanopores with grafted polybases (or polyacids) in the presence of external potentials.

11:51AM W42.00002 Polyelectrolyte brushes in mixed ionic medium studied via intermolecular forces , ROBERT FARINA, NICOLAS LAUGEL, UC-Berkeley, PHILIP PINCUS, UC-Santa Barbara, MATTHEW TIRRELL, UC-Berkeley — The vast uses and applications of polyelectrolyte brushes make them an attractive field of research especially with the growing interest in responsive materials. Polymers which respond via changes in temperature, pH, and ionic strength are increasingly being used for applications in drug delivery, chemical gating, etc. When polyelectrolyte brushes are found in either nature (e.g., surfaces of cartilage and mammalian lung interiors) or commercially (e.g., skin care products, shampoo, and surfaces of medical devices) they are always surrounded by mixed ionic medium. This makes the study of these brushes in varying ionic environments extremely relevant for both current and future potential applications. The polyelectrolyte brushes in this work are diblock co-polymers of poly-styrene sulfonate (N=420) and poly-t-butyl styrene (N=20) which tethers to a hydrophobic surface allowing for a purely thermodynamic study of the polyelectrolyte chains. Intermolecular forces between two brushes are measured using the SFA. As multi-valent concentrations are increased, the brushes collapse internally and form strong adhesion between one another after contact (properties not seen in a purely mono-valent environment).

12:03PM W42.00003 Microsecond MD Simulations of Nano-patterned Polymer Brushes on Self-Assembled Monolayers , CREIGHTON BUIE, LIMING QIU, SOYEUN PARK, MARK VAUGHN, KWAN CHENG, Texas Tech University — Nano-patterned polymer brushes end-grafted onto a self-assembled monolayer interface have unique properties and application potential. However, the molecular-level interactions of these brushes with the substrate interface and the solvent are still not clear. Using a coarse-grained MD simulation approach we investigate the structure and dynamics of brushes of monomer length ranging from 25 to 75 units and an implant density σ of 0.2 to 1.0 nm^{-2} that were end-grafted onto a 5×5 nm^2 well in a self-assembled hexadecane monolayer. The behavior of each polymer-monolayer-water complex was simulated from 3 to 12 μs.The excess width and the extended height of the polymers, the nanosecond-resolved conformational transition kinetics from a compact helical to a random coil-like structure, and the time-averaged monomer density maps were determined. The scaling behavior of these brushes differs from that of previous thermodynamic and computational studies of homogeneous brushes and nanopatterned stripes. Here, we find a weaker dependence of brush height on implant density, $\sigma^{0.29}$ rather than $\sigma^{1/3}$ and near linear scaling of the excess width on σ rather than the $\sigma^{1/2}$. Our structural dynamics data and molecular templates are useful for future experimental and computational investigations of nano-patterned polymer brushes at the nanoscopic length and mesoscopic time scales.

12:15PM W42.00004 Nano-pillars created from the surface-grafted crosslinked polymer chains , SOYEUN PARK, DIPIKA PATEL, FERNANDO MONJARAZ, Texas Tech University, WOLFGANG FREY, The University of Texas at Austin, TEXAS TECH UNIVERSITY, DEPARTMENT OF PHYSICS TEAM, THE UNIVERSITY OF TEXAS AT AUSTIN, DEPARTMENT OF BIOMEDICAL ENGINEERING COLLABORATION — Nano-patterned polymer chains with the controlled mechanical properties are widely applicable to biological and chemical studies. We synthesized linear and crosslinked polymer chains grafted onto micro/nano-patterned substrates by developing a series of unique bottom-up fabrication steps based on the iniferter-driven quasi-living polymerization. We incorporated conventional photolithography and nanosphere lithography. The AFM study provides insight into the influence of the addition of the crosslinker on the configurative, kinetic, mechanical, and wetting properties of polymer chains grafted onto micro/nano-patterns. We found that the addition of crosslinker successfully converts the mushroom-like configuration of nanopatterned polymer chains into the well-standing brush like polymer chains, i.e, soft nano-pillars. By analyzing the AFM force-distance curves obtained in the two-dimensional array and lateral force images, we found that the shear moduli of the obtained soft nano-pillar can be adjusted by varying the concentration of crosslinkers.

12:27PM W42.00005 Polymer brushes: Tools for surface design[1] , CHRISTOPHER OBER, Cornell University — Polymers brushes are ideal materials for interfacing with biological systems as they share many of the same molecular components and properties. Polymer brushes provide remarkable screening power in shielding a substrate from the environment through both steric and charge interactions. However, the majority of biomolecular species will still non-specifically bind to polymer brush surfaces unless some care is given to molecular design. Several polymer brush systems are described to control interaction of biomacromolecules and cells by design of specific and non-specific interactions in polymer brush architectures. "Grown from" and block copolymer brushes are described, both of which provide excellent substrates for study of brush surfaces. Examples of polymer brushes used for sensor creation and for investigation of cellular interaction are given. Brushes used in non-fouling coatings tailored for marine applications and in which amphiphilic structures play an important role are also described.

[1]Support from both NSF and ONR is gratefully acknowledged.

1:03PM W42.00006 Preparation, Patterning, and Electrical Characterization of Conjugated Polymer Brushes , JOSE ALONZO, JIHUA CHEN, ONOME SWADER, NIKOLAY LAVRIK, MARK DADMUN, S. MICHAEL KILBEY II, DEPT. OF CHEMISTRY, UNI. OF TENNESSEE; CENTER FOR NANOPHASE MATERIALS SCIENCES, OAK RIDGE NATL LAB. COLLABORATION — Intimate contact at donor-acceptor interfaces and electrode-film interfaces is considered important for optoelectronic devices. This presentation will describe the formation and characterization of novel conjugated polymer brushes based on end-functionalized poly(3-hexylthiophene) and poly(para-phenylene) (PPP). In each case, end-functionalized polymers were synthesized and grafted to silicon substrates, with changes in film preparation method and polymer molecular weight used to manipulate the grafting density of the interfacial layers. Highly tunable PPP brushes having thickness ranging from 4 to 108 nm were obtained by in situ aromatization of poly(cyclohexadiene) brushes. Exceptionally smooth brush-modified interfaces were prepared, and neutron reflectometry, ellipsometry, AFM, and transmission electron microscopy were used to characterize layer structure and chain density. This presentation will also describe efforts to measure properties of these nanostructured layers using DC conductivity and AC electrical impedance measurements, as well as micro and nano-patterning of conjugated polymer brushes in the context of nanocircuit or organic solar cell applications.

1:15PM W42.00007 Quantifying Fluctuations/Correlations in Polymer Brushes , QIANG WANG, XINGHUA ZHANG, Department of Chemical and Biological Engineering, Colorado State University, PENGFEI ZHANG, BAOHUI LI, Institute of Physics, Nankai University — Fast lattice Monte Carlo (FLMC) simulations with multiple occupancy of lattice sites and Kronecker δ-function interactions give orders of magnitude faster/better sampling of the configurational space of multi-chain systems than conventional lattice MC simulations with self- and mutual- avoiding walks and nearest-neighbor interactions.[1] Using FLMC simulations with Wang-Landau – Transition-Matrix sampling, we have studied polymer brushes in both an implicit and explicit solvent. The various quantities obtained from simulations (including the internal energy, Helmholtz free energy, constant-volume heat capacity, segmental distribution, and chain sizes) are compared with predictions from the corresponding lattice self-consistent field theory and Gaussian fluctuation theory that are based on the same Hamiltonian as in FLMC simulations (thus without any parameter-fitting) to unambiguously and quantitatively reveal the effects of system fluctuations and correlations neglected or treated only approximately in the theories.

[1]Q. Wang, **Soft Matter, 5**, 4564 (2009).

1:27PM W42.00008 Structures of One and Two Polymer Mushrooms , DELIAN YANG, QIANG WANG, Department of Chemical and Biological Engineering, Colorado State University — A polymer mushroom here is referred to as a group of chains end- grafted at the same point on a flat and impenetrable substrate. Using lattice self-consistent field (LSCF) calculations with the Kronecker δ-function interactions (instead of the commonly used nearest-neighbor interactions), we have studied the structures of one and two polymer mushrooms in an explicit solvent as a function of the polymer volume fraction in the system, solvent quality characterized by the Flory-Huggins χ parameter, and distance between the two mushrooms. Since LSCF results are exact only in the limit of number of chains $n \to \infty$, we also use fast lattice Monte Carlo (FLMC) simulations[1] with the same Hamiltonian as in LSCF theory to examine how this limit is approached with increasing n. Direct comparisons between LSCF and FLMC results without any parameter-fitting quantify the fluctuation/correlation effects neglected in LSCF theory.

[1]Q. Wang, **Soft Matter, 5**, 4564 (2009).

1:39PM W42.00009 Tethered chains in good and poor solvent - effects of lateral confinement on adsorption and chain collapse , JUTTA LUETTMER-STRATHMANN, Departments of Physics and Chemistry, The University of Akron, RYAN M. VAN HORN, Department of Chemistry, Allegheny College — The grafting density of a polymer brush affects the response of the system to changes in solvent quality and surface interactions. In this work, we focus on low (mushroom) and intermediate (semi-dilute regime) grafting densities and model a polymer chain in a brush as a single tethered chain subject to an applied force field of cylindrical symmetry that pulls the chain segments toward an axis through the tethering point and normal to the surface. The polymer chain is represented by a bond-fluctuation model with extended range attractive bead-bead interactions and variable bead surface interactions. Monte Carlo simulations with a Wang-Landau type algorithm are performed to determine the density of states in the state space of monomer- monomer contacts, monomer-surface contacts, and lateral chain extension. We present results for the effect of lateral confinement on conformational transitions such as chain adsorption in good and poor solvent.

1:51PM W42.00010 Semiflexible Polymer Brushes , SHILIYANG XU, J.M. SCHWARZ, Physics Department, Syracuse University — Non-crossing flexible polymer brush configurations with N polymers correspond to N vicious random walkers, i.e. the system stalls when any two random walkers meet. We study a system of N vicious accelerating walkers with the velocity undergoing Gaussian fluctations, as opposed to the position, to model semiflexibility. We numerically compute the survival probability exponent, α, for this system, which characterizes the probability for any two semiflexible polymers in the brush not to cross. The data suggest that $\alpha = \frac{1}{8}N(N-1)$. We also numerically study N vicious Levy flights and find, for example, for $N = 3$ and a Levy index $\gamma = 1$ that $\alpha = 1.26 \pm 0.01$.

2:03PM W42.00011 Interfacial properties of statistical copolymer brushes , DAVID TROMBLY, VICTOR PRYAMITSYN, VENKAT GANESAN, University of Texas at Austin — The interfacial properties of statistical copolymers have important ramifications for the design of patterned thin films with preferred morphologies. In order to explore these properties, we study the interfacial properties of random copolymer brushes in contact with a thin film composed of a homopolymer of one of the blocks. We calculate the interfacial widths and interfacial energies between them as a function of different parameters. We find that the interfacial widths decrease (signifying expulsion of the free chains from the brush) with increasing free chain length, grafting density, and Flory interaction parameter χN as well as with decreasing grafted chain length. The interfacial energies show inverse trends to the interfacial widths, except that results for varying grafting density depend on how chemically similar the brush is to the film. We also compare the interfacial efficacies for different types of randomness and find that, except for the case of very blocky chains, blockiness has only little effect on the properties of the interface. We discuss our findings in terms of the design of neutral surfaces and show that our results are consistent with comparable experimental results.

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W43 DPOLY: Morphology and Transport in Charged Polymers, Block Copolymers, Membranes, and Films A306/307

11:15AM W43.00001 Characterization of a Model Polyelectrolyte Membrane Using a Semi-crystalline Block Copolymer , KEITH BEERS, XIN WANG, NITASH BALSARA, UC Berkeley — The microstructured block copolymer sulfonated polystyrene-block-polyethylene is studied as model system for use as a proton exchange membrane in a fuel cell. Self-assembly of this system creates proton conducting hydrophilic channels in the form of sulfonated polystyrene domains, while the polyethylene domains create a hydrophobic matrix to provide mechanical stability. This system serves as a powerful model system since the effects of domain size, morphology and crystallinity on water uptake and proton conductivity can be investigated. Similar systems have shown the ability of small hydrophilic channels to prevent drying at high temperatures in humid air, but have focused on amorphous hydrophobic blocks. The morphology, water uptake, and proton conductivity of this semi-crystalline model system will be discussed.

11:27AM W43.00002 Structure-Property Relationships in Sulfonated Pentablock Copolymers , JAE-HONG CHOI, Department of Materials Science and Engineering, University of Pennsylvania, CARL WILLIS, Kraton Polymers LLC, KAREN I. WINEY, Department of Materials Science and Engineering, University of Pennsylvania — Membranes of pentablock copolymers consisting of poly(*tert*-butyl styrene) (TBS), hydrogenated polyisoprene (HI), and partially sulfonated poly(styrene-*ran*-styrene sulfonate) (SS) were studied using small angle X-ray scattering (SAXS) and transmission electron microscopy (TEM). The TBS-HI-SS-HI-TBS pentablock copolymer in solution forms spherical micelles with a core of SS and a corona of solvated HI and TBS. The spherical micelles in solution compact as the solvent evaporates and some of SS cores merge to form interconnected SS microdomains without substantially changing their shape. The number of connections increases with the volume fraction of the SS block, which increases with sulfonation level. The structure does not have long-range order, because strong ionic interactions prevent extensive rearrangement. The morphologies of the sulfonated pentablock copolymers will be correlated with their transport properties.

11:39AM W43.00003 Interfacial Stability of Solid Block Copolymer Electrolytes for Rechargeable Lithium Metal Batteries , GREG STONE, SCOTT MULLIN, NITASH BALSARA, University of California at Berkeley — Solid electrolytes that can resist dendrite growth from the lithium surface and adhere to the electrode surface are needed for the development of rechargeable batteries with lithium metal anodes. We show that self-assembled block copolymer electrolytes are inherently more stable against lithium metal anodes than homogeneous homopolymers. This is due to an unusual combination of solid-like properties in the bulk to resist dendrite growth, arising from a randomly oriented granular structure, and the liquid-like properties of perpendicularly oriented lamellae that are formed at the lithium-electrolyte interface providing adhesion to the electrode.

11:51AM W43.00004 Local dielectric constant and its effects on the microphase separation in charged-neutral diblock copolymer melts , RAJEEV KUMAR, National Center for Computational Sciences, Oak Ridge National Lab, Oak Ridge, TN- 37831, SCOTT SIDES, Tech-X Corporation, Boulder, CO - 80303, BOBBY SUMPTER, Computer Science and Mathematics Division & Center for Nanophase Materials Sciences, Oak Ridge National Lab, Oak Ridge, TN- 37831 — Using block copolymers as mesoscale templates has potential applications for improved photovoltaic devices and fuel-cells. Charged species in these polyelectrolytic copolymers play a vital role in determining the details of the nanoscale morphologies formed when these systems phase segregate. We have carried out a quantitative analysis of the local dielectric constant for charged-neutral diblock copolymer melts using field-theoretic simulations based on the self-consistent field theory (SCFT). Quantitative expression for the local dielectric constant in terms of the local electric field will be presented along with its effects on the microphase separation in these systems. Using large-scale SCFT simulations, we will explore the effects of different experimental parameters on the morphology diagram. These parameters include the chain length, temperature, degree of ionization and length fraction of the charged block. Also, the effect of added salt on the disorder-order transition temperature and the domain spacings of the ordered morphologies along with the distribution of small ions (counterions and co-ions) will be presented.

12:03PM W43.00005 Magnetically aligned ion-transport polymer membranes[1] , PAWEL MAJEWSKI, MANESH GOPINADHAN, CHINEDUM OSUJI, Yale University — We present the use of magnetic fields to direct the self assembly and impose long-range order in amphiphilic block-copolymers which can be utilized as solid electrolytes for ion-transport membranes or nanomaterials synthesis templates. Our approach allows us to produce highly aligned hexagonally packed cylindrical or lamellar polymer microdomains over macroscopic areas. We systematically explore the influence of several parameters; the strength of magnetic field used for alignment, lithium ion content and temperature on the conductivity of such membranes. A surprising order of magnitude increase in conductivity is found in films aligned in the conduction direction relative to the non-aligned case. The conductivity of field aligned samples shows a non-monotonic dependence on temperature, with a distinct decrease on heating in the proximity of the order-disorder transition of the system before increasing again at elevated temperatures in homogenous melt state. The data suggest that domain-confined ion transport in hexagonally packed cylindrical systems differs greatly in anisotropy compared to lamellar systems.

[1]This work is funded by the NSF under DMR-0847534.

12:15PM W43.00006 The effect of salt-doping on the lamellar phase of AB diblock copolymers , ISSEI NAKAMURA, ZHEN-GANG WANG, Division of Chemistry and Chemical Engineering, California Institute of Technology — We study the effect of adding salts on the lamellar phase of AB diblock copolymers by means of the self-consistent field theory. We consider a model in which the A and B blocks have different dielectric constants. We include the Born energy to account for the preference of salt ions to be solvated by higher dielectric polymer. We first show that the effective χ parameter can be increased upon addition of salt, depending on the size of salt particles, with an accompanied increase in the domain spacing of the lamellar phase. The salt ions tend to be localized in the microphase where the higher dielectric components are dominant. The effect of the incompressibility on the distribution of salt ions is also studied. Moreover, we include a binding interaction between one of the blocks and one of the salt ions (e.g., cations), and study the effects of such strong binding on the distribution of the counterions (anions).

12:27PM W43.00007 Impact of morphology on conductivity of lamellar block copolymer electrolytes for battery applications , VENKAT GANESAN, University of Texas at Austin, VICTOR PRYAMITSYN, The University of Texas at Austin — We use bond fluctuation model based Monte Carlo simulations to study the correlations between structure and the conductivity of the lamella phase of block copolymer electrolytes. We investigate the effects of degree of segregation, polymer molecular weights and the alignment of the lamellae upon the conductivity of the block copolymer lamella. Our results indicate different influences of the preceding factors upon the conductivities parallel and perpendicular to the lamellae. These results are rationalized in terms of the distributions of the ions and the overall inhomogeneous dynamics of the polymer molecules.

12:39PM W43.00008 Dynamics of water in sulfonated poly(phenylene) membranes , NARESH OSTI, THUSITHA ETAMPAWALA, Clemson University, UMESH SHRESTHA, DVORA PERAHIA, Clemson University, CHRISTOPHER CORNELIUS, University of Connecticut — The dynamics of water in networks formed by highly rigid ionic polymers, sulfonated poly(phenylene) as observed by quasi elastic neutron scattering (QENS) is presented. These rigid ionic polymers have potential as effective ion exchange membranes with impact on a large number of applications from water purification to clean energy, where its rigidity distinguishes it from other ionic polymers. Its transport characteristics are affected by its rigidness as well as by direct interactions with the solvent. Our QENS studies as a function of sulfonation levels, temperature and solvent content have shown that on the time scale of the measurement, the polymers are rigid. While macroscopically all samples swell, and transport water, the water molecules appear locally rather confined. Water however remind non-frozen to subzero temperatures. The results will be discussed in view of theoretical models including continues diffusion and hopping of solvent molecules.

12:51PM W43.00009 Morphology and Transport Properties of Phosphonium-containing Styrenic Ionomers with Random Charge Placement , RICK BEYER, KRISTOFFER STOKES[1], JOSHUA ORLICKI, Army Research Laboratory, Aberdeen Proving Ground, MD, YUESHENG YE, YOSSEF ELABD, Drexel University, Philadelphia, PA — Alkaline fuel cell (AFC) technology is currently of interest for portable power supplies due in part to the use of less expensive non-noble metals (nickel, iron, cobalt) as the catalyst material. Wide-spread use of the AFC has been prevented by the use of aqueous KOH as the liquid electrolyte, easily poisoned by CO_2. Development of an semipermeable polymeric alkali anion exchange membrane (AEM) would significantly improve the usefulness of AFCs. We have synthesized a series of random copolymers of styrene and p-vinylbenzyl-trimethylphosphonium chloride, via RAFT polymerization. Detailed ^{1}H-NMR analysis of the polymerization conditions allowed us to refine our approach and generate materials with random monomer addition. ^{1}H-NMR was also used to quantify ion contents, which range from 15 mol% to 100 mol%. In this presentation, we will review the synthesis and characterization of these novel cationomers, and then report on their anion transport characteristics and morphological behavior as characterized via SAXS and TEM.

[1]Current affiliation: Celgard, LLC

1:03PM W43.00010 Morphology of precise acid copolymers neutralized with monovalent cations , MICHELLE SEITZ, University of Pennsylvania, KATHLEEN OPPER, DuPont, KENNETH WAGENER, University of Florida, KAREN WINEY, University of Pennsylvania — Poly(ethylene-co-acrylic acid) copolymers with precisely spaced acid groups along the strictly linear chain backbone form the basis of a new family of ionomers with unprecedented molecular uniformity. These copolymers were neutralized with monovalent cations (Li, Na, and Cs) and their morphologies were studied using X-ray scattering. In order to more fully understand the ionic aggregation in these systems, both the low and high angle features are considered. At low angle a sharp ionomer peak arises from interaggregate interference and shifts with acid spacing. At high angle, the amorphous halo from the average backbone separation is observed. For materials with an acid group on every 9th carbon, additional high angle scattering is observed which may be related to either the internal aggregate structure or isolated ion pairs.

1:15PM W43.00011 Cubic Ordering of Aggregates in Precise Phosphonic Acid Copolymers , FRANCISCO BUITRAGO, University of Pennsylvania, KATHLEEN OPPER, KENNETH WAGENER, University of Florida, KAREN WINEY, University of Pennsylvania — Polyethylene-acid copolymers were synthesized by acyclic diene metathesis (ADMET) chemistry. The result is a series of strictly linear, high molecular weight polyethylenes with pendent acid groups separated by a precisely controlled number of methylene units. Previous studies have been focused on acrylic acid copolymers and ionomers. Here, we focus on phosphonic acid pendent groups in single and geminal architectures. The morphology of these materials has been studied by X-ray scattering at 25 and 150 $^\circ$C, along with transmission electron microscopy. For a geminal acid copolymer with low acid content, the precise molecular structure produces thermally persistent acid aggregates on a cubic lattice. This is the first report of cubic aggregate packing in polyethylene-acid copolymers.

1:27PM W43.00012 The Effect of Sulfonation and Neutralization on the Dynamics of Zn Neutralized Sulfonated Polystyrene Ionomers , ALICIA CASTAGNA, The Pennsylvania State University, WENQIN WANG, KAREN I. WINEY, University of Pennsylvania, JAMES RUNT, The Pennsylvania State University — The effect of sulfonation and neutralization levels on structure and dynamics of Zn neutralized sulfonated polystyrene (SPS) ionomers were investigated using scanning transmission electron microscopy (STEM), X-ray scattering, and dielectric relaxation spectroscopy. STEM and X-ray scattering revealed the presence of spherical aggregates 2 nm in diameter. Successful fitting of the scattering data to the Kinning-Thomas modified hard sphere model revealed that aggregate size is independent of degree of sulfonation and neutralization level, and that aggregate composition becomes increasingly ionic with increasing neutralization. Two segmental relaxations were identified in dielectric loss spectra corresponding to cooperative motion of chain segments in the unrestricted matrix and motions of chain segments restricted by aggregates. A Maxwell-Wagner-Sillars interfacial polarization process was revealed, with relaxation times that were in good agreement with predictions from a simple model of dispersed ionic spheres.

1:39PM W43.00013 Proton Transport in Nanostructured Block Copolymer/Ionic Liquid Membranes , MEGAN HOARFROST, University of California, Berkeley, MADHU TYAGI, NIST Center for Neutron Research, JEFFREY REIMER, RACHEL SEGALMAN, University of California, Berkeley — Nanostructured block copolymer/ionic liquid mixtures are of interest for creating membranes having high proton conductivity coupled with high thermal stability. In these mixtures, it is anticipated that nanoconfinement to block copolymer domains will affect ionic liquid proton transport properties. Using pulsed-field gradient NMR and quasi-elastic neutron scattering, this relationship has been investigated for mixtures of poly(styrene-b- 2-vinylpyridine) (S2VP) with ionic liquids composed of imidazole and bis(trifluoromethane)sulfonimide (HTFSI), where the ionic liquids selectively reside in the P2VP domains of the block copolymer. Proton mobility is highest in the neat ionic liquids when there is an excess of imidazole compared to HTFSI due to proton hopping between hydrogen-bonded imidazoles. As predicted, the amount of proton hopping can be tuned by nanoconfinement, as evidenced by the finding that a lamellar mixture of an imidazole- excess ionic liquid with S2VP has greater proton mobility than a corresponding disordered mixture of the ionic liquid with P2VP homopolymer.

1:51PM W43.00014 Simultaneous Electronic and Ionic Charge Transport in Poly(3-hexylthiophene)-b-Poly(ethylene oxide) , SHRAYESH PATEL, University California, Berkeley and Lawerence Berkeley National Lab, ANNA JAVIER, Lawerence Berkeley National Lab, NITASH BALSARA, University California, Berkeley and Lawerence Berkeley National Lab — Block copolymers can self-assemble to distinct channels, which allows for simultaneous transport of electronic and ionic charge carriers. A potential polymer system is Poly(3-hexylthiophene)-b-Poly(ethylene oxide) (P3HT-b-PEO). P3HT serves as the electronic conducting channel while the PEO serves as the ionic conducting channel. Both conductive blocks are doped to induce simultaneous electronic and ionic conduction. The PEO phase is doped with LiTFSI while the P3HT is doped with F_4TCNQ, which generates hole carriers. In addition, we take into account the case where no electronic dopant is added to P3HT phase. The charge transport properties of the material are analyzed via ac impedance spectroscopy and dc polarization techniques. These experiments provide decoupled electronic and ionic transport in P3HT-b-PEO.

2:03PM W43.00015 Confinement Effects on Watery Domains in Hydrated Block Copolymer Electrolyte Membranes , MOON JEONG PARK, Department of Chemistry, Pohang University of Science and Technology, SUNG YEON KIM, JOOMI YEO — The morphology of a series of diblock copolymers comprising randomly sulfonated polystyrene (PSS) and polymethylbutylene (PMB) blocks equilibrated with humid air was determined by in- situ small angle neutron scattering (SANS). In-situ SANS data were collected over a wide angular range permitting the determination of the superstructure of the hydrophilic PSS-rich and hydrophobic PMB-rich domains and the substructure within the hydrophilic PSS-rich domains. When the characteristic length of the superstructure is larger than 10 nm, the hydrophilic PSS domains are heterogeneous with periodically arranged watery domains. The scattering signature of the watery domains is very similar to the well-established "ionomer peak." This peak vanishes when the neutron scattering length density of the water (H2O/D2O mixture) is matched to that of the PSS block. The spacing between watery domains depends only on sulfonation level of the PSS block. When the characteristic length of the superstructure is less than 10 nm, the watery substructure disappears and homogeneous hydrated PSS-rich domains are obtained.

Thursday, March 24, 2011 11:15AM - 2:03PM –

Session W44 DPOLY: Focus Session: Dynamics of Polymers-Phenomena due to Confinement - Diffusion, Particles, & Pores A309

11:15AM W44.00001 Single-molecule measurements of adsorbed polymer , CHANGQIAN YU, JUAN GUAN, SUNG CHUL BAE, STEVE GRANICK, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign — Single-molecule tracking is used to study the surface mobility of PEG (polyethylene glycol) chains adsorbed to the solid-liquid interface from dilute aqueous solution. The end-labeled chains are visualized by objective-based total internal reflection fluorescence microscopy (TIRFM) and their trajectories are analyzed after cleaning the images with denoising algorithms. Surface mobility, which in this system depends on pH, is decomposed into one family of chains which remains adsorbed over the observation time window, and another family that appears to translate from point to point by hopping. This we quantify with nm-level resolution.

11:27AM W44.00002 Segmental motion in polystyrene thin film: a single molecule fluorescence study[1] , ZHONGLI ZHENG, JIANG ZHAO, Institute of Chemistry, Chinese Academy of Sciences — Single molecule fluorescence de-focus microscopy is used to study the segmental motion by observing the rotational motion of single fluorophores chemically attached to polystyrene chain ends. The collective nature of the rotational motion was noticed: a sudden change of the fraction of rotating fluorophores was discovered at a temperature 60 degree below the glass transition temperature of polystyrene. The dependence of the critical temperature on film thickness and surface chemistry was investigated and the results show that the effect of confinement, surface interaction and free surface.

[1]Project supported by National Natural Science Foundation of China (NSFC).

11:39AM W44.00003 Order of Magnitude Decrease in Dye Diffusion in Nanoconfined Polymer Films: Fluorescence Nonradiative Energy Transfer Technique , HUI DENG, MANISH MUNDRA, JOHN TORKELSON, Northwestern University — A fluorescence nonradiative energy transfer/multilayer film technique was used to determine the diffusion coefficient of the dyes decacyclene and Disperse Red 1 in supported polystyrene (PS) films as a function of film thickness. Previous studies on the glass transition temperature (Tg) of PS show a decrease in Tg as films are nanoconfined. This Tg-reduction is due to the enhanced role of the polymer/air interface which results in a region of increased polymer mobility as thickness is reduced. However, dye diffusion coefficients decrease upon film nanoconfinement, with the onset of diffusion coefficient reduction appearing at film thicknesses much thicker than the onset of Tg-confinement effects. These results can be explained by the fact that Tg reflects the longer time side of the polymer relaxation time distribution while dye diffusion reflects the shorter time side of the relaxation distribution. We hypothesize that confinement suppresses the shorter time side of the relaxation distribution which results in the observed decrease in diffusion coefficients.

11:51AM W44.00004 Non-classical diffusion of PDMS confined in a surface forces apparatus , SUBHALAKSHMI KUMAR, CHANGQIAN YU, University of Illinois, Urbana-Champaign, SUNG CHUL BAE, STEVE GRANICK, University of Illinois, Urbana Champaign — We present FRAP measurements inside a surface forces apparatus. Polydimethylsiloxane (PDMS), well above its glass transition, was confined into molecularly-thin films between atomically smooth mica sheets. Translational diffusion was measured using fluorescence recovery after photobleaching (FRAP) as the polymer film thickness was changed from tens of Rg to 3 Rg . The FRAP recovery curves of confined films are distinctly non-classical. Huge heterogeneity is suggested by stretched exponential behavior in which the power of time varies smoothly from β=1 (thick films) to β=0.3 (confined films) with a sharp transition between these limits.

12:03PM W44.00005 Probing In-Plane Diffusion of Nano-Confined Polymers in Ultrathin Films , JOSHUA KATZENSTEIN, University of Texas at Austin - Department of Chemical Engineering, JUSTIN CHANDLER, University of Texas at Austin, HALEY HOCKER, CHRISTOPHER ELLISON, University of Texas at Austin - Department of Chemical Engineering — In-plane (parallel to the substrate) polymer diffusion at and near interfaces has significant implications for polymeric surfactants used in tertiary oil recovery, exfoliation of clay sheets in polymer nano-composites, and several other high technology applications. Here, we report a study on the in-plane diffusion of whole polymer chains confined between interfaces using fluorescence recovery after photobleaching. Adapted from quantitative biology, FRAP provides a platform to independently study the effect of temperature, molecular weight, and film thickness on in-plane diffusion of polymers confined between interfaces. Fluorescently labeled polymers were synthesized, spin coated onto quartz substrates and the self-diffusion coefficient was measured by irreversibly photobleaching fluorophores in a pre-defined pattern and monitoring recovery of fluorescence over time. Preliminary results indicate that for thick films the diffusion coefficient is consistent with bulk values.

12:15PM W44.00006 Screening Effect of Supercritical Carbon Dioxide on Polymer/Substrate Interactions[1] , PETER GIN, NAISHENG JIANG, MAYA ENDOH, Materials Science and Engineering, Stony Brook University, BULENT AKGUN, SUSHIL SATIJA, NCNR, NIST, TAD KOGA, Materials Science and Engineering, Stony Brook University — The kinetics and thermodynamic properties of polymer melts near interfaces and in confined geometries can vary significantly from their bulk counterparts. This behavior can be attributed to the presence of an immobile layer at the polymer/substrate interface, which has been reported to hinder the mobility of polymer chains in thin films even at a large length scale. Here, we investigate the use of supercritical carbon dioxide ($scCO_2$) as a medium to screen the polymer/substrate interactions and enhance chain mobility in polymer thin films. In-situ neutron reflectivity was utilized to measure the interdiffusion of deuterated polystyrene (d-PS) into various matrices of hydrogenated PS (h-PS) with thicknesses ranging from 0.5 Rg to 5 Rg. We found that at the unique T (36°C) and P (8.2 MPa) conditions, where the anomalous adsorption of CO_2 molecules in polymer thin films occurs, the diffusion constants remained unchanged regardless of bottom layer thickness, while no diffusion occurred below 1Rg at high temperature (170°C).

[1]We acknowledge the financial support provided by NSF CAREER AWARD under funding number CMMI-0846267.

12:27PM W44.00007 The Glass Transition at Silica/PMMA Nanocomposite Interfaces[1] , RAHMI OZISIK, KATELYN PARKER, RYAN T. SCHNEIDER, RICHARD W. SIEGEL, Rensselaer Polytechnic Institute, JUAN CARLOS CABANELAS, BERNA SERRANO, CLAIRE ANTONELLI, JUAN BASELGA, Universidad Carlos III de Madrid — Local glass transition temperatures (Tg) have been measured in the interfaces of solution blended silica/poly(methyl methacrylate) (PMMA) nanocomposites using florescence spectroscopy and compared with Tg measured by differential scanning calorimetry (DSC). It was found that the two types of measurements yielded significantly different information. Combinations of silanes and poly(propylene glycol)- based molecular spacers bound to fluorophores were covalently linked to the surface of the nanoparticles, allowing for variation of the fluorophore response with respect to the distance from the nanofiller surface. Increases in the bulk Tg from the neat PMMA value were found upon the addition of nanofillers, but were independent of the nanofiller concentration when the filler concentration was above 2% by weight. Furthermore, as the size of the grafted molecular spacer was increased, Tg values were found to decrease and approach Tg of the neat PMMA. Owing to variable conformations of the spacers, an effective distribution of fluorophore-silica distances exists, which influences the fluorophores' response to the transition.

[1]Supported by NSF (CMMI-0500324) and CICYT (MAT 2007-63722).

12:39PM W44.00008 Structural Relaxation of 3-Dimensionally Confined Polymer Glasses: Isobaric versus Isochoric Glass Formation , YUNLONG GUO, CHUAN ZHANG, RODNEY PRIESTLEY, Department of Chemical and Biological Engineering, Princeton University — We have measured the glassy-state structural relaxation of aqueous suspended polystyrene (PS) nanoparticles and the corresponding silica-capped PS nanoparticles via modulated differential scanning calorimetry. Suspended and capped-PS nanoparticles undergo glass formation and subsequent physical aging under isobaric and isochoric conditions, respectively. To account for glass transition temperature (Tg) changes with confinement, physical aging measurements were performed at a constant value of Tg minus Ta, where Ta is the aging temperature. With deceasing diameter, aqueous suspended PS nanoparticles exhibited enhanced physical aging rates in comparison to bulk PS. At all values of Tg minus Ta investigated, capped-PS nanoparticles aged at reduced rates compared to the corresponding aqueous suspended PS nanoparticles. Due to differences in paths to glass formation, suspended and capped-PS nanoparticles aged to different apparent equilibrium states. We captured the physical aging behavior of all nanoparticles via the Tool, Narayanaswamy, and Moynihan (TNM) model of structural relaxation.

12:51PM W44.00009 Molecular Dynamics Study of Single Conjugated Polymers Confined to Nanoparticles , SABINA MASKEY, FLINT PIERCE, DVORA PERAHIA, Clemson University, GARY GREST, Sandia National Lab — Optically active polymers confined into nanoparticles are highly fluorescent and have potential applications in intracellular fluorescence imaging, bio-sensors and other optoelectronic devices. Internal conformation and dynamics of the polymers determines their optical properties. Using molecular dynamics (MD) simulations, we have explored the structure and dynamics of nanoparticles formed by conjugated polymers in a collapsed conformation, which is not the most stable conformation of the polymer. Nanoparticles were formed in a collapsed conformation and followed as the function of time in both poor and good solvents. We found that these nanoparticles are stable and remain collapsed in a poor solvent but rapidly expands and unraveled in a good solvent. The lengths of the side chains affect the internal packing of the side chains which in turn affect the size of the nanoparticles. S(q,t) was measured to characterize the internal dynamics of the collapsed nanoparticles.

1:03PM W44.00010 The Glass Transition Temperature of Polymer Nanoparticles under Soft and Hard Confinement , CHUAN ZHANG, YUNLONG GUO, RODNEY PRIESTLEY, Department of Chemical and Biological Engineering, Princeton University — When confined to the nanoscale, the glass transition temperature (Tg) of polymers can deviate substantially from the bulk, i.e., the Tg-confinement effect. Due to ease of processing, most studies have focused on the size-dependent Tg of thin films, while few have extended investigations to other geometries. As polymers confined in higher geometrical dimensions become the enabling material in technologies ranging from drug delivery to plastic electronics, a greater understanding of size effects on Tg is warranted. Here, we investigate the effect of soft and hard three-dimensional confinement on the Tg of polymer nanoparticles. Via modulated differential scanning calorimetry, we show that Tg decreases with size for bare polymer nanoparticles, i.e., the case of soft confinement while Tg is invariant with size for silica-capped polymer nanoparticles, i.e., the case of hard confinement. These results suggest that the free surface is a key factor in Tg reductions of three-dimensionally confined polymer.

1:15PM W44.00011 Statics and dynamics of confined DNA in a nanopit array , ALEXANDER KLOTZ, WALTER REISNER, McGill University, NANOBIOPHYSICS GROUP TEAM — Polymers have been proposed as tools for self-assembly in nanotechnology. There is interest in controlling the movement and conformation of the polymers by modifying the free energy landscape of their environment. It is necessary to understand the free energy and equilibrium behavior of a polymer in a nanoscale environment in order to control its dynamics. In these experiments, DNA molecules are placed in slits on the order of 100 nanometers. The slits are embedded with a lattice of square pits that act as entropic traps for which it is energetically favorable for the DNA to occupy. Based on the geometric properties of the lattice, the molecule in equilibrium will occupy a discrete number of pits. The dynamics of the system can be understood in terms the number of occupied pits. A partition function based on these states can be used to make testable predictions. Measurement of the static conformations of DNA in these pits, as well as the diffusion of the molecule throughout the lattice, as a function of geometric parameters can be used to test models of polymer free energy. Measurements show that the mean occupancy state scales as expected with various pit parameters. Early diffusion results indicate that the diffusion of DNA can be fine tuned by modifying the topography.

1:27PM W44.00012 Modeling of Free Radical Polymerization of Methyl Methacrylate (MMA) in Nanoporous Confinement , FATEMA BEGUM, SINDEE SIMON — Nanoconfinement of methyl methacrylate free radical polymerization is known to impact the molecular weight and molecular weight distribution of the polymer produced, and the results in the literature generally indicate an increase in molecular weight and a concommitant decrease in polydispersity index. In the present work, the mathematical model described by Verros et al. (2005) for free radical bulk polymerization of methyl methacrylate is extended to account for polymerization in nanopores. The model of Verros et al. (2005) incorporates diffusion effects and is capable of describing the conversion and the number- and weight-average molecular weights of the resulting poly(methyl methacrylate) as a function of polymerization time and process conditions. The model is extended by incorporating the effect of nanoconfinement on diffusivity using the scaling reported in the literature. The results indicate that nanoconfinement will lead to higher molecular weights, lower polydispersity, and the gel effect occurs earlier. The results are compared to experimental work and implications discussed.

1:39PM W44.00013 Effect of Nanopore Confinement on the Polymerization Rate of Linear Polymers , PO-HAN LIN, RAJESH KHARE, Texas Tech University — Confinement to a nanopore has a significant impact on the thermal properties as well as the rate of chemical reactions such as polymerization as compared to these processes in the bulk. In this work, we have studied the effect of nanopore confinement on the rate of free radical polymerization by using molecular simulations. In order to capture the physics of this process, we have implemented a coarse-grained model to carry out reactive molecular dynamics simulations. Our simulation method considers the three stages of polymerization process: initiation, propagation and termination. Our simulation results will be used to compare the polymerization rate in the confinement with that in the bulk. The results will be explained by focusing on the dynamics of the reacting species in the confinement.

1:51PM W44.00014 Theoretical Study of Tethered Polymers inside a Cylindrical Tube , TONGCHUAN SUO, MARK WHITMORE, Department of Physics and Astronomy, University of Manitoba, Winnipeg, Manitoba R3T 2N2, Canada — We present a numerical self-consistent mean-field theoretical (SCMFT) study of polymer chains tethered to the inside walls of cylindrical tubes. We consider cases ranging from relatively thin to relatively thick tubes, from low to high tethering densities, and in various solvents. Our focus is on the polymer concentration profiles and the chain end distributions, in particular the concentrations and chain overlap at the tube centers. We show that these quantities depend primarily on only two parameters, and that this dependence becomes exact in the limit of low polymer concentration. We find that there can be significant polymer interpenetration at the tube centers even in cases where the tube radius is greater than the polymer R_{g}, and this can be tuned by changing the solvent quality and/or tethering density.

Thursday, March 24, 2011 11:15AM - 2:15PM –

Session W45 DAMOP: Atom-Light Interactions: Experiment and Theory A310

11:15AM W45.00001 Lattice-induced nonadiabatic frequency shifts in optical lattice clocks , KYLE BELOY, New Zealand Institute for Advanced Study, Massey Univ. — We consider the frequency shift in optical lattice clocks which arises from the coupling of the electronic motion to the atomic motion within the lattice. For the simplest of three-dimensional lattice geometries this coupling is shown to affect only clocks based on blue-detuned lattices. We have estimated the size of this shift for the prospective strontium lattice clock operating at the 390-nm blue-detuned magic wavelength. The resulting fractional frequency shift is found to be on the order of 10^{-18} and is largely overshadowed by the electric quadrupole shift. For lattice clocks based on more complex geometries or other atomic systems, this shift could potentially be a limiting factor in clock accuracy.

11:27AM W45.00002 Magic wavelengths for optically trapped atoms , BINDIYA ARORA, IISER Mohali, India, MARIANNA SAFRONOVA, University of Delaware, CHARLES CLARK, JQI, NIST and the University of Maryland — The ability to trap neutral atoms inside high-Q cavities in the strong coupling regime is of particular importance for quantum computation and communication schemes, where it is essential to precisely localize and control neutral atoms with minimum decoherence. In a far-detuned optical dipole trap, the potentials experienced by an atom in its ground and excited states may be of opposite sign affecting the fidelity of experiments in which excited states are temporarily occupied. "Magic wavelengths" are those for which such potentials are equal. Single-laser schemes offer few cases in which magic wavelengths exist for Rb [Arora et al. PRA 76, 052509 (2007).] Here we explore bichromatic schemes for state-insensitive optical trapping of the Rb. We describe the use of trapping and control lasers to minimize the variance of the potential experienced by a trapped Rb atom in ground and excited states. We have also identified wavelengths $\lambda_{\rm zero}$ where the ground state frequency-dependent polarizabilities in alkali-metal atoms are zero. These are relevant for cooling and trapping experiments involving mixtures such as Rb/Yb, where the vanishing lattice potential for Rb facilitates interesting applications.

11:39AM W45.00003 Laser frequency stabilization for narrow linewidth cooling of ^{6}Li atoms[1] , ADAM REED, The Ohio State University, Department of Physics, KEVIN JOURDE, ESPCI ParisTech, PEDRO DUARTE, RANDALL HULET, Rice University, Department of Physics and Astronomy — Laser cooling to micro-Kelvin temperatures requires a laser with active frequency stabilization. The linewidth Γ of an atomic transition sets a lower bound on the Doppler cooling temperature $k_B T_D = \hbar\Gamma/2$. The $2s-2p$ transition in ^{6}Li has a lower bound temperature of $T_D \approx 140\,\mu$K. In contrast, the $2s-3p$ transition has a narrower linewidth and thus provides a lower temperature limit of $T_D \approx 20\,\mu$K. We present a method for stabilizing a laser to an atomic line in a vapor cell using modulation transfer spectroscopy and a home-built lock-in amplifier. Our results demonstrate successful locking of a 323 nm laser to the $2s-3p$ transition. The stabilized laser provides a second stage of magneto-optical trapping that results in an order of magnitude increase in the phase space density before evaporating to degeneracy in an optical dipole trap.

[1]This work was supported under ARO Award W911NF-07-1-0464 with funds from the DARPA OLE program, and by the NSF, the ONR, the Welch Foundation (grant C-1133) and the Keck Foundation.

11:51AM W45.00004 Demonstration of a ^{6}Li magneto-optical trap using the $2S_{1/2} \rightarrow 3P_{3/2}$ transition , R. HART, P.M. DUARTE, T.L. YANG, J.M. HITCHCOCK, T.A. CORCOVILOS, R.G. HULET, Department of Physics and Astronomy and Rice Quantum Institute, Rice University — We demonstrate narrow linewidth laser cooling on the $2S_{1/2} \rightarrow 3P_{3/2}$ transition of ^{6}Li at 323 nm. Typically, magneto-optical traps (MOTs) of alkali atoms cool on the D2 transition. The linewidth of this transition determines the Doppler limit of cooling which in the case of ^{6}Li is 140 μK, given a 5.9 MHz transition linewidth. Due to a lack of resolved hyperfine structure that prohibits polarization gradient cooling, typical Li MOTs reach minimum temperatures near 300 μK. Cooling on the $2S_{1/2} \rightarrow 3P_{3/2}$ transition, however, allows for a Doppler limit of 20 μK since the transition linewidth is only 790 kHz. We have implemented this cooling scheme and demonstrate ^{6}Li MOT temperatures of 65 μK. With the increased phase space density from this MOT, initial loading of the gas to an optical trap is substantially enhanced. We present our results on the characteristics of the narrow linewidth MOT and our results on the benefits of using this cooling scheme in the preparation of a degenerate gas of fermions.

12:03PM W45.00005 Pulsed Counter-Rotating Source of Slow, Cold Molecules , IGOR LYUKSYUTOV, LES SHEFFIELD, MARK HICKEY, VITALIY KRASOVITSKIY, DAYA RATHNAYAKA, Department of Physics and Astronomy, Texas A&M University, DUDLEY HERSCHBACH, Department of Chemistry and Chemical Biology, Harvard University — We describe the performance of a new design of the counter-rotating source (CRS) of slow molecules introduced originally by Gupta and Herschbach. The CRS produces a supersonic expansion from a nozzle near the tip of a hollow rotor spun at high speed contrary to the exit beam velocity. Thereby the lab velocity can be markedly reduced. Introducing a pulsed feeding system, cryo-cooling, and shutter system has eliminated the main problem of the original CRS apparatus, in which continuous gas flow imposed high background pressure. The new version provides intense pulses, typically of duration 0.1 ms with lab speeds as low as 40 m/s and longitudinal temperature as low as 0.5 K. This device can, in principle, decelerate (or accelerate) any molecule available as a gas; we report experiments producing slow beams of krypton, oxygen, ammonia, and nitrogen dioxide.

12:15PM W45.00006 Nanofriction in Cold Ion Traps , ANDREA VANOSSI, ANDREA BENASSI, International School for Advanced Studies (SISSA), and CNR-IOM DEMOCRITOS, ERIO TOSATTI, International School for Advanced Studies (SISSA), CNR-IOM DEMOCRITOS, and ICTP — Sliding friction between crystal lattices and the physics of cold ion traps are so far non-overlapping fields. Two sliding lattices may either stick and show static friction or slip with dynamic friction; cold ions are known to form static chains, helices, or clusters, depending on trapping conditions. Based on simulations, we show that much could be learnt about friction by sliding (e.g., via an electric field) the trapped ion chains over a periodic corrugated potential. Unlike infinite chains where, according to theory, the classic Aubry transition to free sliding may take place, static pinning always shows up in trapped chains. Nonetheless we find that a properly defined static friction still vanishes Aubry-like at a symmetric-asymmetric structural transition, ubiquitous for decreasing corrugation in both straight and zig-zag trapped chains. Dynamic friction can also be addressed by ringdown oscillations of the ion trap. Long theorized static and dynamic one dimensional friction phenomena could thus become exquisitely accessible in future cold ion tribology.

12:27PM W45.00007 Pattern formation with trapped ions , TONY LEE, MICHAEL CROSS, California Institute of Technology — We propose an experiment to study collective behavior in a nonlinear medium of trapped ions. Using laser cooling and heating and an anharmonic trap potential, one can turn an ion into a nonlinear van der Pol-Duffing oscillator. A chain of ions interacting electrostatically has stable plane waves for all parameters. The system also behaves like an excitable medium, since a sufficiently large perturbation generates a travelling pulse. Small chains exhibit multistability and limit cycles. We account for noise from spontaneous emission in the amplitude equation and find that the patterns are observable for realistic experimental parameters. The tunability of ion traps makes them an exciting setting to study nonequilibrium statistical physics.

12:39PM W45.00008 Spontaneous emission modification via quantum interference with energy shifts remained , SHUAI YANG, Institute for Quantum Studies and Department of Physics, Texas A&M University, College Station, Texas 77843, USA, SHI-YAO ZHU, Beijing Computational Science Research Center, Beijing, 100084, China, M. SUHAIL ZUBAIRY, Institute for Quantum Studies and Department of Physics, Texas A&M University, College Station, Texas 77843, USA — Quantum interference in spontaneous emission from a four-level atom is investigated with the counter rotating terms and the energy shifts included. The atom has two upper levels coupled to a common lower level by the same vacuum modes and is driven by a coherent field to an auxiliary level. The effect of the counter rotating terms in coupling through the vacuum modes is taken into account by a unitary transformation method. We show how the quantum interference due to the energy shifts effects the spontaneous emission spectrum.

12:51PM W45.00009 Optical chirality and superchiral fields , YIQIAO TANG, Department of Physics, Harvard University — A chiral object is any material body whose mirror image may not be superimposed on the original. Electromagnetic (EM) fields may be chiral too, with circularly polarized light as the paradigmatic example. We propose a measure of the local chirality of EM fields, which we call optical chirality. Optical chirality determines the degree of chiral asymmetry in the interaction of light with small molecules. We predict the existence of superchiral forms of light which show larger bias for exciting a single chiral enantiomer, in some regions of space, than does circularly polarized plane waves. We performed a conceptually simple experiment to probe the interaction of superchiral light with a chiral biperylene derivative. We selected this molecule for its strong intrinsic optical activity and fluorescence in the visible. The regions of enhanced chiral selectivity are too thin to detect by absorption, so we used fluorescence instead. We demonstrated experimentally a 12-fold enhancement in the chiral selectivity of superchiral fields for these chiral compounds. The demonstrated chiral enhancement is not a fundamental limit. Larger enhancement may be obtained at the expense of lower overall excitation rate. These results establish that optical chirality is a fundamental property of the electromagnetic field, with possible applications ranging from plasmonic sensors to absolute asymmetric synthesis.

1:03PM W45.00010 Observation of a Red-Blue Detuning Asymmetry in Matter-Wave Superradiance , LU DENG, EDWARD W. HAGLEY, NIST, QIANG CAO, XIAORUI WANG, XINYU LUO, RUQUAN WANG, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, MARVIN G. PAYNE, NIST, FAN YANG, XIAOJI ZHOU, School of Electronics Engineering & Computer Science, Peking University, Beijing 100871, China, XUZONG CHEN, MINGSHENG ZHAN, State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences — We report the first experimental observation of strong suppression of matter-wave superradiance using blue-detuned pump light and demonstrate a pump-laser detuning asymmetry in the collective atomic recoil motion. In contrast to all previous theoretical frameworks, which predict that the process should be symmetric with respect to the sign of the detuning of the pump laser from the one-photon resonance, we find that for condensates the symmetry is broken. With high condensate densities and red-detuned pump light the distinctive multi-order, matter-wave scattering pattern is clearly visible, whereas with blue-detuned pump light superradiance is strongly suppressed. However, in the limit of a dilute atomic gas symmetry is restored.

1:15PM W45.00011 Large and rapidly-responding Kerr nonlinear phase shift using a four-level N-scheme with an active Raman gain core , KE LI, LU DENG, NIST — We report rapidly-responding Kerr nonlinear phase shift using a long pencil-shaped cold ^{85}Rb atom samples. Our system is a four-level N-scheme based on both the D1 and D2 transition lines of Rb atom. The nonlinear phase shift and nonlinear optical index of the cold medium are studied using an interferometric method for various pump and phase-inducing laser intensities.

1:27PM W45.00012 Experimental Observation of Carrier-Envelope Phase Effects in Multi-Cycle Pulses[1] , PANKAJ JHA, Texas A&M University, YURI ROSTOVTSEV, University of North Texas, HEBIN LI, VLADIMIR SAUTENKOV, Texas A&M University, MARLAN SCULLY, Texas A&M University and Princeton University — Using intense RF pulses interacting with the magnetic Zeeman sub-levels of Rubidium (Rb) atoms, we have experimentally and theoretically shown the CEP effects in the population transfer between two bound atomic states interacting with pulses consisting of many cycles (up to 15 cycles) of the field. It opens several exciting applications and interesting possibilities that can be easily transfer to optical range and enhance current and create new set of tools to control CEP of laser pulses. These tools allow researchers to improve laser systems that generate laser pulses with better reproducibility and accuracy and better controlled. Also the tools provide an additional handle to control the process of collisions, and the current approach of extending the duration of the pulses with measurable or controllable CEP allows researchers to extend the coherent control to a new level where they are able to study molecular collisions or electron collisions in nano-structures under the action of strong electromagnetic fields with known CEP. In particularly, the obtained results can be applied to control of chemical reactions.

[1]Heep Foundation and Robert A. Welch Foundation Fellowship

1:39PM W45.00013 Counter-Propagating Coherent Stimulated Raman Spectroscopy for Remote Sensing in Air , LUQI YUAN, Texas A&M University, ANDREW TRAVERSO, DMITRI VORONINE, PANKAJ JHA, KAI WANG, ALEXEI SOKOLOV, MARLAN SCULLY — We analyze phase-matching conditions in various four-wave mixing schemes for coherent nonlinear optical spectroscopy in the counter-propagating beam configuration. Coherent stimulated Raman spectroscopy satisfies the conditions and gives a signal containing specific molecular spectroscopic information. A counter-propagating broadband and a narrowband pulses are used to measure the Raman spectrum with a single shot. In addition, the nonresonant background due to the nondegenerate four-wave mixing is suppressed. Using this technique we develop a new scheme for standoff spectroscopy in atmosphere by using nitrogen molecules in air as a gain medium for remote lasing.

1:51PM W45.00014 Efficient Backward Emission from Optically Pumped Air , ANDREW TRAVERSO, RODRIGO SANCHEZ-GONZALEZ, MICHAEL GRUBB, DMITRI VORONINE, KAI WANG, LUQI YUAN, Texas A&M University, ALEXEI ZHELTIKOV, Texas A&M University/Moscow State University, ARTHUR DOGARIU, JAMES MICHAEL, RICHARD MILES, Princeton University, VLADIMIR SAUTENKOV, ALEXEI SOKOLOV, SIMON NORTH, Texas A&M University, MARLAN SCULLY, Texas A&M University/Princeton University — We demonstrate the generation of backwards emitted coherent light in atmosphere via optical pumping. The backwards emitted light is narrow band centered at 845 nm and is generated from the dissociation of molecular oxygen and then subsequent two photon excitation of these newly dissociated oxygen atoms. Both the dissociation and excitation of oxygen are driven by a single 226 nm $\sim$10 nanosecond pulsed pump beam. The produced 845 nm light is a pulse approximately 10 nanosecond in duration and not only exhibits threshold characteristics, but is also nearly diffraction-limited. This optically-pumped mirror-less light source which propagates back towards the pump source presents a unique opportunity to develop new techniques for remote sensing.

2:03PM W45.00015 Quantum lithography beyond the diffraction limit via Rabi-oscillations[1] , ZEYANG LIAO, Institute for Quantum Studies and Department of Physics and Astronomy, Texas A&M University, College Station, TX 77843-4242, USA, MOHAMMAD AL-AMRI, The National Center for Mathematics and Physics, KACST, P.O.Box 6086, Riyadh 11442, Saudi Arabia, M. SUHAIL ZUBAIRY, Institute for Quantum Studies and Department of Physics and Astronomy, Texas A&M University, College Station, TX 77843-4242, USA — We propose a quantum optical method to do the sub-wavelength lithography. Our method is similar to the traditional lithography but adding a critical step before dissociating the chemical bound of the photoresist. The subwavelength pattern is achieved by inducing the multi-Rabi-oscillation between the two atomic levels. The proposed method does not require multiphoton absorption and the entanglement of photons. This method is expected to be realizable using current technology.

[1]This work is supported by a grant from the Qatar National Research Fund (QNRF) under the NPRP project and a grant from the King Abdulaziz City for Science and Technology (KACST).

Thursday, March 24, 2011 2:30PM - 5:30PM –

Session X1 DCMP: Quantum and Classical Phenomena in Josephson Junction Arrays Ballroom A1

2:30PM X1.00001 Quantum Coherence of the Fluxonium Superconducting Artificial Atom

, MICHEL DEVORET, Yale University — Artificial atoms built from superconducting tunnel junctions illustrate the problem of engineering a controllable electrodynamic quantum system, starting from basic elements. Can circuit architecture mitigate or even eliminate coherence limitations due to defects in the basic electrical constituents? This central question will be discussed from the perspective of recent experimental results of our group, obtained on the fluxonium[1], a novel superconducting quantum circuit. It consists of a Cooper-pair box junction which is shunted by a long array of larger junctions. Immunity to offset charge noise and only a weak sensitivity to flux noise is observed for the qubit transition. The combination of the very large inductance of the array, which has negligible parasitic resistance, and large phase fluctuations of the small junction, distinguishes fundamentally the fluxonium from the flux qubit. Significant improvement of the relaxation time has been obtained, when one compares with qubits of the same family. Finally, fluxonium displays the type of 3-level-atom physics which should prove useful for continuous, high-fidelity monitoring of a state. Work supported by the IARPA, ARO and NSF.

[1] V.E. Manucharyan, Jens Koch, L.I. Glazman and M.H. Devoret, Science 326, 113-116 (2009).

3:06PM X1.00002 Measurement of Quantum Phase-Slips in Josephson Junction Chains[1]

, WIEBKE GUICHARD, Joseph Fourier University — Quantum phase-slip dynamics in Josephson junction chains could provide the basis for the realization of a new type of topologically protected qubit [1] or for the implementation of a new current standard [2]. I will present measurements of the effect of quantum phase-slips on the ground state of a Josephson junction chain. We can tune in situ the strength of the phase-slips. These phase-slips are the result of fluctuations induced by the finite charging energy of each junction in the chain. Our measurements demonstrate that a Josephson junction chain under phase bias constraint behaves in a *collective* way [3]. I will also show evidence of coherent phase-slip interference, the so called Aharonov-Casher effect. This phenomenon is the dual of the well known Aharonov-Bohm interference.

In collaboration with I.M. Pop, Institut Neel, C.N.R.S. and Universite Joseph Fourier, BP 166, 38042 Grenoble, France; I. Protopopov, L. D. Landau Institute for Theoretical Physics, Kosygin str. 2, Moscow 119334, Russia and Institut fuer Nanotechnologie, Karlsruher Institut fuer Technologie, 76021 Karlsruhe, Germany; and F. Lecocq, Z. Peng, B. Pannetier, O. Buisson, Institut Neel, C.N.R.S. and Universite Joseph Fourier.

[1] I. M. Pop, O. Buisson, K. Hasselbach, I. Protopopov, W. Guichard and B. Pannetier, Phys. Rev. B, 78, 104504(2008)
[2] W. Guichard and F. Hekking, Phys. Rev. B 81, 064508 (2010)
[3] I. M. Pop, I. Protopopov, F. Lecocq, Z. Peng, B. Pannetier, O. Buisson and W. Guichard, Nature Physics, 6, 589 (2010).

[1]European STREP MIDAS, ANR QUANTJO

3:42PM X1.00003 Coherent Terahertz Emission of Intrinsic Josephson Junction Stacks in the Hot Spot Regime[1]

, REINHOLD KLEINER, Physics Institute, University of Tuebingen, D72076 Tuebingen, Germany — Having small sized active and tunable devices operating at frequencies up to the Terahertz (THz) range is one of the goals of modern electronics. However, there is still a lack of good active or passive devices, often referred to as the "Terahertz gap." Intrinsic Josephson junctions formed by the layered crystal structure of high temperature superconductors such as $Bi_2Sr_2CaCu_2O_8$ have the potential to operate in this regime. While for a long time the research on THz generation with this type of junctions was carried out with perhaps only modest success, recently synchronous emission, with an estimated output power in the μW range, of stacks consisting of several hundred intrinsic Josephson junctions was achieved [1]. We report on the investigation of THz electromagnetic wave generation in intrinsic junction stacks (mesas) of different geometries, using a combination of transport measurement, direct electromagnetic wave detection and Low Temperature Scanning Laser Microscopy [2,3]. At high enough input power a hot spot (a region heated to above the superconducting transition temperature) coexists with regions being still in the superconducting state. In the "cold" regions cavity resonances can occur, synchronizing the ac Josephson currents and giving rise to strong and stable coherent THz emission. We discuss possible scenarios of the hot spot/wave interaction and its relation to the generation of coherent THz radiation.

[1] L. Ozyuzer, et al., Science **318**, 1291 (2007).
[2] H. B. Wang, et al., Phys. Rev. Lett. **102**, 017006 (2009).
[3] H. B. Wang, et al., Phys. Rev. Lett. **105**, 057002 (2010).

[1]In collaboration with S. Guenon, B. Gross, M. Gruenzweig, D. Koelle, H. B. Wang, J. Yuan, A. Iishi, T. Hatano, Z. Jiang, Y. Zhong, P.H. Wu.

4:18PM X1.00004 Vortex pinning in ferromagnet-superconductor bilayer with tunable domain patterns[1]

, MARTA Z. CIEPLAK, Institute of Physics, Polish Acad. Sciences — Ferromagnet superconductor hybrids provide a fascinating example of systems in which there is a rich interplay between two seemingly incompatible collective phenomena. Particularly interesting is the impact of the ferromagnet on the dynamics of vortices in the superconductor. The magnetic domains control the location of the vortices. Exquisite control of the dynamics can be achieved by careful tuning of the geometry of the magnetic domains. In this talk I will present the results of recent experiments on superconductor(S)-ferromagnet(F) bilayers with a focus on understanding the hitherto unexplained seemingly unpredictable dependence of the critical current density on the parameters of the experiment. In our experiments the S layer is made of niobium, the F layer is a Co/Pt multilayer with perpendicular magnetic anisotropy, and a thin insulating layer in-between eliminates proximity effect. We use various demagnetization procedures to define different domain patterns in the F layer. We show that some domain patterns produce highly inhomogeneous flux penetration and strong vortex confinement at the sample edge, while for others there is remerkable enhancement of the critical current density in excess of 15. This is the highest value reported to date. We have measured, for the first time in a single tunable structure, the dependence of the activation energy for vortex pinning on the domain width, temperature, and magnetic field. In collaboration with L.Y. Zhu, X. M. Cheng and C. L. Chien (Johns Hopkins), Z. Adamus (Polish Acad. Sci.) and M. Konczykowski (Ecole Polytechnique).

[1]Supported by NSF grant DMR05-20491, by the French-Polish Program PICS 4916, and by EU within the European Regional Development Fund, through the Innovative Economy grant POIG.01.01.02-00-108/09

4:54PM X1.00005 Tuning superconductivity by carrier injection

, PAUL MÜLLER, Department of Physics, University of Erlangen, Germany — All high-T_c cuprates are stacking sequences of CuO_2 layers and charge reservoir layers consisting of metal oxides. Upon doping the CuO_2 layers, antiferromagnetic order is destroyed and metallic conductivity is established. Usually doping is achieved by a non-stoichiometric composition of the charge reservoir layer. However, we already have shown that we can change the carrier concentration of $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystals by current injection along the c- axis [1]. Critical temperature, c-axis resistivity and critical current of intrinsic Josephson junctions can be tuned in a large range from underdoping to extreme overdoping. This effect is persistent up to annealing temperatures of approximately 270 K. Using current injection at higher bias, we were able to reduce the carrier concentration again. We investigated in detail the superconducting properties by performing macroscopic quantum tunneling experiments of intrinsic Josephson junctions. The experiments have been carried out repeatedly on samples, whose properties were changed only by current injection. An exponential increase of the critical current density with hole concentration was observed. At the same time, the capacitance of intrinsic Josephson junctions increased significantly. Finally, only by current injection, we were able to convert into the superconducting state a nonsuperconducting, oxygen depleted sample. This work was done in collaboration with Y. Koval, X.Y. Jin, S. Probst, Y. Simsek, C. Steiner (Universität Erlangen), H. B. Wang (NIMS, Tsukuba), and G. Behr, B. Büchner (IFW Dresden).

[1] Y. Koval, X.Y. Jin, C. Bergmann, Y. Simsek, L. Özyüzer, P. Müller, H. B. Wang, G. Behr, B. Büchner, Appl. Phys. Lett. **96**, 082507 (2010).

Thursday, March 24, 2011 2:30PM - 5:30PM –

Session X2 DCMP: Coexistence Between Antiferromagnetism and Superconductivity in Fe-pnictides Ballroom A2

2:30PM X2.00001 Competing phases in the iron pnictides[1] , RAFAEL FERNANDES, Ames Laboratory and Iowa State University, Ames, IA 50011, USA — In this work, we present a theoretical model that consistently describes the interplay between the magnetic, elastic, and superconducting degrees of freedom of the iron pnictides, comparing our results to several experimental observations. First, we show that the outcome of the competition between the antiferromagnetic (AFM) and the superconducting (SC) order depends on the symmetry of the pairing state. In particular, we demonstrate that a conventional phonon-mediated superconducting state cannot coexist microscopically with the itinerant magnetic phase [1,2]. We also show that the magneto-elastic coupling in these materials is mediated by Ising-nematic degrees of freedom, which emerge from the degeneracy of the magnetic ground state. As a result, in the tetragonal phase, nematic fluctuations lead to the *softening* of the lattice in the normal state but to its *hardening* in the SC state, due to the competition between SC and AFM [3]. Accordingly, in the orthorhombic phase, nematic order is suppressed below the SC transition temperature, causing the suppression of the orthorhombic order parameter [4].

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[2] R. M. Fernandes and J. Schmalian, Phys. Rev. B **82**, 014521 (2010).
[3] R. M. Fernandes *et al.*, Phys. Rev. Lett. **105**, 157003 (2010).
[4] S. Nandi *et al.*, Phys. Rev. Lett. **104**, 057006 (2010).

[1]Research supported by the U.S. DOE, Office of BES, Materials Science and Engineering Division.

3:06PM X2.00002 Superconductivity and Magnetism in iron-pnictides: co-existence or not? , ANTON VORONTSOV, Montana State University — In this talk I will review the weak-coupling approach to describe the interplay of two electronic orders: superconductivity (SC) in the form of Cooper pairs, and magnetism in the form of the spin-density waves (SDW). The two orders, traditionally thought as incompatible, are close neighbors in magnetically-active Fe-based superconductors with surprisingly high T_c. Complex multi-band structure, multiple interactions and many families of these materials create a range of possible states of mingling between superconductivity and magnetism. I will present a list of different parameters, including (a) the Fermi surface shape, (b) the order parameter structure, (c) the relative strength of SC and SDW interactions, (d) the external magnetic field, and describe which properties, or their combinations, lead to co-existence or avoidance of SC and SDW orders, and how transition between the two orders occurs upon doping.

3:42PM X2.00003 Superconductivity and magnetism in 111 iron pnictides[1] , SERGEY BORISENKO, Institute for Solid State Research, IFW-Dresden, Helmholtzstrasse 20, 01069, Dresden, Germany — We study different 111 materials at ultra low temperatures by means of angle-resolved photoemission spectroscopy (ARPES). The measurements provide a direct access to the information on the low energy electronic structure, which includes the detailed knowledge of the Fermi surface, band renormalization, electronic self-energy and symmetry of the superconducting order parameter. The results suggest a direct correlation between the fermiology and fundamental physical properties throughout the phase diagram of 111 iron superconductors. In particular, the Van Hove singularity is identified as playing a primary role for the superconductivity.

[1]The project was supported, in part, by the DFG under Grant No. BO 1912/3-1 within the framework of the priority program SPP1458.

4:18PM X2.00004 Antiferromagnetic phase in iron-based superconductors: selection of magnetic order, spin excitations, competition with superconductivity , ILYA EREMIN, Institue for Theoretical Physics III, Ruhr-University Bochum — Recent discovery of superconductivity in the iron-based layered pnictides with Tc ranging between 26 and 56K generated enormous interest in the physics of these materials. The superconductivity has been discovered in oxygen containing RFeAsO (R=La, Nd, Sm) as well as in oxygen free AFe2As2 (A=Ba, Sr, Ca). Like the cuprates, the pnictides are quasi-two-dimensional systems, their parent material shows antiferromagnetic long-range order below 150K and superconductivity occurs upon doping of either electrons or holes into the FeAs layers. In my talk I will analyze the properties of the magnetically ordered state. In particular, I will discuss the selection of the stripe magnetic order in the unfolded BZ within itinerant description. Selecting one hole and two electron pockets we find that SDW order is highly degenerate if electron pockets are circular and interactions involved are between holes and electrons only. Repulsive charge interactions between two electrons as well as ellipticity of the electron pockets break the degeneracy and select metallic (0, π) [(π,0)] SDW state in the unfolded BZ – the same order as seen in the experiments. I will argue that the SDW state remains a metal even for the case of a perfect nesting because one combination of the two hole operators and one combination of two electron operators decouple from the SDW mixing. We also demonstrate that the quasi-one-dimensional nanostructure identified in the quasiparticle interference (QPI) is a consequence of the interplay of the magnetic (π, 0) spin-density wave (SDW) order with the underlying electronic structure. Finally, we address the salient experimental features of the magnetic excitations in the spin-density-wave phase of iron-based superconductors. We use a multiband random-phase approximation treatment of the dynamical spin susceptibility. Weakly damped spin waves are found near the ordering momentum and it is shown how they dissolve into the particle-hole continuum. We show that ellipticity of the electron bands accounts for the anisotropy of the spin waves along different crystallographic directions and the spectral gap at the momentum conjugated to the ordering one. *Work done with A. V. Chubukov, J. Knolle, R. Moessner, and A. Akbari.

[1] J. Knolle, I. Eremin, A. Akbari, and R. Moessner, Phys. Rev. Lett. 104, 257001 (2010).
[2] J. Knolle, I. Eremin, A.V. Chubukov, and R. Moessner, Phys. Rev. B 81, 140506(R) (2010)
[3] I. Eremin and A.V. Chubukov, Phys. Rev. B 81, 024511 (2010)

4:54PM X2.00005 Optical Investigations of the Superconducting State in 122 Iron-Pnictides[1] , DAN WU, Physikalisches Institut, Unversitat Stuttgart, Germany — The new high-Tc iron pnictide superconductors have a pronounced multiband character, which complicates the electronic properties and allows for a variety of possible superconducting ground states. We have used the infrared spectroscopy–one of the most powerful tools to investigate the low-energy electrodynamic properties of superconductors–to study several pnictide families. We made a comparison between them with the aim to answer the following questions: (1) Is it possible to have more than one superconducting gap in iron pnictide? (2) Can their order parameters be distinct from each other? (3) How does the coupling between different bands influence the gap? (4) Do the gaps have a three-dimensional character? (5) Is the gap scenario universal for all the iron pnictides? We could show that the pairing condition depends sensitively on the similarity of geometry and dimension between hole and electron Fermi-surfaces.

[1]The work was done in collaboration with N. Barisic, J. Carbotte, G. H. Cao, P. Gegenwart, B. Gorshunov, B. Holzapfel, E. Schachinger and Z. A. Xu.

Thursday, March 24, 2011 2:30PM - 5:30PM –

Session X3 DCMP: Topological Vortices in Magnets, Ferroelectrics, and Multiferroics Ballroom A3

2:30PM X3.00001 Magnetic vortices: From a hidden parameter to novel switching modes , YVES ACREMANN, Solid State Physics, Physics Dept., ETH Zurich — This abstract not available.

3:06PM X3.00002 Skyrmion Lattices in Chiral Magnets , CHRISTIAN PFLEIDERER, Physik-Department, Technische Universitaet Muenchen, D-85748 Garching, Germany — Skyrmions are topologically stable field configurations with particle-like properties. Using neutron scattering and measurements of the Hall effect we identified the formation of two-dimensional lattices of skyrmion lines, a new form of magnetic order, in metallic and semiconducting B20 compounds, namely MnSi [1,2], $Mn_{1-x}Co_xSi$ [3], $Mn_{1-x}Fe_xSi$ [3] and $Fe_{1-x}Co_xSi$ [4]. The existence of individual skyrmions and skyrmion lattices has recently been confirmed by Lorentz force microscopy for $Fe_{1-x}Co_xSi$ ($x = 0.5$) [5]. The skyrmion lattices in chiral magnets share remarkable similarities with vortex lattices in type II superconductors – they may be understood as vortex lattices of transverse spin supercurrents exhibiting domain formation and complex morphologies. Our studies establish magnetic materials lacking inversion symmetry as an arena for new forms of order composed of topologically stable spin configurations.

[1] S. Mühlbauer, et al. Science **323**, 915 (2009).
[2] A. Neubauer, et al. Phys. Rev. Lett. **102**, 186602 (2009).
[3] C. Pfleiderer, et al. J. Phys. Cond. Matter **22**, 164207 (2010).
[4] W. Münzer, et al. Phys. Rev. B (R) **81**, (2010).
[5] X. Z. Yu, et al. Nature **465**, 901 (2010); C. Pfleiderer, A. Rosch, Nature (N&V) **465**, 880 (2010).

3:42PM X3.00003 Skyrmion crystal and topological Hall effect in B20-type transition-metal compounds , YOSHINORI ONOSE, University of Tokyo — Topological objects in solids such as domain walls and vortices have been attracting much attention for long. Among them the spin texture called skyrmion is an unusual topological object, in which the spins point in all the directions wrapping a sphere. The skyrmion hosts finite spin chirality, and therefore is anticipated to induce novel electromagnetic phenomena such as topological Hall effect. In B20-type transition metal compounds MnSi and $Fe_{1-x}Co_xSi$, the crystallization of skyrmions was observed by the neutron diffraction studies.[1,2] Recently, we have observed the real-space images of skyrmion crystal in thin films of related compounds ($Fe_{0.5}Co_{0.5}Si$ and FeGe) using Lorentz transmission electron spectroscopy.[3,4] We have observed the hexagonal arrangement of skyrmions including the topological defects (chiral domains and dislocations) under the magnetic field normal to the films, and found that the two dimensional skyrmion crystal phase is fairly stabilized by the thin film form of the samples. We have also studied the topological Hall effect caused by the spin chirality of the skyrmion crystal in a related material MnGe. In terms of the Hall measurement, they have shown the real space nature of the fictitious magnetic field caused by the magnetic configuration of the skyrmion crystal, in contrast with the momentum-space fictitious field in another spin chirality system, $Nd_2Mo_2O_7$.[5] This work was done in collaboration with X. Z. Yu, N. Kanazawa, J. H. Park, J. H. Han, K. Kimoto, W. Z. Zhang, S. Ishiwata, Y. Matsui, N. Nagaosa, and Y. Tokura.

[1] S. Mühlbauer *et al.,* Science **323,** 915 (2009).
[2] W. Münzer *et al.,* Phys. Rev. B **81,** 041203 (2010).
[3] X. Z. Yu, *et al.*, Nature, **465,** 901 (2010).
[4] X. Z. Yu, *et al.,* Nature material, *inpress.*
[5] Y. Taguchi *et al.,* Science **291,** 2573 (2001).

4:18PM X3.00004 Multiferroic vortices in hexagonal manganites[1] , WEIDA WU, Department of Physics and Astronomy, Rutgers University — Hexagonal rare earth manganites ($RE MnO_3$) show a unique improper ferroelectricity induced by structural trimerization. Extensive research on these systems has been carried out due to its potential application in memory and the intriguing multiferroicity (coexistence of ferroelectricity and antiferromagnetism). However, the true relationship between ferroelectric domains and structural domains has never been revealed. Using transmission electron microscopy (TEM) and conductive atomic force microscopy (cAFM), we observed an intriguing conductive "cloverleaf" pattern of six domains emerging from one point, all distinctly characterized by polarization orientation and structural antiphase relationships in hexagonal manganites.[2] The nanoscale electric conduction between a sharp tip and the surface is intrinsically modulated by the ferroelectric polarization.[3] The cloverleaf defects are structural vortices where the phase angle goes successively through all six phases.[4] In addition, we discovered that the ferroelectric domain walls and structural antiphase boundaries are mutually locked. Correlated with previous observation of coupled ferroelectric and antiferromagnetic domain walls,[5] our results suggest that these cloverleaf defects are indeed multiferroic vortices. These fascinating results reveal the rich physics of the hexagonal system with a semiconducting bandgap where structural trimerization, ferroelectricity, magnetism and charge conduction are intricately coupled.

[1] NSF-DMR-0844807

[2] T. Choi, et al, "Insulating interlocked ferroelectric and structural antiphase domain walls in multiferroic $YMnO_3$" Nature Materials, **9**, 253-258 (2010).
[3] W. Wu, et al, "Polarization-Modulated Rectification at Ferroelectric Surfaces" Phys. Rev. Lett., **104**, 217601 (2010).
[4] M. Mostovoy, "a whirlwind of opportunities," Nature Materials, **9**, 188-190 (2010).
[5] M. Fiebig, et al, "Observation of coupled magnetic and electric domains," Nature, **419**, 818 (2002).

4:54PM X3.00005 Ferroelectric vortices from atomistic simulations[1] , LAURENT BELLAICHE, University of Arkansas — In 2004, the use of a first-principles-based effective Hamiltonian [1] led to the prediction of a novel structure in zero-dimensional ferroelectrics, in which the electric dipoles organize themselves to form a vortex [2]. Such structure exhibits the so-called spontaneous toroidal moment, rather than the spontaneous polarization, as its order parameter [2]. Subsequently, various original phenomena, all related to vortices, were predicted in ferroelectric nanostructures. Examples of such phenomena are: (i) the existence of a new order parameter, denoted as the hypertoroidal moment, that is associated with many complex dipolar structures (such as double-vortex states) [3]; (ii) the possible control of single and double vortex states by electric fields, via the formation of original intermediate states [4-8]; (iii) the discovery of a new class of quantum materials (denoted as incipient ferrotoroidics), for which zero-point vibrations wash out the vortex state and yield a complex local structure [9]; (iv) the existence of chiral patterns of oxygen octahedral tiltings that originate from the coupling of these tiltings with the ferroelectric vortices [10]. The purpose of this talk is to discuss some of these striking phenomena, as well as, to reveal others (if time allows). These studies are done in collaboration with A.R. Akbarzadeh, H. Fu, I. Kornev, I. Naumov, I. Ponomareva, S. Prosandeev, Wei Ren and D. Sichuga.

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[3] S. Prosandeev and L. Bellaiche, Phys. Rev. B 77, 060101(R) (2008).
[4] S. Prosandeev, I. Ponomareva, I. Kornev, I. Naumov and L. Bellaiche, Phys. Rev. Lett. 96, 237601 (2006).
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[7] S. Prosandeev, I. Ponomareva, I. Kornev, and L. Bellaiche, Phys. Rev. Lett. 100, 047201 (2008).
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[9] S. Prosandeev, A. R. Akbarzadeh and L. Bellaiche, Phys. Rev. Lett. 102, 257601(2009).
[10] David Sichuga, Wei Ren, Sergey Prosandeev, and L. Bellaiche, Phys. Rev. Lett. 104, 207603 (2010).

[1]These works are supported by the NSF grants DMR 0701558 and DMR-0080054 (C-SPIN), DOE grant DE-SC0002220, and ONR grants N00014-08-1-0915 and N00014-07-1-0825 (DURIP).

Thursday, March 24, 2011 2:30PM - 5:30PM –
Session X4 DPOLY: Functional Gels Ballroom A4

2:30PM X4.00001 Micromechanical study of mitotic chromosome structure[1] , JOHN MARKO, Northwestern University — Our group has developed micromanipulation techniques for study of the highly compacted mitotic form of chromosome found in eukaryote cells during cell division. Each metaphase chromosome contains two duplicate centimeter-long DNA molecules, folded up by proteins into cylindrical structures several microns in length. Native chromosomes display linear and reversible stretching behavior over a wide range of extensions (up to 5x native length for amphibian chromosomes), described by a Young modulus of about 300 Pa. Studies using DNA-cutting and protein-cutting enzymes have revealed that metaphase chromosomes behave as a network of chromatin fibers held together by protein-based isolated crosslinks. Our results are not consistent with the more classical model of loops of chromatin attached to a protein-based structural organizer or "scaffold". In short, our experiments indicate that metaphase chromosomes can be considered to be "gels" of chromatin; the stretching modulus of a whole chromosome is consistent with stretching of the chromatin fibers contained within it. Experiments using topoisomerases suggest that topological constraints may play an appreciable role in confining chromatin in the metaphase chromosome. Finally, recent experiments on human chromosomes will be reviewed, including results of experiments where chromosome-folding proteins are specifically depleted using siRNA methods.

[1]Supported by NSF-MCB-1022117, DMR-0715099, PHY-0852130, DMR-0520513, NCI 1U54CA143869-01 (NU-PS-OC), and the American Heart Association.

3:06PM X4.00002 A Molecular View of Liquid Crystalline Elastomers and Gels , JUAN DE PABLO, University of Wisconsin — A combination of Monte Carlo and molecular dynamics simulations is used to examine the order-disorder transitions that arise in model liquid crystalline elastomers and colloidal gels as a function of concentration and strain, respectively. Two models are considered. In the first, a lattice model is used to represent a colloidal gel of nematogens and nanoparticles. In the second, a cross-linked elastomer of Gay-Berne mesogens is adopted to examine the order-disroder transition that arises as a function of strain. The results of simulations are compared to those of recent experiments for these two classes of systems.

3:42PM X4.00003 Gelation of mucin: Protecting the stomach from autodigestion , RAMA BANSIL, Boston University — In this talk I will describe the molecular mechanisms involved in the remarkable ability of the mucus lining of the stomach for protecting the stomach from being digested by the acidic gastric juices that it secretes. These physical properties can be attributed to the presence of a high molecular weight glycoprotein found in mucus, called mucin. Rheology and other measurements show that gastric mucin forms a gel under acidic pH. A model of gelation based on the interplay of hydrophobic and electrostatic interactions will be discussed. Molecular Dynamics simulation studies of folding and aggregation of mucin domains provide further support for this model. The relevance of gelation to the motion of the ulcer causing bacterium H. pylori will be discussed.

4:18PM X4.00004 Responsive gels and membranes , MONICA OLVERA DE LA CRUZ, Northwestern University — We use computer simulations and analytical method to explore and analyze effects of composition heterogeneities in elastic membranes and gels. In particular, we focus on shape pattern formation in thin networks and elastic closed membranes driven by the presence of composition heterogeneities. We study the crumpling of multicomponent elastic membranes in response to changes in external conditions, as well as the spontaneous buckling transition of heterogeneous elastic shells into regular and irregular polyhedra.

4:54PM X4.00005 ABSTRACT WITHDRAWN –

Thursday, March 24, 2011 2:30PM - 5:30PM –
Session X5 FIAP: The Corporate Feel: Atomic Force Microscopy in Industry Ballroom C1

2:30PM X5.00001 Accelerated design and quality control of impact modifiers for plastics through atomic force microscopy (AFM) analysis , GUNTER MOELLER, Arkema Inc. — Standard polymer resins are often too brittle or do not meet other mechanical property requirements for typical polymer applications. To achieve desired properties it is common to disperse so called "impact modifiers", which are spherical latex particles with diameters of much less than one micrometer, into the pure resin. Understanding and control of the entire process from latex particle formation to subsequent dispersion into polymer resins are necessary to accelerate the development of new materials that meet specific application requirements. In this work AFM imaging and nanoindentation techniques in combination with AFM-based spectroscopic techniques were applied to assess latex formation and dispersion. The size and size distribution of the latex particles can be measured based on AFM amplitude modulation images. AFM phase images provide information about the chemical homogeneity of individual particles. Nanoindentation may be used to estimate their elastic and viscoelastic properties. Proprietary creep and nanoscale Dynamic Mechanical Analysis (DMA) tests that we have developed were used to measure these mechanical properties. The small size of dispersed latex inclusions requires local mechanical and spectroscopic analysis techniques with high lateral and spatial resolution. We applied the CRAVE AFM method, developed at NIST, to perform mechanical analysis of individual latex inclusions and compared results with those obtained using nanoscale DMA. NanoIR, developed by Anasys Inc., and principal component confocal Raman were used for spectroscopic analysis and results from both techniques compared.

3:06PM X5.00002 Scanning Probe Evaluation of Electronic, Mechanical and Structural Material Properties[1] , KUMAR VIRWANI, IBM — We present atomic force microscopy (AFM) studies of a range of properties from three different classes of materials: mixed ionic electronic conductors, low-k dielectrics, and polymer-coated magnetic nanoparticles. (1) Mixed ionic electronic conductors are being investigated as novel diodes to drive phase-change memory elements. Their current-voltage characteristics are measured with direct-current and pulsed-mode conductive AFM (C-AFM). The challenges to reliability of the C-AFM method include the electrical integrity of the probe, the sample and the contacts, and the minimization of path capacitance. The role of C-AFM in the optimization of these electro-active materials will be presented. (2) Low dielectric constant (low-k) materials are used in microprocessors as interlayer insulators, a role directly affected by their mechanical performance. The mechanical properties of nanoporous silicate low-k thin films are investigated in a comparative study of nanomechanics measured by AFM and by traditional nanoindentation. Both methods are still undergoing refinement as reliable analytical tools for determining nanomechanical properties. We will focus on AFM, the faster of the two methods, and its developmental challenges of probe shape, cantilever force constant, machine compliance and calibration standards. (3) Magnetic nanoparticles are being explored for their use in patterned media for magnetic storage. Current methods for visualizing the core-shell structure of polymer-coated magnetic nanoparticles include dye-staining the polymer shell to provide contrast in transmission electron microscopy. AFM-based fast force-volume measurements provide direct visualization of the hard metal oxide core within the soft polymer shell based on structural property differences. In particular, the monitoring of adhesion and deformation between the AFM tip and the nanoparticle, particle-by-particle, provides a reliable qualitative tool to visualize core-shell contrast without the use of additional contrast enhancing agents.

[1]In collaboration with Jane Frommer, IBM.

3:42PM X5.00003 Nanomechanical characterization of polypropylene-based materials with multifrequency atomic force microscopy (AFM)-based methods , DALIA YABLON, Exxonmobil Research and Engineering — Atomic force microscopy (AFM) is a powerful technique with broad applications to characterization of surfaces, primarily used for nanoscale quantitative topographic measurements and qualitatively distinguishing between material properties on the surface. We describe recent advances in our capabilities to quantify nanoscale mechanical measurements of surface properties using recently developed high frequency and multifrequency methods. Initial focus of this work is for polymeric materials (and specifically polypropylene based blends), where nanomechanical characterization is critical for effective understanding of structure-property relationships, especially for more complicated multi-component materials such as blends and composites. SPM techniques rely on complicated tip-sample interactions that must be effectively separated and understood if we are to ultimately identify and quantify specific materials and material properties at the nanoscale. We describe different approaches to this problem utilizing a number of AFM based techniques including force curves, bimodal imaging and contact resonance imaging. Ultimately, these techniques yield quantitative maps of conservative and dissipative tip-sample interactions that are then converted into elastic and viscous moduli maps. We describe initial applications of these methods to measure mechanical properties such as storage and loss moduli of model polypropylene containing blends including polypropylene/rubber and polypropylene/polystyrene blends. Finally, quantitative moduli values obtained by methods described above are compared to those obtained by bulk methods.

4:18PM X5.00004 Probing Photovoltaic Performance , DAVID GINGER, University of Washington — A wide range of nanostructured materials including organic bulk heterojunction blends, solution processed colloidal semiconductors, and hybrid organic/inorganic thin films are being explored for solar energy applications. These sytems typically exhibit nanoscale heterogenity in their electronic and optical properties. Scanning probes are critical for building a microscopic picture of the performance of new nanostructured and thin film photovoltaic materials–and may ultimately prove to be a valuable metrology tool for process control during production–because scanning probe microscopy provides a unique opportunity to correlate local charge generation, recombination and transport with local structure in these systems. In this talk I will focus on techniques developed and lessons learned during our group's study of thin film solar cell materials with a particular emphasis on nanostructured organic bulk heterojunction blends.

4:54PM X5.00005 Challenges and opportunities for probe-based information technology[1] , JEREMY LEVY, U. Pittsburgh — Scanning probe microscopes have become standard tools for characterization of materials and devices at the nanoscale. But what about "OEM" versions for information technology? The standard answer is that probe-based lithography or storage is not practical because it cannot scale-their cost and complexity will never allow useful devices to be made with probes. Such was not always the conventional wisdom in the industrial community. The Millipede Project,[2] pioneered by Gerd Binnig at IBM and pursued at other companies such as Hitachi and Seagate, sought to scale the number of probes to ∼1000. In fact, they were successful, but not enough to be competitive with FLASH memory. Since then, order of magnitude improvements have been made both in scaling up to the number of probes past ten million,[3] and in scaling down the minimum bit size below two nanometers.[4] Combining these two approaches may well justify the statement: "There's plenty of room for probes at the bottom."

[1]This work was supported by NSF DMR-0704022 and DARPA Seedling (W911NF-09-10258).

[2]http://www.zurich.ibm.com/st/storage/concept.html

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Thursday, March 24, 2011 2:30PM - 5:30PM –

Session X6 DCOMP DAMOP: Pairing in Imbalanced Fermi Mixtures Ballroom C2

2:30PM X6.00001 Correlated phases in the Fermi Hubbard model with spin and mass imbalance , GIULIANO ORSO, Université Paris Diderot, Laboratoire Matériaux et Phénomènes Quantiques — One dimensional attractive fermions with unequal spin populations provide a direct realization of the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) superfluid state, in which Cooper pairs condense at finite momentum. The presence of an additional mass asymmetry between the two components gives rise to multi-particle bound states, including trimers made of one light and two heavy fermions. I first discuss the stability of these bound states through the exact solution of the three-body problem. Based on Density Matrix Renormalization Group simulations and bosonization theory, I then show that at finite and commensurate densities the ground state of the system is a Luttinger liquid of trimers. In this new phase superconducting FFLO correlations are exponentially suppressed. Finally I explain how the mass asymmetry changes the topology of the grand-canonical phase diagram of the Fermi Hubbard model. [GO, E. Burovski and T. Jolicoeur, PRL 104, 065301 (2010); E. Burovski, GO and T. Jolicoeur, PRL 103, 215301 (2009)]

3:06PM X6.00002 The phase diagram of imbalanced Fermi gases[1] , DANIEL E. SHEEHY, Louisiana State University — Recent experimental and theoretical research has focused on the phases of strongly interacting Fermi gases under an imposed population imbalance between the fermion species. The large difference in chemical potential between the majority and minority species disrupts conventional singlet s-wave pairing, yielding a rich phase diagram including regions of phase separation, Fulde-Ferrell-Larkin-Ovchinnikov superfluidity and magnetic superfluidity. I will discsuss these predicted phases, as well as the behavior at large imbalance where the minority species can induce an effective attraction among the majority fermions and a resulting instability towards p-wave superfluidity.

[1]Research supported by the Louisiana Board of Regents.

3:42PM X6.00003 Pair formation in Fermi systems with population imbalance in one- and two-dimensional optical lattices[1] , GEORGE BATROUNI, University of Nice, Institut Non-Linaire de Nice — I will discuss pairing in fermionic systems in one- and two-dimensional optical lattices with population imbalance. This will be done in the context of the attractive fermionic Hubbard model using the Stochastic Green Function algorithm in d=1 while for d=2 we use Determinant Quantum Monte Carlo. This is the first exact QMC study examining the effects of finite temperature which is very important in experiments on ultra-cold atoms. Our results show that, in the ground state, the dominant pairing mechanism is at nonzero center of mass momentum, i.e. FFLO. I will then discuss the effect of finite temperature in the uniform and confined systems and present finite temperature phase diagrams. The numerical results will be compared with experiments.

[1]With M. J. Wolak (CQT, National University of Singapore) and V. G. Rousseau (Department of Physics and Astronomy, Louisiana State University).

4:18PM X6.00004 Spin imbalanced Fermi gases in 1D and the crossover to 3D[1] , ANN SOPHIE RITTNER, Rice University — The search for the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase, a polarized superfluid with a spatially varying order parameter, has generated large interest in both condensed matter and cold atoms communities. To date, there has been only indirect experimental evidence of FFLO in the heavy fermion superconductor CeCoIn5. A strongly interacting 3D polarized Fermi gas exhibits three phases at low temperature: an unpolarized superfluid, a partially polarized and a fully polarized normal phase, which phase separate in an optical trap. There is no experimental evidence for an FFLO phase in the 3D system and theory predicts that it occupies only a small region in the phase diagram. In a 1D polarized Fermi gas, the FFLO phase is predicted to occupy a large region of the phase diagram. We have implemented a 2D optical lattice in order to explore the phase diagram of an imbalanced spin mixture of ^{6}Li. In in-situ density distributions, we observe in the center of the cloud a partially polarized region surrounded by an either fully polarized or an unpolarized superfluid shell depending on the spin imbalance. The density profiles are quantitatively well described by a finite temperature Bethe ansatz and can be used to extract the 1d phase diagram of the imbalanced 1d Fermi gas. Moreover, the quantitative agreement of experiment and theory paves the way for directly observing the elusive FFLO phase in the system.

[1]Supported by DARPA, NSF, ONR, and The Welch and Keck Foundations

4:54PM X6.00005 Universal Spin Transport in Strongly Interacting Fermi Gases[1] , MARTIN ZWIERLEIN, Massachusetts Institute of Technology — Ultracold gases of fermionic atoms have emerged as a unique platform to study strongly interacting fermion systems. Here we study spin transport in a two-state mixture of fermionic atoms near a Feshbach resonance. Starting with two separate spin domains in an atom trap, we observe the subsequent evolution of the spin mixture towards the eventual ground state, a superfluid of fermion pairs. Initially, the gas clouds of unlike spins almost perfectly bounce off each other, despite densities a million times thinner than air. Only over several seconds, about 100 000 collision times, the spins slowly diffuse into each other and, below a critical temperature, form a superfluid of fermion pairs. We determine the transport properties in this gas as a function of interaction strength and temperature. In particular, we find the spin diffusion coefficient in the strongly interacting, degenerate regime to take on the universal value for a "perfect fluid", $D \simeq \hbar/m = \frac{(100\mu\mathrm{m})^2}{\mathrm{s}}$, where m is the mass of the ^{6}Li atoms. At high temperatures, we find the universal law $D = \alpha \frac{\hbar}{m} (T/T_F)^{3/2}$ with a constant α. The ratio of spin conductivity and spin diffusion coefficient yields the spin susceptibility in these gases, showing the Curie law at high temperatures and a departure from the compressibility at low temperatures, that we interpret as a signature for entering the Fermi liquid regime. Our transport experiments near and far equilibrium have implications on other strongly interacting Fermi systems, suggesting a fundamental lower limit to the spin diffusion coefficient, in the absence of localization, on the order of $\hbar/m$ - a conjecture already made by Onsager. Our spin susceptibility measurements appear to exclude a ferromagnetic ground state on the repulsive side of the Feshbach resonance.

[1]This work was supported by the NSF, AFOSR-MURI, a grant from the Army Research Office with funding from the DARPA OLE program, the David and Lucille Packard Foundation and the Alfred P. Sloan Foundation.

Thursday, March 24, 2011 2:30PM - 5:30PM –

Session X7 DBP: Quantitative Approaches to DNA Replication Ballroom C3

2:30PM X7.00001 Replication domains are self-interacting structural chromatin units of human chromosomes , ALAIN ARNEODO, CNRS — In higher eukaryotes, the absence of specific sequence motifs marking the origins of replication has been a serious hindrance to the understanding of the mechanisms that regulate the initiation and the maintenance of the replication program in different cell types. In silico analysis of nucleotide compositional skew has predicted the existence, in the germline, of replication N-domains bordered by putative replication origins and where the skew decreases rather linearly as the signature of a progressive inversion of the average fork polarity. Here, from the demonstration that the average fork polarity can be directly extracted from the derivative of replication timing profiles, we develop a wavelet-based pattern recognition methodology to delineate replication U-domains where the replication timing profile is shaped as a U and its derivative as a N. Replication U-domains are robustly found in seven cell lines as covering a significant portion (40-50%) of the human genome where the replication timing data actually displays some plasticity between cell lines. The early replication initiation zones at U-domains borders are found to be hypersensitive to DNase I cleavage, to be associated with transcriptional activity and to present a significant enrichment in insular-binding proteins CTCF, the hallmark of an open chromatin structure. A comparative analysis of genome-wide chromatin interaction (HiC) data shows that replication-U domains correspond to self-interacting structural high order chromatin units of megabase characteristic size. Taken together, these findings provide evidence that the epigenetic compartmentalization of the human genome into autonomous replication U-domains comes along with an extensive remodelling of the threedimensional chromosome architecture during development or in specific diseases. The observed cell specific conservation of the replication timing between the human and mouse genomes strongly suggests that this chromosome organization into self-interacting structural and functional units is a general feature of mammalian organisms.

3:06PM X7.00002 Thermal Replication Trap , DIETER BRAUN, Ludwig Maximilians University — The hallmark of living matter is the replication of genetic molecules and their active storage against diffusion. We have argued in the past that thermal convection can host the million-fold accumulation even of single nucleotides and at the same time trigger exponential replication [1]. Accumulation is driven by thermophoresis and convection in elongated chambers, replication by the inherent temperature cycling in convection. Optothermal pumping [2,3] allows to implement the thermal trap efficiently in a toroidal [4] or linear [5] geometry. Based on this method, we were in a position to combine accumulation and replication of DNA in the same chamber [5]. As we are missing a solid chemistry of prebiotic replication, we used as a proxy reaction for to replication the polymerase chain reaction. Convective flow both drives the DNA replicating polymerase chain reaction (PCR) while concurrent thermophoresis accumulates the replicated 143 base pair DNA in bulk solution. The time constant for accumulation is 92 s while DNA is doubled every 50 s. The length of the amplified DNA is checked with thermophoresis. Finite element simulations confirm the findings. The experiments explore conditions in pores of hydrothermal rock which can serve as a model environment for the origin of life and has prospects towards the first autonomous evolution, hosting the Darwin process by molecular selection using the thermophoretic trap. On the other side, the implemented continuous evolution will be able to breed well specified DNA or RNA molecules in the future.

[1] Baaske, Weinert, Duhr, Lemke, Russell and Braun, PNAS 104, 9346 (2007)
[2] Weinert, Kraus, Franosch and Braun, PRL 100, 164501 (2008)
[3] Weinert and Braun, Journal of Applied Physics 104, 104701 (2008)
[4] Weinert and Braun, Nano Letters 9, 4264 (2009)
[5] Mast and Braun, PRL 104, 188102 (2010)

3:42PM X7.00003 Single-molecule measurements of replisome composition and function reveal the mechanism of polymerase exchange , JOSEPH LOPARO, Harvard Medical School — A complete understanding of the molecular mechanisms underlying the functioning of large, multiprotein complexes requires experimental tools capable of simultaneously visualizing molecular architecture and enzymatic activity in real time. I will describe a novel single-molecule assay that combines the flow-stretching of individual DNA molecules to measure the activity of the DNA-replication machinery with the visualization of fluorescently labeled DNA polymerases at the replication fork. By correlating polymerase stoichiometry with DNA synthesis of T7 bacteriophage replisomes, we are able to quantitatively describe the mechanism of polymerase exchange. We find that even at relatively modest polymerase concentration (2 nM), soluble polymerases are recruited to an actively synthesizing replisome, dramatically increasing local polymerase concentration. These excess polymerases remain passively associated with the replisome through electrostatic interactions with the T7 helicase for 50 seconds until a stochastic and transient dissociation of the synthesizing polymerase from the primer-template allows for a polymerase exchange event to occur.

4:18PM X7.00004 Defects and DNA replication: a role for stochasticity[1] , JOHN BECHHOEFER, Simon Fraser University — When a cell replicates its DNA, each base must be copied once and only once per cell cycle. A failure to complete replication normally can lead to cell death, or worse. In this talk, I will discuss how ideas from statistical physics can help understand how replication is organized and controlled. In particular, we describe a formalism based on rate equations similar to those used to describe the kinetics of crystal growth and show how it can describe the normal course of DNA replication. In practice, replication must also deal with numerous kinds of problems. For example, the machinery of replication may stall or strands may be broken. We show how to extend our formalism to include the effects of such damage and conclude that there are two regimes: a normal regime, where the influence of defects is local, and an initiation-limited regime, where the influence of defects is long range. In the latter regime, defects have a global impact on replication. We show that normal, healthy cells have defect densities in the normal regime but cells with "problems" have defect densities that approach the crossover value. The overall conclusion is that passive stochastic control and physical effects such as diffusion are more relevant for DNA replication than had been believed until recently.

[1]Supported by HFSP and NSERC (Canada).

4:54PM X7.00005 Universal Temporal Profile of Replication Origin Activation in Eukaryotes , ARACH GOLDAR, CEA — The complete and faithful transmission of eukaryotic genome to daughter cells involves the timely duplication of mother cell's DNA. DNA replication starts at multiple chromosomal positions called replication origin. From each activated replication origin two replication forks progress in opposite direction and duplicate the mother cell's DNA. While it is widely accepted that in eukaryotic organisms replication origins are activated in a stochastic manner, little is known on the sources of the observed stochasticity. It is often associated to the population variability to enter S phase. We extract from a growing *Saccharomyces cerevisiae* population the average rate of origin activation in a single cell by combining single molecule measurements and a numerical deconvolution technique. We show that the temporal profile of the rate of origin activation in a single cell is similar to the one extracted from a replicating cell population. Taking into account this observation we exclude the population variability as the origin of observed stochasticity in origin activation. We confirm that the rate of origin activation increases in the early stage of S phase and decreases at the latter stage. The population average activation rate extracted from single molecule analysis is in prefect accordance with the activation rate extracted from published micro-array data, confirming therefore the homogeneity and genome scale invariance of dynamic of replication process. All these observations point toward a possible role of replication fork to control the rate of origin activation.

Thursday, March 24, 2011 2:30PM - 5:30PM –
Session X8 FHP FIP: Migrations of Physicists Ballroom C4

2:30PM X8.00001 Migration of scientists and the International Centre for Theoretical Physics – a Personal and Professional Perspective , KATEPALLI R. SREENIVASAN, New York University — Scientists migrate for a variety of reasons: political problems with their governments, lack of professional opportunities in their countries, the lure of better lives, financial security for them and their families, better education for their off-springs, and so forth. Migration usually occurs from poor and oppressed countries–the two categories are not one and the same–to the rich and the open. It has created, over time, a dilemma for the poor countries: in the midst of all their other problems, how to justify spending on higher education and research when that investment often results in the most enterprising of its citizens to leave their countries behind? (When migration has reversed direction occasionally, it is because of certain necessities of the scientists to be back in their countries or for opportunities that some individuals see for wielding greater scientific power.) The ideal of keeping the best scientists in their own countries, still ensuring that they remain scientifically productive and inspiring to the youth, is what provided the motivation for the creation of the International Centre for Theoretical Physics in Trieste, Italy, where I served as Director for some seven years. In this talk, I will present the story behind the formation of the Centre in 1964, explain its rationale, and analyze its evolution over time to accommodate the changing scene in world; I will discuss how some things have remained the same even as more of them have changed over time. Finally, I will remark on the broad needs of developing countries even though such needs are often very specific to a country.

3:06PM X8.00002 Physicists' Forced Migrations under Hitler , ALAN BEYERCHEN, Ohio State University — When the Nazis came to power in early 1933 they initiated formal and informal measures that forced Jews and political opponents from public institutions such as universities. Some physicists retired and others went into industry, but most emigrated. International communication and contact made emigration a viable option despite the desperate economic times in the Great Depression. Another wave of emigrations followed the annexation of Austria in 1938. Individual cases as well as general patterns of migration and adaptation to new environments will be examined in this presentation. One important result of the forced migrations was that many of the physicists expelled under Hitler played important roles in strengthening physics elsewhere, often on the Allied side in World War II.

3:42PM X8.00003 Migrations and the Rise of High Energy Physics in Brazil , ALBERTO SANTORO, State University of Rio de Janeiro, Brazil — There have been five phases in the development and evolution of High Energy Physics (HEP) in Brazil, that I review from a personal perspective. The Founding Phase (1938 - 1955) was followed by the Brasilia Phase that included an attempt by R. Salmeron, the first Brazilian physicist to work at CERN in its early years, to found an HEP institute at the University of Brasilia in 1960 - 1965. This was followed by my return from France during the redemocratization of 1985, after 21 years of miltary rule. The Expansion Phase (1984 - 1999) followed an ambitious plan that led to the spread of high energy physics to many key institutions throughout the country. The Evolutionary Phase (1984 - 2010), initiated with the strong help of Leon Lederman (Nobel Laureate, 1988) began with the strengthening of HEP groups and their participation in the major experimental collaborations, at the Tevatron at Fermilab and more recently at the LHC at CERN, with the strong support of the Brazilian funding agencies. The fifth Partnership phase (2011 -) has just begun, as the high energy physics community and its supporting agencies work to make Brazil an Associate Member of CERN, and in this way to make the Brazilian community a full partner in the global effort aimed at discoveries at the Energy Frontier.

4:18PM X8.00004 Russian, Soviet, and post-Soviet scientific migration: history and patterns , ALEXEI KOJEVNIKOV, University of British Columbia — Immigrant scientists from other European countries (predominantly German) were crucial in establishing the tradition of modern science in the Russian Empire of the 18th and 19th centuries. Since the 1860s, however, outgoing waves of scientific migration started originating in Russia, bringing important innovations to international science. The scale and patterns of migration varied greatly with the turbulent time. The talk will describe several landmark stages of the proceess and their cultural consequences: from opening higher education possibilities for women during the late 19th century, to post-1917 academic refugees and Soviet defectors, to the 1960s brain drain provoked by the launch of Sputnik, and to what can be called the first truly global scientific diaspora of Russophone scientists after 1990.

4:54PM X8.00005 Chinese/American Physicists: A Transnational History[1] , ZUOYUE WANG, Cal State Polytechnic Univ., Pomona — As part of a broader project on "Chinese/American Scientists: Transnational Science during the Cold War and Beyond," this paper examines the movements of American-trained Chinese physicists following the founding of the People's Republic of China in 1949. While a majority of these physicists chose to stay in the US (the "stayees"), a number went back to China in the 1950s (the "returnees") against many obstacles during the McCarthy era. After the reopening of US-China relations in the 1970s, the two groups joined hands in promoting China-US scientific and educational exchanges, leading eventually to the coming to the US of a new generation of Chinese physics students and the return to China of some of the original "stayees." This transnational history of Chinese/American physicists aims to illustrate the nature and extent of the Americanization of international science and the internationalization of American science in the post-World War II era.

[1]This work was supported in part by the National Science Foundation under Grant No. SES-1026879.

Thursday, March 24, 2011 2:30PM - 5:54PM –

Session X9 DFD: Coordination, Coherence and Synchronization through Hydrodynamic Interactions D220

2:30PM X9.00001 Collective motion and density fluctuations in swimming bacteria , HEPENG ZHANG, University of Texas at Austin and Shanghai Jiao Tong University — The emergence of collective motion such as in fish schools, mammal herds, and insect swarms is a ubiquitous self-organization phenomenon. Such collective behavior plays an important role in a range of problems, such as spreading of deceases in animal or fish groups. Current models have provided a qualitative understanding of collective motion, but progress in quantitative modeling in hindered by the lack of experimental data. Here we examine a model microscopic system, where we are able to measure simultaneously the positions, velocities, and orientations of up to a thousand bacteria in a colony. The motile bacteria form closely-packed dynamic clusters within which they move cooperatively. The number of bacteria in a cluster exhibits a power-law distribution truncated by an exponential tail, and the probability of finding large clusters grows markedly as bacterial density increases. Mobile clusters cause anomalous fluctuations in bacterial density as found in mathematical theories and numerical models. Our results demonstrate that bacteria are an excellent system to study general phenomena of collective motion.

3:06PM X9.00002 Collective behavior of spinning particles at fluid/fluid interface[1] , YAOUEN FILY, Syracuse University, APARNA BASKARAN, Brandeis University, M. CRISTINA MARCHETTI, Syracuse Biomaterials Institute and Syracuse University — Rotating particles in a viscous fluid can exhibit interesting behavior due to hydrodynamic interactions. When the particles are driven by an external torque, these interactions result in an effective azimuthal force, leading to swirling motion. It has been shown that small numbers of such particles form precessing atom-like structures. The behavior of large collections of spinning particles is, however, still relatively unexplored. We study the phase diagram of a collection of spinning particles in two dimensions using molecular dynamics simulations. The rotors interact via hydrodynamic interactions and short-range repulsion, in the presence of thermal noise. The repulsive interaction yields transitions from a solid to a liquid to a gas as the density of rotors is decreased. The azimuthal hydrodynamic interaction modifies each of these phases in a distinct way. Both long-range and screened hydrodynamic interactions are considered. Some properties of the various phases are shown to depend critically on the range of the interaction.

[1]Supported by the NSF through grants DMR-0806511 and DMR-1004789.

3:18PM X9.00003 ABSTRACT WITHDRAWN –

3:30PM X9.00004 Synchronization phenomena in systems with magnetodipolar interactions , ANDREJS CEBERS, MIHAILS BELOVS, University of Latvia — Rich pattern formation phenomena under the action of AC field for two dimensional systems of magnetic dipoles floating on the surface of liquid are observed and reproduced numerically by the first-principles model [1]. Here by the study of dynamics of two dipoles interacting with weak dipolar forces it is found that due to series of bifurcations the motion of dipoles in AC field is synchronized. If the dipoles orientation is confined to the plane the synchronous oscillation regime by infinite period bifurcation transforms to the regime of synchronous rotation. This regime is unstable for intermediate values of the field strength and the motion of dipoles is periodic or quasi-periodic. Above the critical value of field strength these regimes transform to rotational regime and the dipoles synchronously rotate in plane. Estimate of the critical parameters of the synchronization according to the dimensionless parameters used in the first-principles model [1] show that the synchronization of the dipoles rotation should be inherent in this model.

[1] M.Belkin, A.Glatz, A.Snezhko, and I.S.Aranson, Phys.Rev.E, 82, 051301(R), (2010)

3:42PM X9.00005 Pattern Formation in a Rotating Suspension of Non-Brownian Buoyant Particles , PENGER TONG[1], Department of Physics, Hong Kong University of Science and Technology, MAKRAND KALYANKAR, BRUCE ACKERSON, Department of Physics, Oklahoma State University, W.R. MATSON, Department of Physics, DePaul University — This study examines concentration and velocity patterns observed in a horizontal rotating cylinder completely filled with a monodisperse suspension of non-Brownian buoyant particles. The unique patterns or phases are mapped by varying both the rotation rate and the solvent viscosity. Individual phases are identified using both frontal and axial views. Phase boundaries are compared to those obtained recently for suspensions of non-buoyant particles. Expressing the boundaries in terms of dimensionless parameters unifies the data for several samples at low rotation rates. When centrifugal force dominates, the behavior becomes quite different from previous studies.

[1]Work supported in part by the Research Grants Council of Hong Kong SAR.

3:54PM X9.00006 Shear-induced hydrodynamic diffusion of a flowing suspension of elastic capsules , MARCUS HWAI YIK TAN, DUC VINH LE, KENG-HWEE CHIAM, Mechanobiology Institute, National University of Singapore and A*STAR Institute of High Performance Computing — In flowing suspensions of soft and deformable elastic capsules, the shear flow causes hydrodynamic interaction among the capsules, resulting in an effective hydrodynamic diffusion that is not Brownian in origin. Recent experiments have suggested that hydrodynamic diffusion of red blood cells may play an important role in the pathophysiological processes of vasoocclusion and thrombosis. To study hydrodynamic diffusion further, we have developed accurate three-dimensional numerical simulations based on the immersed boundary method and thin shell theory to study the deformation of a large number of elastic capsules enclosed by thin shells moving in a shear flow. Using these simulations, we have calculated the effective hydrodynamic diffusion coefficient and showed how it varies with bulk flow velocity and capsule properties such as the volume fraction, size, and stiffness of spherical and biconcave capsules. We also compared them to scaling arguments and experimental measurements done for red blood cell suspensions.

4:06PM X9.00007 Artificial Microfluidic Squirmers , SHASHI THUTUPALLI, M.P.I. for Dynamics and Self Organisation, Gottingen, Germany, RALF SEEMANN, Physics Faculty, University of Saarlandes, Saarbrucken, Germany, STEPHAN HERMINGHAUS, M.P.I. for Dynamics and Self Organisation, Gottingen, Germany — While there is a growing consensus on the propulsion mechanisms of swimmers at low Reynolds' numbers, many questions remain open regarding the hydrodynamic effects on such swimmers, in particular the coupling between swimmers. Here we present experiments on artificial swimmers, where hydrodynamics is seen to be responsible for a wide range of collective behavior and interactions. Using droplet microfluidics with a surfactant laden continuous oil phase, we create monodisperse aqueous droplets containing chemicals that produce a steady source of Bromine ions. The surfactant (mono-olein) reacts at the droplet interface with the Bromine produced within the droplets, and a dynamic instability leads to gradients of interfacial tension at the droplet interface. These gradients set up Marangoni flows propelling the droplets, in a manner similar to the classical squirmer model of swimming. The flow around the swimmers as well as its effect on the droplet motion are measured using particle image velocimetry (PIV). The PIV analysis reveals the far field flows generated by the swimmers in the surrounding liquid, leading to the emergence of bound states and oriented clusters. We discuss the interaction mechanisms and compare it to previous theoretical work and simulations.

4:18PM X9.00008 Characterizing particle transport due to actuated cilia with adhesive tips , AMITABH BHATTACHARYA, Department of Chemical Engineering, University of Pittsburgh, GAVIN BUXTON, Department of Science, Robert Morris University, ALEXANDER ALEXEEV, Department of Mechanical Engineering, Georgia Institute of Technology, O. BERK USTA, Harvard Medical School, ANNA C. BALAZS, Department of Chemical Engineering, University of Pittsburgh — Biological tissues and organisms commonly utilize arrays of cilia to manipulate microparticles of different sizes. Motivated by biology, we use numerical simulations to study the interaction of microparticles with an array of actuated cilia, immersed in fluidic microchannel. For each cilium in the array, one end is tethered to the wall, while the other end is actuated by an external periodic force. Also, an adhesive force is introduced between the cilia tip and the microparticle. The simulations are performed using the Lattice Boltzmann Method for the flow, with a chain of point-forces, connected by springs, used to represent each cilium. We observe that a combination of hydrodynamic and adhesive forces can lead to size-specific control of microparticle transport. For instance, for certain adhesion strength and particle sizes, it is possible to trap and release particles by varying the actuation frequency. Also, for a given actuation frequency, the average particle speed is maximized at a particular adhesion strength. We will present the parameter range where we can observe the above behavior.

4:30PM X9.00009 Harnessing self-oscillating polymer gels to design active ciliated surfaces , PRATYUSH DAYAL, AMITABH BHATTACHARYA, OLGA KUKSENOK, ANNA C. BALAZS, University of Pittsburgh — Via theory and simulations, we design active surfaces capable of replicating characteristics of biological cilia. Our approach harnesses the use of polymer gels that undergo photosensitive Belousov-Zhabotinsky (BZ) reaction. Powered by internalized BZ reaction these polymer gels swell and de-swell autonomously due to the chemo-mechanical transduction and therefore are ideal materials for designing our system. We have successfully developed an efficient hybrid approach by combining our three dimensional gel lattice spring model (3D-gLSM) and Lattice Boltzmann Method (LBM) which allows us to capture the interactions between the cilia and the surrounding fluid. Using our gLSM-LBM hybrid model we determine the factors that govern the bending and beating of individual cilium and also their collective dynamic behavior. Our findings provide guidelines for designing ciliated surfaces that can exhibit biomimetic functionality.

4:42PM X9.00010 Designing active cilial sensors , YI YANG, ALEXANDER ALEXEEV, Georgia Institute of Technology — We employ a hybrid lattice Boltzmann / lattice spring computational model to simulate the three-dimensional hydrodynamic interactions among actuated and sensory elastic cilia tethered to a wall of a microfluidic channel. These actuated and sensory cilia are arranged a chessboard pattern on the channel wall. The actuated cilia are driven by a sinusoidal force applied to their free ends and induce periodic oscillations of a viscous fluid filling the microchannel. The passive, sensory cilia are used to measure the force arising due to fluid oscillations. We show that the combination of sensory and actuated cilia allows us to evaluate distances to solid objects located in a fluid-filled microchannel, thereby yielding a useful active sensor for microfluidic and biomedical applications.

4:54PM X9.00011 Nonlinear dynamics of flagellar bundling , PIETER JANSSEN, MICHAEL GRAHAM, University of Wisconsin - Madison — Flagella are long thin appendages of microscopic organisms used for propulsion in low-Reynolds environments. In many bacterial species, helical-shaped flagella driven by a molecular motor will bundle up. This bundling process is poorly understood, and the exact roles of hydrodynamic interactions, helix elasticity, and mechanical contact are unclear. To investigate the bundling, we consider two flexible helices next to each other, as well as several flagella attached to a spherical body. Each helix is modeled as several prolate spheroids connected by springs. For HI, we consider the flagella to made up of point forces, while the finite size of the body is incorporated via Faxén's laws. Before flagella can bundle, they must synchronize. Synchronization occurs fast relative to the bundling process. For flagella next to each other, the initial stage of bundling is governed by rotlet interactions generated by the rotating helices. At longer times, once bundling has occurred, we find that a sharp distinction can be made between "tight" and "loose" bundles, indicated by the local distance between the flagella. As function of the anchor point distance, a sharp transition from tight to loose is found when starting from the completely unbundled state. Incremental steps from stationary situations give multiple stationary for a single anchor distance. We show that the balance between elasticity and strong non-linear hydrodynamic interactions is responsible for this bifurcation behavior.

5:06PM X9.00012 Spontaneous transitions in the synchronisation states of a Chlamydomonas mutant , KIRSTY WAN, KYRIACOS LEPTOS, MARCO POLIN, University of Cambridge, IDAN TUVAL, IMEDEA, Mallorca, Spain, RAYMOND GOLDSTEIN, University of Cambridge — The mechanisms by which eukaryotic flagella are found to synchronise is poorly understood; the origins being dependent upon the hydrodynamics, as well as the underlying molecular biochemistry. Exemplifying how available phenotypic variations in a species may be exploited to extend our mathematical models for flagellar coupling, we turn to ptx1 - a non-phototactic mutant strain of the biflagellated alga *Chlamydomonas* with seemingly intact flagellar apparatus, which does not exhibit any gross motility defects. Intriguingly however, our high-speed imaging analysis of flagellar dynamics in ptx1 have revealed that rather unlike their wildtype predecessors, which beat mostly in synchrony interrupted by brief periods of drifts or slip [1], the two flagella of ptx1 are observed to consistently revert from synchrony to a state of stable, coupled, anti-phase beating dynamics. Incorporating the interpretation of the flagella pair as coupled noisy oscillators, we show how such behaviour corroborates readily with a secondary contribution to the coupling, which is further conjectured to be inherent in the wildtype.
[1] Polin M et al. *Science*, 487-490, **2009**.

5:18PM X9.00013 Emergence of synchronisation in flagella of variable length[1] , MARCO POLIN, DAMTP, University of Cambridge, IDAN TUVAL, IMEDEA, Mallorca, Spain, RAYMOND GOLDSTEIN, DAMTP, University of Cambridge — *Chlamydomonas reinhardtii* is a unicellular green alga that can swim by the concerted breaststroke-like beating of its two flagella. When the flagella are synchronised the organism moves along a straight helical path, while a large difference in the two beating frequencies induces sharp turns. Even in the synchronous state, however, the two flagella have slightly different intrinsic frequencies, and synchrony is guaranteed only by the presence of a sufficiently strong interflagellar coupling. Although the magnitude of this coupling is consistent with the value derived from a rough hydrodynamic estimate, no direct experimental test for the role of hydrodynamic in interflagellar coupling is available. In order to better understand the origin of interflagellar coupling, we employ high- speed imaging to study the dynamics of the two flagella of *Chlamydomonas* as they regrow after mechanically induced deflagellation. Our results show that the duration of synchronised motion is strongly dependent on flagellar length. We discuss this dependence in light of hydrodynamic models of flagellar synchronisation.

[1]MP acknowledges the support of the EPSRC.

5:30PM X9.00014 Fluid dynamics and noise in bacterial scattering , JORN DUNKEL, KNUT DRESCHER, University of Cambridge, LUIS CISNEROS, University of Arizona, SUJOY GANGULY, RAYMOND GOLDSTEIN, University of Cambridge — Bacterial communication through chemical and physical channels is permanently challenged by internal and external noise. While the role of stochastic fluctuations in quorum sensing has been widely studied both theoretically and experimentally, our understanding of hydrodynamic interactions between bacteria is limited by the absence of empirical data. Here, we report the first direct measurement of the fluid flow generated by an individual bacterium far away from and near to a wall. The experiments show that the micro-hydrodynamics of E. coli are considerably different from that of more complex eucaryotes as, for example, Chlamydomonas algae. We discuss the implications of our results for bacterial cell-cell and cell-wall interactions.

5:42PM X9.00015 ABSTRACT WITHDRAWN –

Thursday, March 24, 2011 2:30PM - 5:30PM –

Session X10 DMP: Focus Session: Growth, Structure, Dynamics, and Function of Nanostructured Surfaces and Interfaces – Organic Molecules D221

2:30PM X10.00001 Identification of the Atomic Scale Structures of the Molecule-Metal Interfaces of Single-Molecule Nanowires[1] , FIRUZ DEMIR, GEORGE KIRCZENOW, Simon Fraser University, Burnaby, Canada — We show theoretically how inelastic tunneling spectroscopy can identify the atomic scale structures of the molecule-metal interfaces of single-molecule nanowires bridging pairs metal electrodes, and thus resolve a long standing problem that is central to the field of single-molecule nanoelectronics. As an example we consider the propanedithiol (PDT) molecules bridging gold nanocontacts in the recent experiment of Hihath *et al.* [Nano Lett. **8**, 1673 (2008)]. Based on *ab initio* density functional and semi-empirical calculations we identify the features observed in the experimental inelastic tunneling spectra of these molecules at phonon energies near 46, 40 and 42 meV as arising from sulfur atoms (that have lost their thiol hydrogen atoms) bonding to the gold contacts in top site, bridge site and mixed bridge-top site geometries respectively. PDT molecules in which the sulfur atoms retain their thiol hydrogen atoms and bond strongly to gold in the top site geometry give rise to an IETS feature in the phonon energy range 54-57 meV.

[1]This work was supported by CIFAR and NSERC.

2:42PM X10.00002 The adsorption geometries of C60 monolayer on Ag(111) and Au(111)[1] , RENEE DIEHL, HEEKEUN SHIN, Penn State University, KATARIINA PUSSI, Lappeenranta University of Technology — C_{60} films on metal surfaces are of particular interest as model van der Waals systems, and for applications such as molecular electronics. The electronic properties of these films are known to depend strongly on their structures and the relative molecular orientations of the C_{60} molecules, yet there are few detailed structure determinations for C_{60} films. When grown at room temperature and annealed to a sufficiently high temperature, C_{60} on Au(111) and Ag(111) form $(2\sqrt{3}\times 2\sqrt{3})$R30° structures with one C_{60} molecule per unit cell. We present a LEED study of their surface geometries, which are similar in some ways, but differ in others. They both form vacancy site structures that are thermally activated, they both form monolayers that are composed of a mixture of hex-down and 6:6 bond down molecules. The details of the 6:6 bond molecule geometries are different on both substrates, and the temperature dependence of the mixture is different.

[1]This research is supported by NSF-DMR-0505160 and the Academy of Finland.

2:54PM X10.00003 Mechanical Properties of a vdW molecular monolayer at a metal surface: Structural Polymorphism leading to facile compression , DEZHENG SUN, DAEHO KIM, UC Riverside, DUY LE, UC Florida, ØYVIND BORCK, Norwegian University of Science and Technology, KRISTIAN BERLAND, Chalmers University of Technology, KWANGMOO KIM, University of Maryland, WENHAO LU, YEMING ZHU, MIAOMIAO LUO, JON WYRICK, ZHIHAI CHENG, UC Riverside, T.L. EINSTEIN, University of Maryland, TALAT RAHMAN, UC Florida, PER HYLDGAARD, Chalmers University of Technology, LUDWIG BARTELS, UC Riverside — Intermolecular force plays an important role in self-assembly and surface pattern formation. Anthracene and similar unsubstituted arenes attach to a metallic substrate predominantly through van der Waals interaction leading. In this contribution we present images how anthracene on Cu(111) forms a large number of highly ordered patterns that feature a broad array of structural motifs. Density functional theory modeling including vdW interactions allows us to model the energetic of the pattern formation at high fidelity. Moreover, it allows us to deduce the strain energy associated with films of varying coverage. From this work, we obtain the Young's modulus and Poisson Ratio of a molecular monolayer, which resemble properties conventionally found for porous materials. These patterns are in marked contrast to those found after introduction of functional groups in the molecules, such as carbonyls or thiols.

3:06PM X10.00004 Monte Carlo Study of the Fish-like Patterns of Anthracenes on Cu(111)[1] , KWANGMOO KIM, T.L. EINSTEIN, University of Maryland, College Park, DEZHENG SUN, DAE-HO KIM, LUDWIG BARTELS, University of California, Riverside — Using Monte Carlo calculations of the two-dimensional triangular lattice with a 2-component 3-state Potts model, we demonstrate a mechanism for the spontaneous formation of fish-like patterns of anthracene (AC) molecules on Cu(111) by sputtering and annealing, then cooling to $\sim$ 80 K. The two components are an AC on a hollow site and another on a bridge site of Cu(111).[2] The liquid crystal model with two separate parts, positional and orientational, only explains a part of the fish-like pattern, not the whole regular pattern. Our model fixes the positional order of AC's into the triangular lattice and the orientational order into three angles as observed in the experiments. The variation of the coverages of AC's is reflected in the change of the ratio of two components in our model. We also try to understand the compression of AC's with the introduction of Gaussian dispersion of AC's about their triangular lattice sites.

[1]Supported primarily by NSF Grants CHE 07-50334 with a secondary support from NSF-MRSEC at the University of Maryland, DMR05-20471. Work at UCR supported primarily by NSF CHE 07-49949.
[2]Dezheng Sun *et al.*, Phys. Rev. B **82**, xxx(R) (2010).

3:18PM X10.00005 Self-assembly of metal phthalocyanines modulated by different substrates , WENDE XIAO, Institute of Physics, Chinese Academy of Sciences, YUHANG JIANG, JICHUN LIAN, LIWEI LIU, ZHIHAI CHENG, LI GAO, SHIXUAN DU, HONGJUN GAO — The self-assembly of organic molecules on solid surfaces has made tremendous progresses due to potential applications in organic nano-devices. Among the organic molecular building blocks, metal phthalocyanines (MPcs) have been attracting considerable interests because of their novel electronic and magnetic properties. The self-assembly and physical properties of MPcs on various surfaces have been investigated by scanning tunneling microscopy and spectroscopy (STM/STS). In this presentation, we will report on the self-assembly of iron phthalocyanine (FePc), manganese phthalocyanine (MnPc) and nickel phthalocyanine (NiPc) on Pb(111) and monolayer graphene (MG) epitaxy on Ru (0001) by means of low temperature (LT) STM. Highly ordered close-packed islands with square lattice are observed for all three kinds of MPcs growth on Pb(111), whereas regular dislocation lines are formed in the molecular islands of FePc on Pb(111). We find that the Kondo resonance of MnPc on Pb(111) is strongly location-dependant. For FePc, MnPc and NiPc growth on MG, dispersive single molecules, dispersive molecular lines and small patches of Kagome lattice are observed, respectively.

3:30PM X10.00006 Structural and electronic properties of polymer-silicon semiconductor heterojunctions using hybrid functionals , JOSEPH TURNBULL, North Carolina State University, WENCHANG LU, JERRY BERNHOLC, North Carolina State University, Department of Physics, Center for High Performance Simulation; Oak Ridge National Laboratory — Combining organic and inorganic components to form semiconductor heterostructures provides the basis for an enormous number of potential optoelectronic device designs. We report here on the use of hybrid-DFT calculations to study the structural and electronic properties of semiconductor interfaces between silicon and pi-conjugated polymers. Using large supercells and exact-exchange-corrected hybrid functionals, we explore different attachment motifs for polymer monolayers, as well as the role of screening, in particular in the context of predicting semiconductor band-offsets.

3:42PM X10.00007 Tuning Structural and Mechanical Properties of Two-Dimensional Molecular Crystals: The Roles of Carbon Side Chains , H.-J. GAO, H.Y. CUN, Y.L. WANG, S.X. DU, L. ZHANG, L.Z. ZHANG, W.A. HOFER, S.J. PENNYCOOK, INSTITUTE OF PHYSICS, CHINESE ACADEMY OF SCIENCES, PR CHINA TEAM, SURFACE SCIENCE RESEARCH CENTRE, UNIVERSITY OF LIVERPOOL, UK COLLABORATION, MATERIALS SCIENCE AND TECHNOLOGY DIVISION, OAK RIDGE NATIONAL LABORATORY, USA COLLABORATION — Organic-molecule based flexible electronics has been of significant interest due to its potential to challenge conventional silicon-based technologies. The crucial properties of these devices rely on the largely invariant physical properties of organic compounds or films when they are mechanically deformed. In this present work, by choosing quinacridone with flexible carbon chains as a model system, we developed a theoretical scheme to evaluate the contributions of various interactions to the molecular self-assembly process and find that such a process should be considered as a collective interaction between molecules and substrates rather than from the viewpoint of an isolated molecule. Importantly, the data provide insight into the origin and an estimate of the magnitude of the Young's modulus of the molecular film, which suggests that the elastic properties of molecular films can be tuned through control of side chain length.

3:54PM X10.00008 Formation of Molecular Networks: Tailored Quantum Boxes and Behavior of Adsorbed CO in Them[1] , JON WYRICK, DEZHENG SUN, DAE-HO KIM, ZHIHAI CHENG, WENHAO LU, YEMING ZHU, MIAOMIAO LUO, UC Riverside, YONG SU KIM, ELI ROTENBERG, LBL Berkeley, KWANGMOO KIM, T.L. EINSTEIN, U. Maryland, LUDWIG BARTELS, UCR — We show that the behavior of CO adsorbed into the pores of large regular networks on Cu(111) is significantly affected by their nano-scale lateral confinement and that formation of the networks themselves is directed by the Shockley surface state. Saturation coverages of CO are found to exhibit persistent dislocation lines; at lower coverages their mobility increases. Individual CO within the pores titrate the surface state, providing crucial information for understanding formation of the network as a result of optimization of the number N of electrons bound within each pore. Determination of N is based on quinone-coverage-dependent UPS data and an analysis of states of particles in a pore-shaped box (verified by CO's titration); a wide range of possible pore shapes and sizes has been considered.

[1]Work at UCR supported by NSF CHE 07-49949; at UMD by NSF CHE 07-50334 & UMD NSF-MRSEC DMR 05-20471

4:06PM X10.00009 Origin of the Giant Honeycomb Network of Quinones on Cu(111)[1] , T.L. EINSTEIN, KWANGMOO KIM, U. Maryland, JON WYRICK, ZHIHAI CHENG, LUDWIG BARTELS, UC Riverside, KRISTIAN BERLAND, PER HYLDGAARD, Chalmers U. Tech. — We discuss the factors that lead to the amazing regular giant honeycomb network formed by quinones on Cu(111). Using a related lattice gas model with many characteristic energies, we can reproduce many experimental features. These models require a long-range attraction, which can be attributed to indirect interactions mediated by the Shockley surface state of Cu(111). However, Wyrick's preceding talk gave evidence that the network self-selects for the size of the pore rather than for the periodicity of the superstructure, suggesting that confined states are the key ingredient. We discuss this phenomenon in terms of the magic numbers of 2D quantum dots. We also report calculations of the effects of anthraquinones (AQ) in modifying the surface states by considering a superlattice of AQ chains with various separations. We discuss implications of these results for tuning the electronic states and, thence, superstructures.

[1]Supported by (TLE) NSF CHE 07-50334 & UMD MRSEC DMR 05-20471, (JW & LB) NSF CHE NSF CHE 07-49949, (KB & PH) Swedish Vetenskapsrådet VR 621-2008-4346.

4:18PM X10.00010 Tunneling and Time-Reversal Invariance in the Diffusion of Polyatomic Molecules at a Metal Surface , ZHIHAI CHENG, ERIC CHU, DEZHENG SUN, DAEHO KIM, YEMING ZHU, MIAOMIAO LUO, GREG PAWIN, KIN WONG, KI-YOUNG KWON, ROBERT CARP, MICHAEL MARSELLA, LUDWIG BARTELS, UCR — Rectangular molecules with 1 or 2 oxygen substrate linkers attached to each of their long sides diffuse in a uniaxial fashion, despite the threefold symmetry of the Cu(111) substrate. They achieve this by sequential placement of their substrate linkers and are hence dubbed "molecular walkers". VT-STM monitoring of their motion reveals a striking difference between the diffusion prefactors of the quadrupedal and bipedal species, with the latter being very low. DFT modeling of the diffusion barrier and WBK-based estimation of the potential for tunneling suggest that this discrepancy lies in the prevalence of tunneling for species, whose motion is only blocked by a barrier affecting one of their substrate linkers. In contrast, if the diffusion barrier affects two substrate linkers simultaneously, tunneling will not occur and conventional prefactors are observed. This finding may actually have far-reaching implications for the modeling of molecular motion in general, as it highlights that blocking of a single atoms is insufficient for confinement of molecular motion. We also investigated an asymmetric "molecular walkers", showing a symmetric diffusion in agreement with time-reversal invariance despite a saw-tooth shape of the diffusion barrier experienced.

4:30PM X10.00011 Hydrogen Bonding Controls the Dynamics of Catechol Adsorbed on a TiO_2(110) Surface , ULRIKE DIEBOLD[1], SHAO-CHUN LI, Department of Physics and Engineering Physics, Tulane University, New Orleans, LA 70118, USA, LI-NA CHU, XUE-QING GONG, Labs for Advanced Materials, Research Institute of Industrial Catalysis, East China University of Science and Technology, Shanghai, P. R. China — Direct studies of how organic molecules diffuse on metal oxide surfaces can provide insights into catalysis and molecular assembly processes. We studied individual catechol molecules, $C_6H_4(OH)_2$, on a rutile TiO_2(110) surface with scanning tunnelingmicroscopy. Surface hydroxyls enhanced the diffusivity of adsorbed catecholates. The capture and release of a proton caused individual molecules to switch between mobile and immobile states within a measurement period of minutes. Density functional theory calculations showed that the transfer of hydrogen from surface hydroxyls to the molecule and its interaction with surface hydroxyls substantially lowered the activation barrier for rotational motion across the surface. Hydrogen bonding can play an essential role in the initial stages of the dynamics of molecular assembly.

[1]Institute of Applied Physics, Vienna University of Technology, Wiedner Hauptstrasse 8-10, Vienna, Austria

4:42PM X10.00012 Reversible rectification in sub-monolayer molecular heterojunctions[1] , JOE SMERDON, CHRIS GIEBINK, Center for Nanoscale Materials, Argonne National Laboratory, MATTHIAS BODE, Univ. Wuerzburg, NATHAN GUISINGER, JEFFREY GUEST, Center for Nanoscale Materials, Argonne National Laboratory — Pentacene and C_{60} are archetypal molecules for optically active acceptor-donor heterojunctions and have been used as the active materials in bilayer solar cells. We will discuss UHV STM and STS measurements on these bi-molecular films deposited sequentially to form heterojunctions on Cu(111). It is observed that rectification can be detected at the single-junction limit, and that the direction of rectification flips in accordance with the polarity of the heterojunction. The morphology of heterolayers will also be discussed. It is found that the density of a Pn monolayer can be affected by choice of growth conditions, and in turn can affect the overall morphology of the heterolayer and the rectification behavior of the heterojunctions. We will also briefly discuss progress towards probing the photophysical behavior of these systems. The correlation of atomic-scale structure and electronic behavior at the single-junction limit has important implications for applications of such heterojunctions, such as solar cells or OLEDs.

[1]This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357 and "SISGR" Contract No. DE-FG02-09ER16109.

4:54PM X10.00013 Molecular self-assembly of dichloropentacene and C_{60} for a model organic solar cell heterojunction , JUN WANG, AMANDA BROWN, IRVINDER KAUR, JIAN-MING TANG, GLEN MILLER, KARSTEN POHL, Univ. of New Hampshire — Organic molecular self-assembly is a bottom-up approach to create molecular architectures that are suitable for a variety of applications including functional materials and molecular electronics. Specifically, the co-assembly of functionalized acenes (electron-donor materials) and fullerenes (electron-acceptor materials) on metal substrates provides a model for studying the structural and electronic properties for novel organic photovoltaic heterojunctions. Previously, we have fabricated a persistent self-assembled monolayer composed of single-domain 6,13-dichloropentacene (DCP) over large areas on the stepped Au(788) surface. Here we present the subsequent growth of C_{60} on a DCP monolayer covered gold surface by STM investigation and ab-initio calculations. After mild annealing C_{60} molecules are forced to the Au(788) step edges forming very long C_{60} chains, in contrast to the short C_{60} chains reported on bare vicinal gold steps. These final structure formations are attributed to the delicate intermolecular interactions and molecule-substrate interactions.

5:06PM X10.00014 BEEM Study of Interface Properties in PVDF-graphite Heterojunctions[1] , LE ZHANG, CLAY UPTON, ANDREI SOKOLOV, University of Nebraska - Lincoln — Since the prediction of giant electroresistance, tunnel junctions with ferroelectric (FE) barrier attract significant experimental and theoretical attention due to potential application as non-volatile data storage devices. The ferroelectric polymer, polyvinylidene fluoride (PVDF), is of particular interest thanks to its outstanding electromechanical, dielectric, and mechanical properties. However, direct experimental study of organic FE interface properties as a function of its polarization is extremely challenging. We employ ballistic electron emission microscope (BEEM) technique for nanometer size characterization of P(VDF-TrFE)/HOPG heterostructure. This method offers STM scale of spatial resolution and is immune to the contact quality of top electrode. By comparing the voltage dependence of ballistic current for different polarization states, we observe the change in tunnel barrier properties as the sign of FE polarization reverses. High-quality thin films of PVDF were fabricated using a Langmuir-Blodgett (LB) technique. Results will be also compared with thermally evaporated PVDF film and its isomorphic analog, polyethylene.

[1]Support from NSF MRSEC

5:18PM X10.00015 Reverse self assembly: (111)-oriented gold crystallization at thiol monolayer templates[1] , AHMET UYSAL, BENJAMIN STRIPE, PULAK DUTTA, Physics and Astronomy, Northwestern University, BINHUA LIN, MATI MERON, CARS, The University of Chicago — Certain microorganisms can reduce gold ions from aqueous solutions to form gold nano/micro particles in a controlled way [1]. Understanding how biomolecules control the crystallization process may result in cheap and environment-friendly techniques in many different applications, including organic-inorganic hybrid molecular technologies and shape controlled gold nanoparticle production. To better understand the organic-inorganic interactions, we studied the crystallization of gold under octadecanethiol monolayers at the air-water interface. We used synchrotron x-rays in the grazing incidence geometry to determine the orientation of the gold crystals as well as the organic monolayer structure *in situ*. These x-rays also act as the gold reducing agent in this experiment. We see that the (111) faces of gold crystals are parallel to the monolayer surface. The monolayer structure changes with time and becomes commensurate with the gold (111) face, similar to a $\sqrt{3} \times \sqrt{3}$ self-assembled monolayer of thiol on gold.

[1] K. B. Narayanan, and N. Sakthivel, Advances in Colloid and Interface Science 156, 1 (2010).

[1]This work was supported by the US Department of Energy under grant no: DE-FG02-84ER45125.

Thursday, March 24, 2011 2:30PM - 5:30PM –
Session X11 FIAP: Integer Quantum Hall Effect D222

2:30PM X11.00001 Imaging quantum Hall Coulomb islands inside a quantum ring , FREDERICO MARTINS, BENOIT HACKENS, SEBASTIEN FANIEL, VINCENT BAYOT, Universite catholique de Louvain, Louvain-la-Neuve 1348, Belgium, MARCO PALA, MINATEC, Grenoble, France, HERMANN SELLIER, SERGE HUANT, Institut Neel, Grenoble, LUDOVIC DESPLANQUE, XAVIER WALLART, IEMN, Villeneuve d'Ascq, France — In the quantum Hall regime near integer filling factors, electrons are transmitted through edge states confined at the borders of the device. In mesoscopic samples, however, edge states may be sufficiently close to allow electrons to tunnel, or to be transmitted through localized states ("Coulomb islands") [1]. Here, we use the biased tip of a low temperature scanning gate microscope to alter tunneling through quantum Hall Coulomb islands localized inside a quantum ring patterned in an InGaAs/InAlAs heterostructure. Simultaneously, we map the quantum ring resistance and observe different sets of concentric resistance fringes, due to charging/discharging of each Coulomb island. Tuning the magnetic field and the tip voltage, we reveal the rich and complex behaviour of these fringes [2].

[1] B. Rosenow and B. I. Halperin, PRL 98, 106801 (2007).
[2] B. Hackens et al., Nature Communications 1, 39 (2010).

2:42PM X11.00002 Emergent Dissipation in the $\nu = 1$ Quantum Hall Bilayer[1] , GANPATHY MURTHY, University of Kentucky, HERBERT FERTIG, Indiana University — Disorder is known to be central to the $\nu = 1$ bilayer [1]. Building on our previous study of the bilayer $\nu = 1$ system in a periodic potential [2] to capture the nonperturbative effects of disorder, we construct a $T = 0$ effective theory, in which the XY angle is coupled to an emergent Ising spin. We uncover a $z = 2$ quantum phase transition with emergent dissipation. Calculations of the interlayer tunnelling conductance and counterflow conductivity will be presented.

[1] H. A. Fertig and G. Murthy, Phys. Rev. Lett. **95**, 156802 (2005).
[2] J. Sun, G. Murthy, H. A. Fertig, and N. Bray-Ali, Phys. Rev. B, **81**, 195314 (2010).

[1]NSF DMR-0703992 and DMR-0704033.

2:54PM X11.00003 Microwave induced electron heating in the regime of radiation-induced magnetoresistance oscillations in the GaAs/AlGaAs system[1] , A.N. RAMANAYAKA, R.G. MANI, Georgia State University, W. WEGSCHEIDER, Laboratorium fuer Festkoerperphysik, ETH Zurich — We examine the influence of microwave photoexcitation on the amplitude of Shubnikov-de Haas (SdH) oscillations at large filling factors in a two dimensional GaAs/AlGaAs electron system. A SdH lineshape analysis indicates that increasing the incident microwave power has a weak effect on the amplitude of the SdH oscillations, in comparison to the influence of modest temperature changes at liquid Helium temperatures on the dark-specimen SdH effect. The results indicate negligible electron heating under modest microwave photoexcitation, in good agreement with theoretical predictions for this regime.

[1]ARO W911NF-07-01-0158, DOE DE-SC0001762

3:06PM X11.00004 Transport study under microwave photoexcitation in epitaxial graphene[1] , RAMESH MANI, Georgia State University, JOHN HANKINSON, CLAIRE BERGER[2], WALT DE HEER, Georgia Institute of Technology — Single layers of carbon known as graphene are a promising new electronic material with potential for high frequency applications. For electronics, top-gated graphene field-effect transistors fabricated on large area epitaxial graphene wafers have already indicated switching cutoff frequencies up to 100 GHz [1]. Microwave and terahertz radiation-sensing constitutes another area of interest. Hence, we examine the electrical photo-response of graphene devices in the microwave band, and report transport measurements under microwave photo-excitation (f $<$ 120 GHz) carried out on micron sized Hall bars at liquid Helium temperatures.

[1] Y-M Lin et al., Science 327, 662 (2010).

[1]Work at GSU has been supported by the ARO under W911NF-07-01-0158, and by the DOE under DE-SC0001762.
[2]CNRS-LEPES, Grenoble, France

3:18PM X11.00005 Quantized Anomalous Hall Insulator in a Nanopatterned Two-Dimensional Electron Gas , YONGPING ZHANG, CHUANWEI ZHANG, Department of Physics and Astronomy, Washington State University — We propose that a quantum anomalous Hall insulator (QAHI) can be realized in a nanopatterned two-dimensional electron gas (2DEG) with an in-plane magnetic field. The Berry curvatures originating from the in-plane magnetic field and Rashba and Dresselhaus spin-orbit coupling, in combination with a nanoscale honeycomb lattice potential modulation, lead to topologically nontrivial insulating states in the 2DEG. In the bulk insulating gaps, the anomalous Hall conductivity is quantized -e^2/h, corresponding to a finite Chern number -1. There exists one gapless chiral edge state on each edge of a finite size 2DEG.

3:30PM X11.00006 Remote sensing of transport in microwave photo-excited GaAs/AlGaAs heterostructure devices[1] , TIANYU YE, G. CHAND, A.N. RAMANAYAKA, R.G. MANI, W. WEGSCHEIDER, GEORGIA STATE UNIVERSITY COLLABORATION, ETH-ZURICH, SWITZERLAND COLLABORATION — The GaAs/AlGaAs two dimensional electron system (2DES) exhibits magnetoresistance oscillations under microwave and terahertz photo-excitation at liquid Helium temperatures. Such oscillations are understood in terms of the displacement and inelastic models for photo-excited transport in this system. In order to identify the relative physical contributions, we report on transport measurements and concurrent "remote" sensing of the 2DES. Hence, measurements under microwave photo-excitation were carried out on Hall bars fabricated from high mobility GaAs/AlGaAs single heterostructures, as a sensor above the specimen served to look for concurrent changes in response. We report here on the observed noticeable changes in the remote sensor and correlate the observations with the observed transport response of the photo-excited 2DES.

[1]Work has been supported by the ARO under W911NF-07-01-0158, and by the DOE under DE-SC0001762.

3:42PM X11.00007 Microscopic conductivity imaging of the quantum Hall edge states by a microwave impedance microscope , KEJI LAI, WORASOM KUNDHIKANJANA, MICHAEL KELLY, ZHI-XUN SHEN, Stanford University, JAVAD SHABANI, MANSOUR SHAYEGAN, Princeton University — Spatially resolved studies of the quantum Hall edge channels are usually challenging because most high mobility two-dimensional electron gas (2DEG) systems are buried underneath the surface. Using a cryogenic microwave impedance microscope, we demonstrate the conductivity mapping of the bulk and edge states in a GaAs/AlGaAs 2DEG. Narrow strips with either metallic or insulating screening properties are observed along edges of the 2DEG. The sizes and positions of these strips as a function of the magnetic fields agree with the self-consistent electrostatic picture. The quantitative local conductivity information provides a complete microscopic description of the evolution through the bulk filling factor $\nu = 2$. The imaging was performed without DC electrodes, vividly manifesting that the quantum Hall edges are equilibrium states and do not depend on externally supplied currents.

3:54PM X11.00008 Study of integer quantum Hall transition in long-ranged potentials[1] , RAVINDRA BHATT, Department of Electrical Engineering, Princeton University, Princeton, NJ 08544-5263, A. CHANDRAN, Princeton University, Princeton, NJ 08544 — We present results of a numerical study of a two-dimensional system of noninteracting electrons in a random correlated potential in the lowest Landau level in the presence of a perpendicular magnetic field. We use spatially uncorrelated and unbiased random gaussian potentials as well as potentials $V(r)$ with long-range, power-law correlations $\langle V(0)V(r)\rangle \propto r^{-\alpha}$ for different exponents α as models of disorder. We compute the Hall conductance σ_{xy} as well as the Thouless conductance as a function of size L of the sample, and use finite size scaling to determine the exponent ν characterizing the divergence of the localization length ξ at the quantum Hall transition. We also study the scaling of the diagonal conductivity as a function of L and compare our results to those obtained previously through different methods.

[1]This work was supported by Department of Energy under Grant DE-SC20002140

4:06PM X11.00009 High-Resolution Tunneling Spectroscopy of 2D Holes in the Quantum Hall Regime , B. HUNT, Dept. of Physics, MIT, O.E. DIAL, Dept. of Physics, Harvard, R.C. ASHOORI, Dept. of Physics, MIT, L.N. PFEIFFER, K.W. WEST, Department of Electrical Engineering, Princeton — We use Time-Domain Capacitance Spectroscopy (TDCS)[1], a method for extracting precise, high-resolution tunneling spectra, to determine the single-particle spectrum of the 2D hole system (2DHS) in the presence of high magnetic fields. The 2DHS has a variable density from zero to $3 \times 10^{11}\,\mathrm{cm}^{-2}$ and $T = 100\,\mathrm{mK}$. Owing to the heavy mass of holes in GaAs quantum wells, much higher values of r_s are attainable compared to 2D electron systems(2DES). Basic structure in the spectra appear very different from those observed in the 2DES[1]. For instance, a magnetic-field-induced Coulomb gap [1] appearing about the Fermi energy has a strong dependence on electron density (with a larger gap at low densities) that is not present for the 2DES. In addition, structure created by the exchange enhancement of spin splittings has an entirely different appearance from that seen in the 2DES. Ultimately, at lower temperatures, a high-resolution TDCS study of the 2DHS may show features related to the 2D metal-insulator transition.

[1] O.E. Dial et al, Nature 448, 176-179 (2007).

4:18PM X11.00010 High quality two-dimensional hole system on hydrogen terminated silicon (111) surfaces , BINHUI HU, TOMASZ M. KOTT, ROBERT N. MCFARLAND, BRUCE E. KANE, University of Maryland — We have previously developed a novel field effect transistor structure, in which high mobility two-dimensional electrons are induced at a hydrogen-terminated Si(111) surface by a positive gate voltage through an encapsulated vacuum dielectric [1]. In this talk, we will demonstrate that a similar structure can also be used to define a high quality two-dimensional hole system (2DHS) at the H-Si(111) surface with a negative gate voltage. Hole concentrations up to 7.1×10^{11} cm^{-2} are obtained. The longitudinal and Hall resistivities are measured as functions of magnetic fields up to 12 T. Preliminary data show Shubnikov-de Haas (SdH) oscillations at B $>$ 3 T at T= 5 K. Until now the studies on 2DHSs on Si(111) surfaces are limited, primarily due to the lack of high quality 2DHSs on them. The high quality 2DHS here can provide some new opportunities.

[1] K. Eng, R. N. McFarland, and B. E. Kane, Appl. Phys. Lett. 87, 052106 (2005).

4:30PM X11.00011 Microwave photo-voltaic oscillations in the GaAs/AlGaAs system[1] , GANESH CHAND, T. YE, A. RAMANAYAKA, R.G. MANI, Georgia State University, W. WEGSCHEIDER, ETH-Zurich — Microwave photo-excitation of the GaAs/AlGaAs system produces oscillations in the diagonal resistance that lead into novel zero-resistance states in the low temperature limit. Such photo-excitation also produces concomitant photo-voltage oscillations. Here, we examine this microwave photo-voltaic effect and correlate the results with observed magneto-transport over the frequency range $30 \leq f \leq 120GHz$ in Hall bars fabricatedfrom material characterized by n = 2x $10^{11}cm^{-2}$.

[1]Work has been supported by the ARO under W911NF-07-01-0158, and by the DOE under DE-SC0001762.

4:42PM X11.00012 Terahertz Coherent Control of Cyclotron Resonance in the Quantum Hall Regime , T. ARIKAWA, X. WANG, J. KONO, Rice University, D.J. HILTON, University of Alabama at Birmingham, J.L. RENO, W. PAN, Sandia National Laboratories — We report on the creation and coherent control of a superposition of many-electron quantum states (or a qubit) in a Landau-quantized GaAs two-dimensional electron gas (2DEG) using a sequence of coherent terahertz (THz) pulses. The first pulse excites electrons from the highest-filled Landau level (LL) to the lowest-unfilled LL, creating a superposition of the two LLs which re-emits a coherent THz wave. We found that the second THz pulse incident within the decoherence time stops or enhances the THz re-emission depending on its arrival phase. These results show that an arbitrary coherent control of the LL qubit is possible using THz pulses. We also performed a simulation within the framework of single-particle optical Bloch equations, which reproduced the experimental results surprisingly well. This agreement shows that the 2DEG behaves in the same way as a single-electron two-level system despite the fact that it contains a large density of interacting electrons. This finding extends the Kohn's theorem to a more general level of coherent dynamics.

4:54PM X11.00013 THz quantum Hall conductivity in a two dimensional electron gas , A.V. STIER, H. ZHANG, C.T. ELLIS, D. EASON, G. STRASSER, B.D. MCCOMBE, J. CERNE, University at Buffalo, The State University of New York — We investigate the THz Hall conductivity through measurement of the Faraday effect at 84 cm^{-1} near the cyclotron resonance (CR) in a two dimensional electron gas formed at a GaAs/(AlGa)As interface. Motivated by predictions of novel step-like features in the optical Hall conductivity (σ_{xy}) by Morimoto et.al. (Phys. Rev. Lett. 2009), we measure the THz σ_{xy} as a function of filling factor and temperature using polarization modulation techniques (Grayson, Phys. Rev. Lett. 2002). We observe plateaus in the Faraday rotation near integer filling factors of 1, 2 and 3 which we attribute to the THz integer quantum Hall effect. In electron density dependent studies, we observe a slight non-monotonic shift of the plateaus as a function of filling factor at magnetic fields above CR. A comparison of this effect with the shift in temperature shows that this cannot be explained by a simple electronic heating effect. This research was funded through NSF-DMR1006078.

5:06PM X11.00014 Superconducting Transport Mediated by Quantum Hall Edge Modes , STEPHANIE LAW, University of Illinois at Urbana-Champaign, MICHAEL VISSERS, ALLISON DOVE, NADYA MASON, JAMES ECKSTEIN — We report transport measurements between superconducting leads separated by a small gap consisting of quantum Hall edge modes. The NbTi superconducting layer is grown in-situ on top of the semiconducting heterostructure to allow good contact. The samples are then fabricated into Hall bars with narrow gaps between the superconducting leads. Differential resistance and IV characteristics are measured in two and four terminal setups at 300mK both on and off quantum Hall plateaus. We will show that in the smallest gaps when we are on a plateau, we see a chiral supercurrent the direction of which is controlled by the field. With larger gaps we see either a zero bias resistance minimum or maximum. Data taken on and off plateaus show marked differences, indicating that quantum Hall modes are crucial. Results for samples with different heterostructures will also be shown.

5:18PM X11.00015 In-plane Field Tuned Subband Quantum Hall Ferromagnetism , DAGIM TILAHUN, ALLAN MACDONALD — Motivated by the recent experimental work of Guo *et al.* (Phys. Rev. B 78, 233305 (2008)), we study the effects of an in-plane magnetic field on quantum Hall states in which subband, Landau level, and spin degrees of freedom compete. We find that the phase diagram identified by these authors can be explained qualitatively by using only single-electron properties, whereas the energy gap behavior can be explained only by considering electron-electron interactions. We predict a series of in-plane field tuned first order phase transitions in high-mobility samples.

Thursday, March 24, 2011 2:30PM - 5:30PM –

Session X13 GSNP: Focus Session: Continuum Description of Particulate Media D225/226

2:30PM X13.00001 A nonlocal enhancement to granular elasto-plasticity , KEN KAMRIN, MIT, GEORG KOVAL — A general, three-dimensional law to predict granular flow in an arbitrary geometry has been an elusive goal for decades. Recently, an elasto-plastic continuum model has shown the ability to approximate steady flow and stress profiles in multiple inhomogeneous flow environments. However, the model does not capture some of the characteristic phenomena observed in the slow, creeping flow regime. As normalized flow-rate decreases, granular stresses are observed to become largely rate-independent and a dominating length-scale emerges in the mechanics. This talk attempts to account for these effects with a nonlocal correction term that modifies the continuum law when the inertial number drops below a critical value. The correction depends on stress and strain-rate gradients and brings in a natural dependence on the particle diameter. We implement the modified law in multiple geometries and validate its predictions against discrete particle simulations.

2:42PM X13.00002 Effective temperature in elastoplasticity of amorphous solids[1] , IDO REGEV[2], Los Alamos National Laboratory, LAURENT BOUE, JACQUES ZYLBERG, ITAMAR PROCACCIA, The Weizmann institute of Science, GEORGE HENTSCHEL, Emory University — An effective temperature $T_{\rm eff}$ which differs from the bath temperature is believed to play an essential role in the theory of elasto-plasticity of amorphous solids. The definition of a measurable $T_{\rm eff}$ in the literature on sheared solids suffers however from being connected to a fluctuation-dissipation theorem which is correct only in equilibrium. Here we introduce a natural definition of $T_{\rm eff}$ based on measurable structural features without recourse to any questionable assumption. The value of $T_{\rm eff}$ is connected, using theory and scaling concepts, to the flow stress and the mean energy that characterize the elasto-plastic flow.

[1]This work was supported in part by the Israel Science Foundation and the German Israeli Foundation

[2]Formerly, the Weizmann institute of Science

2:54PM X13.00003 Shock driven jamming and periodic fracture of particulate rafts , MAHESH BANDI, SEAS, Harvard Univeristy. CNLS & MPA-10, Los Alamos National Laboratory, TUOMAS TALLINEN, L. MAHADEVAN, SEAS, Harvard University — A tenuous monolayer of hydrophobic particles at the air-water interface often forms a scum or raft. When such a monolayer is disturbed by localized surfactant introduction, a radially divergent shock emanates and packs the particles into a jammed, compact, annular band that grows with time. The resulting two-dimensional, disordered, elastic solid locally has a packing fraction that saturates at random close packed density (ϕ_{RCP}) and fractures as it is driven radially outwards, to form periodic triangular cracks with robust geometrical features. We find that the number of cracks N varies monotonically with the initial particulate packing fraction ϕ_{init}, as does the compaction band radius R^* at fracture onset. However, its width W^* is constant across all ϕ_{init}. A simple geometric theory that treats the compaction band as an elastic annulus, and accounts for mass conservation allows us to deduce that $N \simeq 2\pi R^*/W^* \simeq 4\pi\phi_{RCP}/\phi_{init}$, a result that we experimentally verify over the range ($0.1 \leq \phi_{init} \leq 0.64$).

3:06PM X13.00004 Application of Classical Nucleation Theory to Cavitation in Metallic Glass , MICHAEL FALK, Departments of Materials Science and Engineering; Mechanical Engineering; and Physics and Astronomy, Johns Hopkins University — In order to predict the fracture toughness of amorphous solids such as metallic glasses it is necessary to understand the physics of the process zone. Theories of plastic deformation provide information about response to shear, but on their own these theories provide limited insight into the microscopic mechanisms that mediate the free surface generation critical to crack propagation. Previous molecular dynamics simulations indicate that cavitation likely plays this role. We have undertaken a series of molecular dynamics simulations of cavitation under hydrostatic tension in a binary metallic glass analog using pair-wise potentials. We compare the rate of cavity nucleation directly to homogeneous nucleation theory to examine the role of surface energy and irreversible deformation in the cavitation process. We find that both the reduction of the surface energy at small cavity size and the plastic deformation required for the cavity to grow play important roles in setting the strain-dependent free energy barrier to cavitation.

Work done in collaboration with Michael Spector, Materials Science and Engineering, Johns Hopkins University, Baltimore; Shuo Lu, Materials Science and Engineering, Beihang University; and Pavan K. Valavala, Materials Science and Engineering, Johns Hopkins University.

3:42PM X13.00005 Macroscopic transport and topological transitions in ordered suspensions in parallel-wall channels[1] , JERZY BLAWZDZIEWICZ, Texas Tech University, NIDHI KHURANA, Yale University, ELIGIUSZ WAJNRYB, IPPT, Warsaw, Poland — Our recent investigations of ordered suspensions in parallel-wall channels revealed complex nonlinear dynamics, including formation of defects in a particle lattice, dynamic order-disorder transitions, buckling of particle lattice, and fingering instabilities. We will describe hydrodynamic mechanisms that govern this collective particle behavior.

[1]Supported by NSF grant CBET–0931504

3:54PM X13.00006 Continuum Mean-Field Theories for Molecular Fluids, and Their Validity at the Nanoscale[1] , C.B. HANNA, Boise State University, F. PEYRONEL, University of Guelph, C. MACDOUGALL, St. Francis Xavier University, A. MARANGONI, University of Guelph, D.A. PINK, St. Francis Xavier University, AFMNET-NCE COLLABORATION — We present a calculation of the physical properties of solid triglyceride particles dispersed in an oil phase, using atomic- scale molecular dynamics. Significant equilibrium density oscillations in the oil appear when the interparticle distance, d, becomes sufficiently small, with a global minimum in the free energy found at $d \approx 1.4$ nm. We compare the simulation values of the Hamaker coefficient with those of models which assume that the oil is a homogeneous continuum: (i) Lifshitz theory, (ii) the Fractal Model, and (iii) a Lennard-Jones 6-12 potential model. The last-named yields a minimum in the free energy at $d \approx 0.26$ nm. We conclude that, at the nanoscale, continuum Lifshitz theory and other continuum mean-field theories based on the assumption of homogeneous fluid density can lead to erroneous conclusions.

[1]CBH supported by NSF DMR-0906618. DAP supported by NSERC. This work supported by AFMNet-NCE.

4:06PM X13.00007 Coarse-Graining of a Physical Granular System , JIE ZHANG, Indiana University-Purdue University-Fort Wayne, ISAAC GOLDHIRSCH[1], Tel Aviv University, ROBERT BEHRINGER, Duke University — We present results, including particle displacements and rotations, as well as strain and stress fields, obtained by applying a resolution-controlled coarse-graining method to an experiment comprised of bidisperse disks subject to pure shear. We briefly review the experimental methods which involve determing inter-particle contact forces using the photoelastic properties of the disks. We then consider the philosophical and technical approaches of the coarse-graining methods used here. We particularly consider the emergence of shear bands, which are manifest in the displacements, rotations, and some strain fields, but not in the stress. Correlations of the displacement fluctuations decay on a very small scale, of the order of a few particle diameters, even close to jamming, which in this case, is induced by shear. We report an unexpected but simple correlation between particle rotation angles and the rotation field.

[1](deceased)

4:18PM X13.00008 Nonequilibrium Thermodynamics of Driven Disordered Materials , ERAN BOUCHBINDER, Weizmann Institute of Science — We present a nonequilibrium thermodynamic framework for describing the dynamics of driven disordered solids (noncrystalline solids near and below their glass temperature, soft glassy materials such as colloidal suspensions and heavily dislocated polycrystalline solids). A central idea in our approach is that the set of mechanically stable configurations, i.e. the part of the system that is described by inherent structures, evolves slowly as compared to thermal vibrations and is characterized by an effective disorder temperature. Our thermodynamics-motivated equations of motion for the flow of energy and entropy are supplemented by coarse-grained internal variables that carry information about the relevant microscopic physics. Applications of this framework to amorphous visco-plasticity (Shear-Transformation-Zone theory), glassy memory effects (the Kovacs effect) and dislocation-mediated polycrystalline plasticity will be briefly discussed.

4:54PM X13.00009 Breakdown of Granular Constitutive Relations for Flow through a Narrow Vertical Channel[1] , DONALD CANDELA, KEVIN FACTO, University of Massachusetts Amherst — We have used NMR/MRI techniques to study flow profiles and fluctuations in the dense, gravity-driven flow of a granular medium through a relatively narrow vertical channel (channel diameter approximately 20 grain diameters). Although the flow is macroscopically steady, the NMR experiments reveal large velocity fluctuations that can be characterized as random, short-lived jamming of the flow. Constitutive relations have been successfully developed for granular shear flows in constant pressure conditions, such as flow in open chutes or wide vertical channels. For the narrow-channel flow probed in our experiments, the constant-pressure constitutive relations are not appropriate. An alternative equation of state based on constant-volume conditions may be appropriate for the narrow-channel case, or it can be modeled using a piling-jamming model that abandons the constitutive-equation approach altogether.

[1]Supported by NSF Grant CBET-0651397

5:06PM X13.00010 Dynamic Structure Factor and Transport Coefficients of a Homogeneously Driven Granular Fluid in Steady State[1] , KATHARINA VOLLMAYR-LEE, Bucknell University, USA, ANNETTE ZIPPELIUS, TIMO ASPELMEIER, Georg-August-Universitaet Goettingen, Germany — We study the dynamic structure factor of a granular fluid of hard spheres, driven into a stationary nonequilibrium state by balancing the energy loss due to inelastic collisions with the energy input due to driving. The driving is chosen to conserve momentum, so that fluctuating hydrodynamics predicts the existence of sound modes. We present results of computer simulations which are based on an event driven algorithm. The dynamic structure factor $F(q, \omega)$ is determined for volume fractions 0.05, 0.1 and 0.2 and coefficients of normal restitution 0.8 and 0.9. We observe sound waves, and compare our results for $F(q, \omega)$ with the predictions of generalized fluctuating hydrodynamics which takes into account that temperature fluctuations decay either diffusively or with a finite relaxation rate, depending on wave number and inelasticity. We determine the speed of sound and the transport coefficients and compare them to the results of kinetic theory.

[1]K.V.L. thanks the Institute of Theoretical Physics, University of Goettingen, for financial support and hospitality.

5:18PM X13.00011 Discrete-continuum mapping for fiber network mechanics , CATALIN PICU, ALI SHAHSAVARI, HAMED HATAMI-MARBINI, Rensselaer Polytechnic Institute — Semi-flexible random fiber networks are the structural element of many biological and non-biological systems such as the cytoskeleton, artificial tissue and cellulose-based products. We have shown that in these systems the density, as well as mechanical fields (elastic moduli, strain energy etc), are long-range power-law correlated. The correlation length evolves during deformation. A procedure to map the elasticity of the discrete system to continuum representations is developed. The method is used to solve boundary value problems defined over large fiber network domains. However, the mapping can be performed only in some situations, limitations which are discussed in this talk.

Thursday, March 24, 2011 2:30PM - 5:30PM –

Session X14 GSNP: Focus Session: Extreme Mechanics: Elasticity and Deformation IV D227

2:30PM X14.00001 Harnessing Instabilities in Polymers under Electric Fields , XUANHE ZHAO, Duke University — Subject to a voltage, a layer of a polymer reduces thickness and expands area, so the same voltage will induce an even higher electric field. The positive feedback may cause the polymer to thin down drastically, resulting in an electrical breakdown. This electromechanical instability has been long recognized in the electrical power industry as a major failure mode for polymer insulators. In this talk, we will present recent new observations and understandings of the electromechanical instability. For example, what will happen if the polymer is bonded on a rigid substrate to prevent the area expansion? We show that a new mode of instability will set in. Once the electric field reaches a critical value, the initially flat surface suddenly folds upon itself, deforming into a pattern of creases. As the electric field further rises, the creases increase in size and decrease in density, and strikingly evolve into holes in the polymer. The critical electric field for the creasing instability scales with square root of the polymer's modulus. We show that linear stability analysis overestimates the critical electric field for the instability. A theoretical model has been developed to predict the critical field by comparing the potential energies in the creased and flat states. The theoretical prediction matches consistently with experimental results. We further show that the instability can be harnessed with promising applications in many areas including high-breakdown-field organic capacitors, electrostatic lithography, dynamic pattern formations, fabrication of semi-permeable membranes, and energy harvesting.

3:06PM X14.00002 Ultrasoft Electronics for Hyperelastic Strain, Pressure, and Direct Curvature Sensing[1] , CARMEL MAJIDI, REBECCA KRAMER, ROBERT WOOD, Harvard University — Progress in soft robotics, wearable computing, and programmable matter demands a new class of ultrasoft electronics for tactile control, contact detection, and deformation mapping. This next generation of sensors will remain electrically functional under extreme deformation without influencing the natural mechanics of the host system. Ultrasoft strain and pressure sensing has previously been demonstrated with elastomer sheets (eg. PDMS, silicone rubber) embedded with microchannels of conductive liquid (mercury, eGaIn). Building on these efforts, we introduce a novel method for direct curvature sensing that registers the location and intensity of surface curvature. An elastomer sheet is embedded with micropatterned cavities and microchannels of conductive liquid. Bending the elastomer or placing it on a curved surface leads to a change in channel cross-section and a corresponding change in its electrical resistance. In contrast to conventional methods of curvature sensing, this approach does not depend on semi-rigid components or differential strain measurement. Direct curvature sensing completes the portfolio of sensing elements required to completely map hyperelastic deformation for future soft robotics and computing.

[1]NSF MRSEC DMR-0820484

3:18PM X14.00003 ABSTRACT WITHDRAWN –

3:30PM X14.00004 Tensile shock waves in rubber , KRISHNASWAMY RAVI-CHANDAR, University of Texas, JOHNATHAN NIEMCZURA, Army Research Laboratory — We examine the propagation of waves of finite deformation in rubbers through experiments and analysis; in particular attention is focused on the propagation of one-dimensional tensile shock waves in strips of latex and nitrile rubber. Tensile wave propagation experiments were conducted at high strain-rates by holding one end fixed and displacing the other end at a constant velocity. A high-speed video camera was used to monitor the motion and to determine the evolution of strain and particle velocity in rubber strips. Shock waves have been generated under tensile impact in pre-stretched rubber strips; analysis of the response yields the tensile shock adiabat for rubbers. The propagation of shocks is analyzed by developing an analogy with the theory of detonation; it is shown that the condition for shock propagation can be determined using the Chapman-Jouguet shock condition.

3:42PM X14.00005 Kinetic features of pattern transformation and recovery in periodic hydrogel membranes , XUELIAN ZHU, RONG DONG, JI FENG, CHI-MON CHEN, SHU YANG, University of Pennsylvania, DEPT. OF MATER. SCI. & ENG., UNIV. OF PENNSYLVANIA TEAM — Pattern transformation triggered by mechanical instabilities is an attractive bottom-up method to create complex structures over a wide range of length scales. However, how to dynamically control the transformation and its recovery is yet to be studied. Here, we present a systematic study of the kinetic pattern transformation and its recovery using a model system from poly(2-hydroxyethyl methacrylate) hydrogel membrane with a square lattice of micron-sized cylindrical holes. The hydrogel membrane undergoes (1) a breathing mode (i.e. the hole reduces size but retains the shape) when exposed to DI-water; (2) a phase transition to a diamond plate pattern driven by capillarity during drying process; and (3) a recovery upon re-exposure to water. During drying, many antiphase boundaries (APBs) appear in the diamond plate pattern, which then act as embryos that determine the kinetic path for recovery. The boundary morphology (either random or aligned) can be manipulated by the moving speed of the waterfront. To reveal the underlying mechanism of pattern transformation and APB arrangement, as well as the role of APB in recovery, we utilized the dynamic Monte Carlo method to simulate the kinetic process of pattern transformation and recovery, which qualitatively matched well with the experiments.

3:54PM X14.00006 Cavitation in elastomeric solids: A defect-growth theory[1] , OSCAR LOPEZ-PAMIES, State University of New York at Stony Brook, MARTIN IDIART, TOSHIO NAKAMURA — A new theory is introduced to study the phenomenon of cavitation in soft solids that, contrary to existing approaches, simultaneously: (i) applies to large (including compressible and anisotropic) classes of nonlinear elastic solids, (ii) allows to consider general 3D loading conditions with arbitrary triaxiality, and (iii) incorporates direct information on the initial shape, spatial distribution, and mechanical properties of the underlying defects at which cavitation can initiate. The basic idea is to cast cavitation in elastomeric solids as the homogenization problem of nonlinear elastic materials containing random distributions of zero-volume cavities, or defects. In spite of the generality of the proposed approach, the relevant calculations amount to solving tractable Hamilton-Jacobi equations, in which the initial size of the cavities plays the role of "time" and the applied load plays the role of "space."

[1]Work supported by the National Science Foundation through Grant NSF/DMS–1009503.

4:06PM X14.00007 The aerodynamics of jumping rope , JEFFREY ARISTOFF, HOWARD STONE, Department of Mechanical and Aerospace Engineering, Princeton University — We present the results of a combined theoretical and experimental investigation of the motion of a rotating string that is held at both ends (i.e. a jump rope). In particular, we determine how the surrounding fluid affects the shape of the string at high Reynolds numbers: the string bends toward the axis of rotation, thereby reducing its total drag. We derive a pair of coupled non-linear differential equations that describe the shape, the numerical solution of which compares well with asymptotic approximations and experiments. Implications for successful skipping will be discussed.

4:18PM X14.00008 Helical Root Buckling: A Transient Mechanism for Stiff Interface Penetration , JESSE SILVERBERG, Department of Physics, Cornell University, ROSLYN NOAR, UNCSU, Dept of Plant Pathology, MICHAEL PACKER, Department of Physics, Cornell University, MARIA HARRISON, Boyce Thompson Institute, Cornell University, ITAI COHEN, CHRIS HENLEY, Department of Physics, Cornell University, SHARON GERBODE, School of Engineering and Applied Sciences, Harvard University — Tilling in agriculture is commonly used to loosen the topmost layer of soil and promote healthy plant growth. As roots navigate this mechanically heterogeneous environment, they encounter interfaces between the compliant soil and the underlying compacted soil. Inspired by this problem, we used 3D time-lapse imaging of Medicago Truncatula plants to study root growth in two-layered transparent hydrogels. The layers are mechanically distinct; the top layer is more compliant than the bottom. We observe that the roots form a transient helical structure as they attempt to penetrate the bi-layer interface. Interpreting this phenotype as a form of buckling due to root elongation, we measured the helix size as a function of the surrounding gel modulus. Our measurements show that by twisting the root tip during growth, the helical structure recruits the surrounding medium for an enhanced penetration force allowing the plants access to the lower layer of gel.

4:30PM X14.00009 Increasing Digging Efficiency Using Two Biologically-Inspired Techniques[1] , DAWN WENDELL, PEKO HOSOI, MIT — The mechanics of digging through granular materials often neglect the inhomogeneities present in granular packings. This work reports on two biologically-inspired mechanisms that aim to increase the efficiency of digging through granular materials by taking advantage of the variety of forces found in granular packings. First, flexible diggers demonstrate that a slight increase in flexibility can lead to more efficient digging using a completely passive mechanism. Secondly, a digger with an actuated tip is investigated to find optimum parameters for energy efficient digging with actuated mechanisms.

[1]This work is funded by Schlumberger-Doll Research.

4:42PM X14.00010 Pattern switches in granular crystals , KATIA BERTOLDI, JONGMIN SHIM, Harvard University, FATIH GONCU, University of Twente, STEPHEN WILLSHAW, TOM MULLIN, University of Manchester, STEFAN LUDING, University of Twente — We report an experimental and numerical study of a pattern transformation in a regular array of macroscopic cylindrical particles with contrasting dimensions and stiffnesses. The initial structure is a square lattice with a pair of large (soft) and small (hard) particles at each lattice site. The application of a uniaxial compression produces a new periodic structure and the transformation principally depends on the size ratio of the particles. At small ratios it is homogeneous and approximately reversible i.e. the initial geometry is almost recovered after unloading. In contrast, when the size ratio is increased the final pattern is reached after a sudden rearrangement of the particles which involves the formation of a shear band. The structural reorganization of the granular crystal will have a significant effect on wave propagation properties and we suggest that this could have interesting applications in phononic and photonic crystals.

4:54PM X14.00011 Evidence for a mechanical instability, via folding, of the vein network in leaves , PILNAM KIM, Princeton University, MANOUK ABKARIAN, Universite Montpellier 2 / CNRS, HOWARD A. STONE, Princeton University — The venation pattern of leaves is the archetype of a self-organized transport network whose efficiency and robustness stems from the connectivity of its hierarchical branching structure, but whose underlying principles of formation are not understood. Here we propose that the folding instability of the inner tissues of the leaf provides such a hierarchical venation pattern. Using a multi-layered polymeric system under an equibiaxial compressive stress, which mimics both growth and the layered structure of a leaf tissue, we show that a repetitive wrinkling-to-folding transition can achieve a hierarchical network of folds by continual, local reorganization of the stress field. We find that the resulting network topology, including closed loops, is the result of a spontaneous evolution of both terminal and segmental branching of the fold network and shares basic topological properties with venation patterns. This folding transition gives new insights into the role of mechanical stress as a possible feedback mechanism for cell differentiation in early veins.

5:06PM X14.00012 Minimal resonances in annular non-Euclidean strips , BRYAN CHEN, Department of Physics and Astronomy, University of Pennsylvania, CHRISTIAN SANTANGELO, Department of Physics, University of Massachusetts, Amherst — Differential growth processes play a prominent role in shaping leaves and biological tissues. Using both analytical and numerical calculations, we consider the shapes of closed, elastic strips which have been subjected to an inhomogeneous pattern of swelling. The stretching and bending energies of a closed strip are frustrated by compatibility constraints between the curvatures and metric of the strip. To analyze this frustration, we study the class of "conical" closed strips with a prescribed metric tensor on their center line. The resulting strip shapes can be classified according to their number of wrinkles and the prescribed pattern of swelling. We use this class of strips as a variational ansatz to obtain the minimal energy shapes of closed strips and find excellent agreement with the results of a numerical bead-spring model. We derive and test a surprising resonance condition for strips with minimal bending energy along the strip center line to exist.

5:18PM X14.00013 Deflation of elastic surfaces , CATHERINE QUILLIET, Laboratory of Interdisciplinary Physics (ex "Spectro") — The deflation of elastic spherical surfaces has been numerically investigated, and show very different types of deformations according the range of elastic parameters, some of them being quantitatively understood through simple theoretical considerations. In particular, the role of the Poisson ratio is closely investigated. This work allowed to retrieve various shapes observed on hollow deformable shells (from colloidal to centimeter scale), on lipid vesicles, or on some simple biological objects. Conversely, it shows how high deformations can tell observers about mechanical properties of a body. Such investigations have been extended to other geometries, in order to provide clues to understand deformations of vegetal or animal tissues.

Thursday, March 24, 2011 2:30PM - 5:30PM –

Session X15 DMP GMAG FIAP: Focus Session: Spins in Semiconductors - Manipulation of Dopant Spins D171

2:30PM X15.00001 Quantum information in silicon: Initialization, manipulation, storage and readout[1] , GAVIN W. MORLEY, London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, UK — Spin qubits in silicon are exciting because of their long coherence times [1] and the electrical readout of the state of one electron spin [2]. In a single experiment we demonstrate initialization [3], manipulation, storage and electrical readout of quantum information with a small ensemble of phosphorus electronic and nuclear spins in silicon [4]. Our electrical readout does not destroy the electron spin coherence which is limited instead by naturally-occurring ^{29}Si nuclear spins. These experiments require a pulsed electron spin resonance spectrometer operating at high magnetic fields [5]. Silicon quantum computers would benefit from having a second dopant species which can be addressed selectively [6-8], and we find that bismuth atoms are well suited for this role [9]. They offer long spin coherence times [9,10] as well as new opportunities [11] when compared with phosphorus.

[1] A M Tyryshkin & S A Lyon, Phosphorus electron spin coherence time can be over 10 s, Private communication (2010)
[2] A Morello *et al*, Nature **467**, 687 (2010)
[3] D R McCamey, J van Tol, G W Morley & C Boehme, Phys Rev Lett **102**, 027601 (2009)
[4] G W Morley *et al*, Phys Rev Lett **101**, 07602 (2008)
[5] G W Morley, L-C Brunel & J van Tol, Rev Sci Instrum **79**, 064703 (2008)
[6] A M Stoneham, A H Harker & G W Morley, J Phys Condens Matter **21**, 364222 (2009)
[7] A M Stoneham, A J Fisher & P T Greenland, J Phys Condens Matter **15**, L447 (2003)
[8] P T Greenland *et al*, Nature **465**, 1057 (2010)
[9] G W Morley *et al*, Nature Mater **9**, 725 (2010)
[10] R E George *et al*, Phys Rev Lett **105**, 067601 (2010)
[11] M H Mohammady, G W Morley & T S Monteiro, Phys Rev Lett **105**, 067602 (2010)

[1]Work supported by the Royal Commission for the Exhibition of 1851, EPSRC, NSF and the State of Florida.

3:06PM X15.00002 Crystal orientation induced spin Rabi beat oscillations of point defects at the c-Si(111)/SiO_2 interface , SEOYOUNG PAIK, SANG-YUN LEE, CHRISTOPH BOEHME, University of Utah — Spin-dependent electronic transitions such as certain charge carrier recombination and transport processes in semiconductors are usually governed by the Pauli blockade within pairs of two paramagnetic centers. One implication of this is that the manipulation of spin states, e.g. by magnetic resonant excitation, can produce changes to electric currents of the given semiconductor material. If both spins are changed at the same time, quantum beat effects such as beat oscillation between resonantly induced spin Rabi nutation becomes detectable through current measurements [1]. Here, we report on electrically detected spin Rabi beat oscillation caused by pairs of ^{31}P donor states and P_b interface defects at the phosphorous doped Si(111)/SiO_2interface. Due to the g-factor anisotropy of the P_b center we can tune the intra pair Larmor frequency difference (so called Larmor separation) through orientation of the sample with regard to the external magnetic field. As the Larmor separation governs the spin Rabi beat oscillation, we show experimentally how the crystal orientation can influence the beat effect.

[1] D. R. McCamey, et al. *Phys. Rev. Lett.* **104**, 017601 (2010).

3:18PM X15.00003 Dynamic Response of the Kondo Resonance in a Single-Electron Transistor in the Presence of Magnetic Field , BRYAN HEMINGWAY, TAI-MIN LIU, ANDREI KOGAN, University of Cincinnati, STEVEN HERBERT, Xavier University, MICHAEL MELLOCH, Purdue University — We report a sharp peak in the differential conductance of a Single-Electron Transistor (SET) in the Kondo regime irradiated with microwaves, plotted as function of an external, in-plane magnetic field, B. The peak emerges at frequencies, hf, above $\sim T_K/2$ and shifts approximately linearly with the microwave signal frequency. At frequencies significantly below the Kondo scale, T_K/h (M. Hettler and H. Schoeller Phys. Rev. Lett. 74, 4907-4910 (1995)), no such peak is present and the conductance data agree with the predictions based on static measurements. In the Coulomb Blockade regime, we find good agreement with the photon-assisted resonant tunneling model and experiments (T.H. Oosterkamp et al., Phys. Rev. Lett. 78 (1997)) . Our SETs are fabricated lithographically using GaAs/AlGaAs heterostructure with sheet density 4.8×10^{11} cm^{-2} and mobility 5×10^5 cm^{2}V^{-1}sec^{-1} and have the lithographic dot size approximately 130 nm in diameter.

3:30PM X15.00004 Jahn-Teller induced multiple ferromagnetic exchange interactions in magnetic semiconductors[1] , HANNES RAEBIGER, TAKESHI FUJITA, Yokohama National University, Yokohama — Ferromagnetic interactions among $3d$ impurities in compound semiconductors (II-VI, III-V, etc) are usually rationalized via "double exchange", "p-d exchange", and "superexchange" type interactions, which ensue a description of the $3d$ impurity electronic configuration based on host symmetries. Obviously Jahn-Teller distortions break these symmetries and yield completely different, closed shell, electronic configurations for the impurities, which most theories [1] simply describe as magnetically inactive. Nonetheless, such Jahn-Teller distorted $3d$ impurities e.g. in the AlN host exhibit strong short range ferromagnetic interactions. Superexchange models may offer some insight to "closed shell" magnetic interactions, not applicable to the present case, however. We investigate such peculiar magnetic interactions via density-functional calculations, and find that a Jahn-Teller distortion can trigger the formation of a 3d-3d chemical bond that stabilizes ferromagnetism via direct exchange [2], and further facilitates a double exchange type interaction. This multiple exchange is what aligns parallel the spins of e.g. Cr impurities in AlN.

[1] A. Zunger, S. Lany, and H. Raebiger, Physics **3**, 53 (2010).
[2] H. Raebiger, S. Lany, and A. Zunger, PRL **99**, 167203 (2007).

[1]Funded by JSPS Grant-in-Aid for Young Scientists (A) No. 21686003.

3:42PM X15.00005 Detecting excitation and magnetization of individual dopants in a semiconductor two-dimensional electron gas[1] , JENS WIEBE, Institute of Applied Physics, Hamburg University — Magnetic atoms doped into a semiconductor are the building blocks for bottom up spintronic and quantum logic devices. They also provide model systems for the investigation of fundamental effects. In order to correlate the dopant's atomic structure with its magnetism magnetically sensitive techniques with atomic resolution are a prerequisite. Here, I show electrical excitation and read-out [1] of single magnetic dopant associated spins in a two-dimensional electron gas (2DEG) confined to a semiconductor surface [2] using spin-resolved scanning tunneling spectroscopy [3]. I will review our real-space study of the quantum Hall transition in the 2DEG [2] and of the magnetic properties of the dopants [1]. Finally, I will demonstrate that the dopant serves as an atomic scale probe for local magnetometry of the 2DEG. This work was done in collaboration with A. A. Khajetoorians, B. Chillian, S. Schuwalow, F. Lechermann, K. Hashimoto, C. Sohrmann, T. Inaoka, F. Meier, Y. Hirayama, R. A. Römer, M. Morgenstern, and R. Wiesendanger.

[1] A. A. Khajetoorians *et al.*, Nature **467**, 1084 (2010).
[2] K. Hashimoto *et al.*, Phys. Rev. Lett. **101**, 256802 (2008).
[3] J. Wiebe *et al.*, Rev. Sci. Instrum. **75**, 4871 (2004).

[1]We acknowledge financial support from ERC Advanced Grant "FURORE", by the DFG via SFB668 and GrK1286, and by the city of Hamburg via the cluster of excellence "Nanospintronics".

4:18PM X15.00006 Coherent spin precession of multiple spins in an inhomogeneous environment , V. KORTAN, M.E. FLATTÉ, University of Iowa Department of Physics and Astronomy — Mn dopants in GaAs, whose core spins are bound anti-aligned to a hole, forming a J=1 ground state of the neutral acceptor, are very sensitive to their environment, including strain [1] and electric fields [2]. This sensitivity affects spin precession by broadening resonance lines and shifting/adding resonant frequencies. Using a low energy Hamiltonian developed for a single Mn ion-hole complex in GaAs [1,2] we have studied spin dynamics of a small collection of spins in the presence of bias electric fields and strain fields. Each Mn ion-hole complex is locally subject to a random electric field in addition to bias fields to determine if coherent spin precession persists. Using these calculations we predict the possible observation of coherent spin precession of small numbers of Mn spins via optical polarization measurements [3], and estimate the strength of the random field necessary to destroy the signal of coherent spin precession. This work supported by NRI through WIN.

[1] A. M. Yakunin, et al, Nature Mat. 6, 512 (2007).
[2] J.-M Tang, Jeremy Levy, and M. E. Flatté, Phys. Rev. Lett. 97, 106803 (2006).
[3] R. C. Myers, et al, Nature Mat. 7, 203 (2008).

4:30PM X15.00007 Study of spin interactions between InAs surface electrons and local magnetic moments by antilocalization measurements , YAO ZHANG, R.L. KALLAHER, V. SOGHOMONIAN, J.J. HEREMANS, Virginia Tech — Spin-orbit coupled electrons in the InAs surface accumulation layer can be used as a sensitive system to experimentally study the interactions and exchange between electrons and local magnetic moments in semiconductors. We use antilocalization measurements as a probe of quantum states, by comparing measurements on patterned InAs accumulation layers where Sm^{3+}, Gd^{3+} and Ho^{3+} have been deposited, with those where no magnetic species are deposited. The randomly distributed ions modify the spin-orbit scattering time and the magnetic spin-flip time, identified via the antilocalization signal and characterized over temperature. The magnetic spin-flip time carries information about magnetic interactions. Experiments indicate that the spin-orbit scattering times display a weak temperature dependence. The Sm^{3+} and Gd^{3+} cases yield temperature-independent magnetic spin-flip times, while Ho^{3+} shows a spin-flip time obeying $T^{-1/2}$ at low temperatures. Similar results as observed in the Ho^{3+} case have in the literature been attributed to Kondo-like behavior. We thus interpret the results as indicative of a Kondo interaction with a Kondo temperature considerably above 5 K, of which antilocalization measurements can identify the low-temperature tail (partial support from DOE DE-FG02-08ER46532).

4:42PM X15.00008 Spin relaxation dynamics for an electron gas with localized magnetic impurities near the ferromagnetic transition[1] , MATTHEW MOWER, GIOVANNI VIGNALE, University of Missouri — We study the spin relaxation dynamics of electrons in Mn-doped GaAs. Modeling the Mn as magnetic impurities embedded in an electron gas, we construct effective electron-electron and impurity-impurity interactions. This model exhibits a ferromagnetic transition as the temperature is lowered. Near the ferromagnetic transition, strong spin fluctuations cause an enhancement of the electron scattering rate, which affects the spin relaxation time of spin polarized electrons. This is especially notable in the D'yakonov-Perel' spin relaxation time which is proportional to the electron scattering rate. We will elucidate the behavior of the spin relaxation time and other spin-dependent kinetic coefficients near the ferromagnetic transition.

[1]Work supported by NSF DMR-0705460 and DOE DE-FG02-05ER46203

4:54PM X15.00009 Intrinsic Magnetism at Silicon Surfaces , STEVEN ERWIN, Naval Research Laboratory, FRANZ HIMPSEL, University of Wisconsin-Madison — It has been a long-standing goal to create magnetism in a nonmagnetic material by manipulating its structure at the nanometer scale. Many structural defects have unpaired spins; an ordered arrangement of such defects can give rise to a magnetically ordered state. Here we predict theoretically [1] that stepped silicon surfaces stabilized by adsorbed gold realize this goal by self-assembly, creating linear chains of polarized electron spins with virtually perfect structural order. The spins are localized at the silicon step edges, which have the form of graphitic hexagonal ribbons. The predicted magnetic state is indirectly supported by recent experimental observations, such as the coexistence of double- and triple-period distortions and the absence of edge states in photoemission. Ordered arrays of spins at a surface offer access to local probes with single spin sensitivity, such as spin-polarized scanning tunneling microscopy. The integration of structural and magnetic order is crucial for technologies involving spin-based computation and storage at the atomic level.

[1] S.C. Erwin and F.J. Himpsel, Nature Communications 1:58 (2010).

5:06PM X15.00010 Magnetic Si Atoms at the Step Edges of Si(553)-Au , PAUL SNIJDERS, ORNL, NATHAN GUISINGER, ANL, PHILLIP JOHNSON, UW-Madison, STEVEN ERWIN, NRL, FRANZ HIMPSEL, UW-Madison — A recent calculation predicts the possibility of magnetism at step edges of vicinal Si(111) surfaces decorated with gold [1]. Graphene-like Si ribbons are formed, which contain spin-polarized Si atoms at their edges. Those atoms form a six-fold superlattice at low temperature. Scanning tunneling spectroscopy (STS) of the magnetic broken bond orbitals reveals two peaks below 50 K. They match the calculated majority and minority spin states. The peaks merge into a single, broad peak at 300 K due to rapid spin fluctuations.

[1] Steven C. Erwin and F. J. Himpsel, Nature Communications 1:58 (2010).

5:18PM X15.00011 Electronic structure of Gd impurities in GaN on Ga, N and Ga-N adjacent sites and the role of N interstitials , TAWINAN CHEIWCHANCHAMNANGIJ, WALTER LAMBRECHT, Case Western Reserve University — Gd-doped GaN is one of the most interesting dilute magnetic semiconductors. However, the origins of its magnetic properties are still unclear. Previous studies have focused on the role of intrinsic defects, such as Ga vacancies and N or O interstitials. Here, we study Gd doped in pairs on adjacent Ga and N sites, which were suggested to be required to explain the X-ray linear dichroism signals in Gd L-edge spectra by Ney et al. JMMM 322, 1162 (2010). By using the FP-LMTO method in the LSDA+U, we find that the Gd on N site is pushed to the interstitial site after the relaxation and there is no extra magnetic moment besides the seven Bohr magneton from the 4f half-filled shell on each Gd atom. In spite of the relaxation, we find the energy of formation of this cluster to be of order 10 eV, which shows that the Gd doped on Ga-N adjacent sites is unlikely to occur. We also study Gd doped on a single N site and find an excess magnetic moment of 3 Bohr magneton which is spread over Gd, the nearest neighbor Ga atoms, and second nearest neighbor N atoms. However, its energy of formation is also large that this kind of impurity is unlikely to occur. We critically examine previous work on the role of N interstitials in the magnetism of Gd-doped GaN by studying the magnetic properties of the split interstitials, their interaction with each other and with Gd.

Thursday, March 24, 2011 2:30PM - 5:06PM –

Session X16 GMAG DMP: Focus Session: Spins in Carbon-Based Materials – Graphene, CNT, and C60 D173

2:30PM X16.00001 Enhanced spin injection and spin lifetime in Graphene[1] , WEI HAN, KEYU PI, KATHLEEN MCCREARY, YAN LI, ROLAND KAWAKAMI — Graphene is an attractive material for spintronics due to the low intrinsic spin-orbit and hyperfine coupling, which should lead to excellent spin transport properties. Earlier studies on spin injection and transport in graphene present two major challenges: low spin injection efficiency and short spin lifetimes compared to the theoretical predictions. In our work, we utilized TiO2 Seeded MgO barriers and achieved tunneling spin injection into single layer. As a result, large nonlocal magnetoresistances were observed at room temperature, with high spin injection efficiency up to 30%. Surprisingly, enhanced spin lifetimes of graphene are obtained, which is due to reducing the contract-induced spin relaxation by inserting tunnel barrier between graphene and Co electrodes.

[1]Thanks to the support of ONR and NSF.

2:42PM X16.00002 Electrical Detection of Spin Transport in Epitaxial Graphene Grown on the Si-face of Hexagonal SiC(0001) , J. ABEL, A. MATSUBAYASHI, J. GARRAMONE, University at Albany, C. DIMITRAKOPOULOS, A. GRILL, C.Y SUNG, IBM T.J Watson Research Center, V. LABELLA, University at Albany — Graphene has great potential for use as a spin transport channel due to its low spin orbit coupling and high mobility. Spin diffusion lengths in the microns have been demonstrated on exfoliated graphene at room temperature[1]. We will present our measurements of spin relaxation in both exfoliated graphene and epitaxially grown graphene on SiC from IBM using non-local Hanle measurements as a function of temperature. The diffusion lengths on epitaxial graphene were comparable to those found in exfoliated flakes. The initial results show the diffusion length is limited by contact induced relaxation that occurs at the metal/graphene interface in agreement with results from exfoliated flakes.

[1]Wei Han, et al. PRL 105, 167202 (2010).

2:54PM X16.00003 Room Temperature Spin Transport in C_{60}-based spin valves.[1] , LUIS HUESO, CIC nanoGUNE / IKERBASQUE, MARCO GOBBI, ROGER LLOPIS, FEDERICO GOLMAR, CIC nanoGUNE, FELIX CASANOVA, CIC nanoGUNE / IKERBASQUE — Carbon-based materials offer a unique playground for spin transport studies by merging relatively small spin relaxation mechanisms with the potential chemical versatility of some organic molecules. However, how the spin travels inside such materials is far from understood. In this work, we present magneto-transport studies in vertical spin valves containing a C_{60} non-magnetic spacer and simple ferromagnetic (Co and Py) electrodes. Large magnetoresistance values (up to 5%) are recorded at room temperature for fullerene thickness up to 30 nm. Remarkably, magnetoresistance is also present at relatively high bias (1 Volt), highlighting the robustness of the spin transport in this material. By choosing such a simple carbon system we are also able to introduce a simple multi-step tunneling model, which explain the electronic transport data and which is compatible with coherent spin transport over long distances.

[1]We acknowledge financial support from Spanish MICINN project MAT2009-08494 and from the European Comission Marie Curie grant PIRG06-GA-2009-256470

3:06PM X16.00004 Spin-orbit coupling in graphene: from single layers to graphite[1] , JAROSLAV FABIAN, Institute for Theoretical Physics, University of Regensburg — The spin-orbit interaction in graphene is full of contrasts. First, this relativistic interaction destroys the ideal relativistic "touching cones" electronic dispersion at the K points. A finite, albeit small, gap appears, giving a finite mass to the electrons. Then, while the spin-orbit splitting in the carbon atom is about 10 meV, the electronic states at the K points have a gap of only about 24 micro eV. Finally, it turns out that this quintessential sp material has its spin-orbit coupling derived almost exclusively from d orbitals. In this talk I will give first-principles [1] and tight-binding [2] perspectives on the spin-orbit coupling in graphene in the presence of a transverse electric field. The field, which would normally come from the substrate or the gates, breaks the space inversion symmetry and gives the extrinsic (Bychkov-Rashba) splitting of the states. It also brings interesting band-structure topologies, from gapped at low electric fields (the topological insulator phase), through a mixture of genuine touching Dirac cones and parabolic bands (the intrinsic and extrinsic spin-orbit strengths equal), to gapples, dominated by the extrinsic effects [1]. The intrinsic coupling is dominated by d orbitals, while the extrinsic by the field induced hybridization of the s and p orbitals. It turns out that similar physics holds for bilayer and trilayer graphene, ultimately also in graphite. I will also discuss the problem of the spin relaxation in graphene. The main issue is that conventional theories predict microseconds for the spin relaxation time, while experiments seem to consistently yield 100 ps. One possibility [3] is that that spin relaxation in graphene is due to adatoms that pull out the carbon-like spin-orbit coupling of the p electrons and lead to the larger spin relaxation of the Dyakonov-Perel type.

[1] M. Gmitra et al., Phys. Rev. B 80, 235431 (2009);
[2] S. Konschuh et al., Phys. Rev. B (in press);
[3] C. Ertler et al., Phys. Rev. B(R) 80, 041405 (2009).

[1]This work has been funded by the DFG SFB 689 and SPP1285.

3:42PM X16.00005 Ferromagnetism in Mn-implanted HOPG[1] , SAMARESH GUCHHAIT, The University of Texas at Austin, HENDRIK OHLDAG, Stanford Synchrotron Radiation Lightsource, DOMINGO FERRER, SANJAY BANERJEE, The University of Texas at Austin — 20 keV energy Mn ions were implanted on HOPG samples at 300°C. SQUID magnetometer measurements show ferromagnetic ordering and magnetic hysteresis at very low temperatures. Mn K-edge XAS spectra show presence of Mn and O in our sample and XMCD data shows ferromagnetic ordering of Mn at 14 K, but not at 300 K. SIMS data show presence of Mn and O with carbon, besides other elements. Raman spectroscopy results indicate disorder graphite phase and high resolution TEM images confirm amorphous Mn-implanted region with presence of nanocrystallites.

[1]This work was supported by SWAN and NSF DMR 0605828.

3:54PM X16.00006 Organic spin-valves based on fullerene C60[1] , RAN LIN, FUJIAN WANG, MARKUS WOHLGENANNT, University of Iowa, CHUNYONG HE, XIAOFANG ZHAI, YURI SUZUKI, University of California at Berkeley, MARKUS WOHLGENANNT TEAM[2], YURI SUZUKI TEAM[3] — Recent work suggests that the spin-transport length in organic semiconductors is limited by hyperfine coupling. Therefore, to potentially overcome this limitation, we fabricated spin-valves based on C60 for which the hyperfine coupling is minute. However, our devices do not show a significantly larger spin-diffusion length. This suggests that either a mechanism other than hyperfine coupling causes the loss of spin-polarization, or that in thick devices an increasing conductivity mismatch limits spin-injection.

[1]This work was supported by Army MURI Grant No. W911NF-08-1-0317 and NSF Grant No. ECS 07-25280.
[2]at University of Iowa
[3]at University of California at Berkeley

4:06PM X16.00007 On the Role of Spin-Orbit Coupling in the Spin Response of C_{60}-based Spintronics Devices[1] , THO NGUYEN, FIJIAN WANG, Department of Physics & Astronomy, University of Utah, 115 South 1400 East, Salt Lake City, Utah 84112, USA, XIAO-GUANG LI, Hefei National Laboratory for Physical Sciences at Microscale, People's Republic of China, EITAN EHRENFREUND, Technion-Israel Institute of Technology, Israel, VALY VARDENY, Department of Physics & Astronomy, University of Utah, 115 South 1400 East, Salt Lake City, Utah 84112, USA — We report comprehensive studies of the spin response in C_{60}-based spintronics devices such as spin valves and diodes. The buckeyball C_{60} molecules are composed of ∼99% ^{12}C carbon atoms having spinless nuclei with zero hyperfine interaction. Therefore it was believed that the spin diffusion length in C_{60}-based spin-valves is large, and the magnetoresistance (MR) in C_{60} diodes is negligible small. Surprisingly, we obtained a small spin diffusion length which we believe to be due to a relatively strong spin-orbit (SO) coupling in the material. We also found that the MR in C_{60} diodes is relatively small, with characteristic magnetic field response dominated by the SO coupling with strength, $\xi \approx 1/2$ μeV, more than ten times larger than the HFI constant. This was verified by measuring the response of ^{13}C-rich C_{60} diodes.

[1]This work was supported in part by the Department of Energy (Grant No. 04-ER461090.

4:18PM X16.00008 Kondo effect of magnetic impurities on nanotubes[1] , PIER PAOLO BARUSELLI, SISSA, Via Bonomea, 265 34136 Trieste (Italy), CNR-IOM Democritos, ALEXANDER SMOGUNOV, SISSA, CEA Saclay, MICHELE FABRIZIO, ERIO TOSATTI, SISSA, ICTP, CNR-IOM Democritos — The effect of magnetic impurities on the ballistic conductance of nanocontacts is, as suggested in recent work, amenable to ab initio study [1]. Our method proceeds via a conventional density functional calculation of spin and symmetry dependent electron scattering phase shifts, followed by the subsequent numerical renormalization group solution of Anderson models – whose ingredients and parameters are chosen so as to reproduce these phase shifts. We apply this method to investigate the Kondo zero bias anomalies that would be caused in the ballistic conductance of perfect metallic (4,4) and (8,8) single wall carbon nanotubes, ideally connected to leads at the two ends, by externally adsorbed Co and Fe adatoms. The different spin and electronic structure of these impurities are predicted to lead to a variety of Kondo temperatures, generally well below 10 K, and to interference between channels leading to Fano-like conductance minima at zero bias.

[1] P. Lucignano, R. Mazzarello, A. Smogunov, and E. Tosatti, Nature Materials 8, 563 (2009).

[1]Sponsored by PRIN/COFIN contract 20087NX9Y7.

4:30PM X16.00009 Electric-field control of magnetism in graphene quantum dots: A route to spin field effect transistors[1] , LUIS AGAPITO, NICHOLAS KIOUSSIS, Department of Physics, California State University Northridge, EFTHIMIOS KAXIRAS, Department of Physics, Harvard University — Graphene is a promising candidate for all-carbon electronics because of its outstanding electrical, mechanical, and thermal properties. Also, the relentless drive for miniaturization leads to the use of ever smaller graphene fragments; at nanoscopic dimensions ($<$ 10nm), edge states become more relevant. Edge states are important because they lie in the vicinity of the Fermi level and hence are relevant to transport properties. Furthermore, edge states exhibit magnetism. We have employed ab-initio electronic structure and Landauer-Büttiker transport calculations to study the magnetoelectro effects of graphene patches. We will present results of (1) how specific geometries (such as "diamond" shape) favor specific magnetic states, (2) how those magnetic states can be controlled by an external electric field [1], and (3) we will demonstrate how a graphene fragment containing different edge geometries can be employed as a spin-polarized field effect transistor.

[1] Agapito et al., PRB Rap. Com. 82, (2010)

[1]Supported by Grants NSF-PREM DMR-00116566 and DMR-0958596 and by NIH 3SC3GM084838-02S1 and 1SC3GM084838-02.

4:42PM X16.00010 Evidence for magnetic behavior in chemically modified graphene , JOEL THERRIEN, KYLE TWAROWSKI, ECE, U. Massachusetts Lowell, VAIBHAV MATHUR, Physics, U. Massachusetts Lowell, ANTONIO H. CASTRO-NETO, Physics, Boston University — Although graphene has exceptional electronic and structural properties, there is very little experimental evidence that graphene by itself shows strong electron-electron correlations. In fact, in spite of a large amount of theoretical work, recent experiments have shown that pure and clean graphene shows no signs of correlated many-body states such as magnetism or superconductivity. We will report on the observation of room temperature magnetism in mechanically exfoliated, chemically modified, graphene. The effect has been found using both magnetic force microscopy and magnetization tests. It was shown that the graphene can be brought back to a non-magnetized state by removing the surface chemistry. The search for correlated electronic states in graphene generates an enormous interest because of its low dimensionality, which is prone to strong quantum and thermal effects, and also because it would open up doors for a plethora of technological applications, from permanent two-dimensional magnets to spintronics.

4:54PM X16.00011 QMC study of molecules for spintronics and photoswitching[1] , MATUS DUBECKY, RENE DERIAN, LUCIA HORVATHOVA, Inst. of Physics, Slovak Academy of Sciences, Bratislava, Slovakia, LUBOS MITAS, Dept. of Physics, North Carolina State University, Raleigh, 27695, U.S.A., IVAN STICH, Inst. of Physics, Slovak Academy of Sciences, Bratislava, Slovakia — A combination of QMC and quantum chemistry (CAS-SCF) techniques are used to study two large molecules: azobenzene (AB) imporatnt as a photoswitch and vanadbenzene (VB), frequently used in spintronics [1]. In AB higher singlet state, S_2 the fingerprint of AB in excitation spectra has been calculated in addition to the low singlet states S and S_1 [2]. We have also calculated the lowest triplet T_1 vertical excitation, identified by EELS [3] as well as adiabatic T_1 excited state. All calculated energies are in excellent agreement with available experiments [3, 4]. In VB we focus initially on PES for dissociation and excited state of the vanadium cation.

[1] V.V. Maslyuk et al., Phys.Rev.Lett. 97, 201, (2006). [2] M. Dubecky et al., J.Chem.Phys, accepted (2010). [3] M. Allan, private communication. [4] J.-Å. Andersson, R. Petterson, L. Tegnér, J. Photochem. **20**, 17 (1982).

[1]Financial support from APVV projects APVV-0091-09, LPP-0392-09 and by ERDF OP R&D, CE QUTE ITMS 26240120009 are acknowledged.

Thursday, March 24, 2011 2:30PM - 5:30PM –

Session X17 GMAG DMP: Focus Session: Magnetic Oxide Thin Films - Multiferroic Heterostructures and Europium Oxide D174

2:30PM X17.00001 Electric field control of magnetism in multiferroic heterostructures[1] , CARLOS A.F. VAZ, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — Much interest is being devoted to designing systems where magnetic and ferroelectric orders coexist (multiferroics), and where the presence of magnetoelectric coupling could enable the electrostatic control of magnetism in the solid state. In particular, proximity effects can be tailored to design novel electronic structures with enhanced magnetoelectric couplings in composite heterostructures [1]. A striking example of this approach is our recent demonstration of a large, charge-mediated, magnetoelectric coupling in epitaxial PZT/LSMO heterostructures [2], which explores the sensitivity of the magnetic properties of the doped manganites to charge. Through magnetic, electric, structural and spectroscopic characterization, we demonstrate that the magnetoelectric coupling in PZT/LSMO heterostructures is electronic in origin, and results from the modulation in the valency of the Mn upon switching the PZT ferroelectric polarization [3]. In particular, we conclude that the interfacial spin ordering is modified upon charge doping, which explains the large magnetoelectric response found in this system [4]. This ability to control spin via electric fields opens a new pathway for the development of novel spin-based technologies.

[1] Vaz et al. Adv. Mater. 22:2900, 2010.
[2] Molegraaf et al. Adv. Mater. 21:3470, 2009.
[3] Vaz et al. Phys. Rev. Lett., 104:127202, 2010.
[4] Vaz et al. Appl. Phys. Lett., 97:042506, 2010.

[1]Work carried out at the Deparment of Applied Physics, Yale University, New Haven, CT 06520.

3:06PM X17.00002 Ferroelectric field effect modulation of magnetism in composite multiferroics , JASON HOFFMAN, CARLOS VAZ, YARON SEGAL, MATTHEW MARSHALL, FRED WALKER, CHARLES AHN, Yale University — This work harnesses the strong charge-driven magnetoelectric coupling in $Pb(Zr_{0.2}Ti_{0.8})O_3/La_{0.8}Sr_{0.2}MnO_3$ (PZT/LSMO) heterostructures to explore the sensitivity to charge of the electron transport and magnetic behavior of complex oxides. Epitaxial LSMO films that exhibit a highly ordered crystalline structure, as determined by *in situ* reflection high energy electron diffraction (RHEED) measurements and *ex situ* x-ray diffraction and transmission electron microscopy are grown by oxide molecular beam epitaxy. Off-axis RF magnetron sputtering is used to grow the PZT gate dielectric, which is characterized by square polarization-electric field hysteresis loops, with a large polarization and low leakage current. We use a combination of low-field magneto-transport and magneto-optic Kerr effect (MOKE) magnetometry to study the ferroelectric field effect induced changes in the magnetic coercive field in PZT/LSMO bilayers. A reversible shift in the coercive field is observed for the two polarization states of the ferroelectric, with a larger coercive field in polarization state that accumulates hole carriers at the PZT/LSMO interface. The reversible electrical control of magnetism in engineered heterostructures is opens new directions in the field of spintronics.

3:18PM X17.00003 Pulsed Laser Deposition of $Cr_{2-x}Fe_xTeO_6$ Thin Film[1] , JUNLEI WANG, KIRILL D. BELASHCHENKO, PETER A. DOWBEN, CHRISTIAN BINEK, Department of Physics & Astronomy, University of Nebraska-Lincoln — Promising spintronic concepts such as Cr_2O_3 based voltage-controlled exchange bias system [1] employ electric controlled boundary magnetization. Symmetry arguments reveal that equilibrium boundary magnetization is a generic property of magnetoelectric antiferromagnets [2]. However, experimental evidence of the boundary magnetization is scarce. Here we explore non-traditional growth of magnetoelectric oxides with tri-rutile structure using pulsed laser deposition (PLD) methodology. We grow and characterize structurally and magnetically various magnetoelectric thin films of the $Cr_{2-x}Fe_xTeO_6$ family starting from x=2 in order to take advantage of the reduced chemical complexity of Fe_2TeO_6 and the beneficial high temperature onset of antiferromagnetic order at 230K in comparison to 90K of Cr_2TeO_6. Our investigation aims on an experimental test of the predicted generality of the equilibrium boundary magnetization in magnetoelectric antiferromagnets.

[1]. He, Xi et al., Nature Materials 9, 579 - 585 (2010)
[2]. Belashchenko, K.D., Phys. Rev. Lett. 105, 147204 (2010)

[1]This project is supported by MRSEC Supplement.

3:30PM X17.00004 Properties of the Predicted Multiferroic $Ca_3Mn_2O_7$ - Experiment , R. MISRA, The Pennsylvania State University, University Park, PA, C. ADAMO, N.A. BENEDEK, Cornell University, NY, S.A. DENEV, A. SENGUPTA, The Pennsylvania State University, University Park, PA, J.A. MUNDY, Cornell University, NY, J.H. LEE, The Pennsylvania State University, University Park, PA, D.A. MULLER, Cornell University, NY, V. GOPALAN, The Pennsylvania State University, University Park, PA, C.J. FENNIE, D.G. SCHLOM, Cornell University, NY, P. SCHIFFER, The Pennsylvania State University, University Park, PA — We have studied the properties of epitaxial films of $Ca_3Mn_2O_7$, an $n = 2$ Ruddlesden-Popper phase. This material has been predicted to have novel multiferroic properties, including electric field switching of the magnetization [1]. 50 nm thick unstrained $Ca_3Mn_2O_7$ films were grown by reactive MBE on (110) $YAlO_3$ single crystal substrates. XRD shows that the $Ca_3Mn_2O_7$ films are single phase and epitaxial with (001) $Ca_3Mn_2O_7$ // (110) $YAlO_3$. Our films show a transition to a weakly ferromagnetic or canted antiferromagnetic state below 120K. The magnetic properties have strong anisotropy with a clear transition visible with an in-plane applied field, but none along the out of plane direction. Second harmonic generation results show that a weak polar order exists at room temperature and it persists until $\sim$700°C. We also report on the low temperature dielectric properties of the material.

[1] N. A. Benedek and C. J. Fennie, arXiv:1007.1003v1.

3:42PM X17.00005 Robust isothermal electric control of exchange bias at room temperature[1] , CHRISTIAN BINEK, University of Nebraska-Lincoln — Voltage-controlled spintronics is of particular importance to continue progress in information technology through reduced power consumption, enhanced processing speed, integration density, and functionality in comparison with present day CMOS electronics. Almost all existing and prototypical solid-state spintronic devices rely on tailored interface magnetism, enabling spin-selective transmission or scattering of electrons. Controlling magnetism at thin-film interfaces, preferably by purely electrical means, is a key challenge to better spintronics. Currently, most attempts to electrically control magnetism focus on potentially large magnetoelectric effects of multiferroics. We report on our interest in magnetoelectric Cr_2O_3 (chromia). Robust isothermal electric control of exchange bias is achieved at room temperature in perpendicular anisotropic Cr_2O_3(0001)/CoPd exchange bias heterostructures. This discovery promises significant implications for potential spintronics. From the perspective of basic science, our finding serves as macroscopic evidence for roughness-insensitive and electrically controllable equilibrium boundary magnetization in magnetoelectric antiferromagnets. The latter evolves at chromia (0001) surfaces and interfaces when chromia is in one of its two degenerate antiferromagnetic single domain states selected via magnetoelectric annealing. Theoretical insight into the boundary magnetization and its role in electrically controlled exchange bias is gained from first-principles calculations and general symmetry arguments. Measurements of spin-resolved ultraviolet photoemission, magnetometry at Cr_2O_3(0001) surfaces, and detailed investigations of the unique exchange bias properties of Cr_2O_3(0001)/CoPd including its electric controllability provide macroscopically averaged information about the boundary magnetization of chromia. Laterally resolved X-ray PEEM and temperature dependent MFM reveal detailed microscopic information of the chromia (0001) surface magnetization and provide a coherent interpretation of our results on robust isothermal electric control of exchange bias. The latter promise a new route towards purely voltage-controlled spintronics and an exciting way to electrically control magnetism.

[1]Financial support by NSF through Nebraska MRSEC, SRC/NSF Supplement to Nebraska MRSEC, CAREER DMR-0547887, NRI, and Cottrell Research Corporation.

4:18PM X17.00006 Europium Chalcogenide Magnetic Semiconducting Nanocrystals , JAMES DICKERSON, Vanderbilt Univ — This abstract not available.

4:54PM X17.00007 First-principles analysis of magnetic interaction in electron-doped EuO , JOONHEE AN, KIRILL BELASHCHENKO, University of Nebraska, Lincoln, KIRILL BELASHCHENKO'S GROUP TEAM — Using linear response calculations within the linear muffin-tin orbital method, we analyze the exchange interaction in electron-doped EuO. The 4f shell is treated within the LDA+U method. Calculations in the virtual crystal approximation show that the RKKY interaction mediated by the conduction band qualitatively explains the observed doping dependence of the Curie temperature in EuO. Further, to understand the role of a particular rare earth dopant, we consider EuO supercells with a substitutional Gd atom, as well as with an oxygen vacancy. Important differences with the virtual crystal approximation are found. The behavior of the exchange interaction in real space is analyzed, and its mechanisms are sorted out. The applicability of the magnetic polaron picture to Gd-doped EuO is evaluated.

5:06PM X17.00008 Curie temperature of electron-doped EuO - is there an intrinsic limit? , A. SCHMEHL, T. MAIROSER, University of Augsburg, Augsburg, Germany, A. MELVILLE, T. HEEG, Cornell University, Ithaca, N.Y., USA, L. CANELLA, P. BÖNI, Technische Universitaet Muenchen, Garching, Germany, W. ZANDER, J. SCHUBERT, Forschungszentrum Juelich GmbH, Juelich, Germany, D.E. SHAI, E.J. MONKMAN, K. M. SHEN, D.G. SCHLOM, Cornell University, Ithaca, N.Y., USA, J. MANNHART, University of Augsburg, Augsburg, Germany — Increasing the Curie temperature (T_C) of the ferromagnetic semiconductor europium monoxide is the key problem to make this versatile material attractive for wide use. Its half-metallic behavior and its structural and electronic compatibility with Si, GaN and GaAs make EuO a promising material for semiconductor-based spintronics. By doping EuO with donor impurities, T_C can substantially be increased. This increase is attributed to an additional exchange interaction that is mediated via the conduction electrons. Here we report on Hall measurements on Gd doped EuO films grown over a wide range of doping concentrations and growth conditions. We demonstrate that only a small fraction of the introduced impurities actually act as donors even for optimized growth parameters. Too high growth temperatures even render the dopants completely inactive. These results open the exciting question, if further raising the charge carrier density will elevate the Curie temperature way above today's maximum value of 170 K.

5:18PM X17.00009 The Effect of Lu Doping on Ferromagnetic EuO , ALEXANDER MELVILLE, Cornell University, THOMAS MAIROSER, ANDREAS SCHMEHL, JOCHEN MANNHART, University of Augsburg, DARRELL SCHLOM, Cornell University, CORNELL UNIVERSITY TEAM, UNIVERSITY OF AUGSBURG COLLABORATION — Europium Oxide (EuO) is a poorly understood ferromagnetic semiconductor whose spin-ordering temperature (T_C) can be greatly influenced by the inclusion of dopants such as oxygen vacancies or one of several trivalent ions. The ability to grow high-quality crystalline and stoichiometric EuO by adsorption-controlled growth using molecular-beam epitaxy is imperative in separating the effect of oxygen vacancies from that of trivalent dopants. In this study, we have prepared 5% Lu-doped EuO and characterized the effects of this doping on the magnetic and electronic properties. We show for the first time that Lu is a viable dopant material for EuO, increasing the T_C up to 120K as a result of an increase in the carrier concentration to $1.8\text{x}10^{26}\text{m}^{-3}$ from $1.0\text{x}10^{23}\text{m}^{-3}$. This is on par with other EuO films grown in an adsorption-controlled environment and doped with La or Gd. Furthermore, we find that EuO maintains a high spin-polarization (>80%) at this doping level. As a result of the simultaneously high T_C and high spin-polarization, EuO can be considered for spintronic applications at much higher temperatures than possible for undoped EuO.

Thursday, March 24, 2011 2:30PM - 5:30PM –

Session X18 GMAG DMP: Focus Session: Low D/Frustrated Magnetism - Spin Chains & Ladders D172

2:30PM X18.00001 Quantum criticality, kink confinement, and emergent symmetries in coupled Ising chains and ladders , ALAN TENNANT, Helmholtz Center Berlin — In this talk I cover the physics in three of the central quantum phase transitions in 1D. First, the transverse Ising model which is realized in CoNb2O6. While this is perhaps the simplest textbook case of a quantum phase transition, a remarkable emergence of E8 symmetry arises close to the quantum critical point. This manifests itself in an octave of bound states. We observe these experimentally and in particular the interval of the first two resonances on this octave which are found to match the golden ratio 1.618... - just as predicted for the emergence of this extraordinary symmetry. I then plan to show with the example of the Heisenberg chain how we can probe the quantum critical volume experimentally and show the characteristic scaling behaviour in space and time. The third example is of a spin ladder CaCu2O3 which is near the long sought after Wess-Zumino-Novikov-Witten quantum critical point.

3:06PM X18.00002 Evidence for strong orbital fluctuations below the Jahn-Teller transition in $Sr_3Cr_2O_8$, J. DEISENHOFER, ZHE WANG, M. SCHMIDT, A. GÜNTHER, S. SCHAILE, N. PASCHER, F. MAYR, Y. GONCHAROV, H.-A. KRUG VON NIDDA, A. LOIDL, Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany, D.L. QUINTERO-CASTRO, A.T.M.N. ISLAM, B. LAKE, Helmholtz-Zentrum Berlin für Materialien und Energie, D-14109 Berlin, Germany — We report on the magnetic and phononic excitation spectrum of SrCrO determined by THz and infrared (IR) spectroscopy, specific heat, and electron spin resonance measurements. We identify the singlet-triplet excitations in the dimerized ground state and observe an extended temperature range $T^*(= 125\text{ K}) < T < T_{JT}(= 285\text{ K})$ below the Jahn-Teller transition, where the IR active phonons change only gradually with decreasing temperature. A clear anomaly in the specific heat marks the onset of orbital ordering at T_{JT}, but a detailed analysis of the orbital contribution to the specific heat shows the persistence of strong fluctuations down to T^* in agreement with the IR data. Due to these fluctuations we can observe electron spin resonance absorptions only below T^* with a linewidth $\propto \exp(-\Delta/k_BT)$ indicating an Orbach-type spin relaxation via the excited orbital state of the Cr e doublet split by $\Delta/k_B = 388$ K.

3:18PM X18.00003 NMR in the high-field magnetic phase of $LiCuVO_4$, WOLFGANG KRAETSCHMER, NORBERT BUETTGEN, ALOIS LOIDL, Center for Electronic Correlations and Magnetism, University of Augsburg, LEONID E. SVISTOV, LYUDMILA A. PROZOROVA, Kapitza Institute, Moscow, ANDREY PROKOFIEV, Institute for Solid State Physics, TU Vienna — $LiCuVO_4$ is a quasi-one-dimensional antiferromagnetic spin-$1/2$ system with strong magnetic frustration due to competing interactions within the Cu spin chain. Consequently, a complex magnetic phase diagram with three critical magnetic field values evolves [arXiv:1005.5668]. Furthermore, spiral spin order below T_N=2.7K induces ferroelectricity thus rendering $LiCuVO_4$ multiferroic. The ferroelectric polarization can be switched by reorienting the spin helix through application of external magnetic fields [PRB **77**, 144101 (2008)]. Above $H > H_{c2}$ $LiCuVO_4$ becomes paraelectric and the magnetic order changes to a collinear spin-modulated phase. Employing Nuclear Magnetic Resonance we study the nature of this high-field phase by analysis of ^{7}Li and ^{51}V spectra recorded around $H > H_{c2}$=7.5T. We find, together with simulations for different scenarios, that Cu-spins of neighboring planes along the c-axis have a random phase-relation thus implying a two-dimensional character of the spin order [PRB **77**, 144101 (2008)].

3:30PM X18.00004 Density Functional Study of the magnetic structure on spin frustrated $MnSb_2S_4$ and Sr_2MOsO_6 (M = Cu, Ni) , CHUAN TIAN, CHANGHOON LEE, ERJUN KAN, North Carolina State University, FANG WU[1], Nanjing Forestry University, MIKE WHANGBO, North Carolina State University — We explored the electronic structures of two spin-frustrated magnetic systems monoclinic $MnSb_2S_4$ and Sr_2MOsO_6 (M = Cu, Ni) on the basis of first principles DFT calculations. The spin exchanges of $MnSb_2S_4$ are frustrated within each MnS_4 chain and between adjacent MnS_4 chains, which explains the observed helical spin order of $MnSb_2S_4$. We predict that $MnSb_2S_4$ is multiferroic with ferroelectric polarization of $\sim$14 μC/m^2 along the chain direction, and a field-induced reversal of the ferroelectric polarization occurs by reversing the direction of the helical spin rotation. The ordered double perovskites Sr_2MOsO_6 (M = Cu, Ni), reported to be half-metallic, are found to be magnetic insulators. The magnetic structures of Sr_2MOsO_6 were probed by evaluating their spin exchanges.

[1]People's Republic of China

3:42PM X18.00005 Ultra-slow Magnetic Order-Order Transition in the Spin Chain Antiferromagnet Ca3Co2O6

, O.A. PETRENKO, University of Warwick, Department of Physics, Coventry, CV4 7AL UK, S. AGRESTINI, C.L. FLECK, L.C. CHAPON, C. MAZZOLI, A. BOMBARDI, M.R. LEES — We report the observation of a highly unusual time-dependent magnetic phenomena in which a transition from one long-range magnetically ordered state to another occurs over a timescale of several hours. We have used powder neutron diffraction to investigate the magnetic structure of Ising spin chain compound $Ca_3Co_2O_6$. Our investigation focuses on the low-temperature regime ($T < 14$ K$<< T_N = 25$ K) where previous neutron diffraction studies have shown that there is an increasing instability in the spin density wave (SDW) order within this material. The results of the present work reveal that there is an order-order transition from the SDW structure to a new commensurate antiferromagnetic phase. The extraordinary time dependence of the magnetic reflections demonstrates that this transition occurs via a very slow transformation process. As the temperature is reduced the characteristic time of the transition process increases rapidly and at low temperatures the magnetic states become frozen. Calculations show that the commensurate AFM phase has a lower exchange energy than the SDW structure and is therefore expected to be ground state of $Ca_3Co_2O_6$. Our neutron data confirm the theoretical predictions, but also show that the SDW phase is preferred for 12 K $< T < T_N$.

3:54PM X18.00006 Magnetic structure and superexchange pathways in CsV_2O_5

, ANDRES SAUL, CINaM/CNRS (Marseille, France), GUILLAUME RADTKE, IM2NP (Marseille, France) — The study of low dimensional spin-1/2 quantum systems has been a very prolific field of condensed matter physics during the last decades. The family of vanadates, in particular, has provided a rich variety of compounds with different behaviours and topologies. Their magnetic structure and properties are primarily determined by the magnitude and the sign of the different exchange couplings arising between magnetic ions and therefore on the very details of their atomic and electronic structures. The sole consideration of the topology of a compound, based on idealized crystal structures, is often incomplete and even misleading. In this work, the magnetic properties of the layered compound CsV_2O_5 have been investigated using density-functional calculations. The results show that this compound is built from strongly dimerized alternating chains oriented along the **c** axis. Moreover, we demonstrate that the largest interaction along the chains direction arises *between* the structural dimers, involving a superexchange pathway through the covalently bonded $V^{(5+)}O_4$ bridging groups.

4:06PM X18.00007 Thermal Conductivity due to Magnon Heat Transport in $Ca_{2+x}Y_{2-x}Cu_5O_{10}$[1]

, RAHEEM BELLO, Department of Physics, Department of Astronomy University of Texas, ISAAC MANZANERA ESTEVE, JOHN MARKERT, Department of Physics, University of Texas — In the spin-chain structure $Ca_{2+x}Y_{2-x}Cu_5O_{10}$, the thermal conductivity in some samples is observed to exhibit two peaks attributed to the thermal transport contributions by phonons and magnons. We have built a thermal conductivity probe, with a 2D rotation stage, to study the magnon contribution to the thermal conductivity of ceramic samples over the range 4–300 K. We plan to measure changes in the magnon contribution by varying the orientation of the lattice with respect to the magnetic field. We have prepared a set of samples with small deviations in oxygen stoichiometry to examine the effects of the defects on magnon thermal transport.

[1]NSF DMR-060528, Welch F-1191, HHMI- S2005907, NSF-26-1127-6950

4:18PM X18.00008 The origin of the incommesurate phase in the spin Peierls compound TiOCl

, ARIEL DOBRY, DIEGO MASTROGIUSEPPE, CLAUDIO GAZZA, Instituto de Física de Rosario — TiOX (X=Cl,Br) are recently characterized Spin-Peierls compounds. They are unusual due to the appearance of an intermediate incommensurate phase between the dimerized and the uniform ones. We show that the incommensurate phase is stabilized by a linear dependency of the phononic dispersion near the dimerized mode. A model based on antiferromagnetic chains with position dependent exchanges accounts for the evolution of the atomic coordinates with temperature within the incommensurate phase. The magnetic gap closes in the intermediate phase. Finally, we find that the magnetic static structure factor has incommensurate peaks situated at twice the wave vector of the structural ones. These peaks could be found in future elastic neutron scattering measurements.

4:30PM X18.00009 Singlet-Triplet Excitations in the Unconventional Spin-Peierls System TiOBr

, J.P. CLANCY, B.D. GAULIN, McMaster University, C.P. ADAMS, St. Francis Xavier University, G.E. GRANROTH, A.I. KOLESNIKOV, T.E. SHERLINE, Oak Ridge National Laboratory, F.C. CHOU, National Taiwan University — TiOBr belongs to a select group of quasi-one-dimensional materials which undergo a spin-Peierls (SP) phase transition and develop a dimerized singlet ground state at low temperatures. However, unlike conventional SP systems, TiOBr exhibits not one, but two successive phase transitions upon cooling: a continuous transition into an incommensurate SP state at $T_{C2} \sim 48$ K, followed by a discontinuous transition into a commensurate SP state at $T_{C1} \sim 27$ K. We have performed time-of-flight neutron scattering measurements on powder samples of TiOBr using the fine-resolution Fermi chopper spectrometer (SEQUOIA) at the Spallation Neutron Source. These measurements reveal two branches of magnetic excitations within the commensurate and incommensurate SP phases, which we associate with n = 1 and n = 2 triplet excitations out of the singlet ground state. This study represents the first direct measure of the singlet-triplet energy gap in TiOBr, which we have determined to be $E_g = 21.2 \pm 1.0$ meV.

4:42PM X18.00010 Field-Induced Gap in a Quantum Spin-1/2 Chain in a Strong Magnetic Field[1]

, S. ZVYAGIN, M. OZEROV, J. WOSNITZA, Dresden High Magnetic Field Laboratory (HLD/FZD), Dresden, Germany, E. ČIŽMÁR, CLTP/P.J. Safarik University, Košice, Slovakia, R. FEYERHERM, HZB, Berlin, Germany, S.R. MANMANA, JILA, Dept. of Physics, University of Colorado, Boulder, USA, F. MILA, Inst. for Theor. Physics, EPF Lausanne, Lausanne, Switzerland — Magnetic excitations in copper pyrimidine dinitrate, a spin-1/2 antiferromagnetic chain with alternating g-tensor and Dzyaloshinskii-Moriya interactions that exhibits a field-induced spin gap, are probed by means of pulsed-field electron spin resonance spectroscopy. In particular, we report on a minimum of the gap in the vicinity of the saturation field $H_{sat} = 48.5$ T associated with a transition from the sine-Gordon region (with soliton-breather elementary excitations) to a spin-polarized state (with magnon excitations). This interpretation is fully confirmed by the quantitative agreement over the entire field range of the experimental data with the DMRG investigation of the spin-1/2 Heisenberg chain with a staggered transverse field.

[1] This work was partly supported by the DFG, EuroMagNET (EU contract No. 228043), APVV-VVCE-0058-07, APVV-0006-07, PIF-NSF (grant number 0904017), the Swiss National Fund and MaNEP.

4:54PM X18.00011 Non-equlibrium energy dynamics in spin chains and ladders

, FABIAN HEIDRICH-MEISNER, STEPHAN LANGER, MARKUS HEYL, LMU Munich, Germany, IAN MCCULLOCH, U Queensland, Brisbane, Australia — We investigate the real-time dynamics of the energy density in spin-1/2 chains and ladders, starting from initial states with an inhomogeneous profile of bond energies, extending our previous work on the dynamics of spin-density wave packets [1]. These simulations are carried out using the adaptive time-dependent density matrix renormalization group algorithm. We analyze the time-dependence of the spatial variance of the bond energies which yields necessary criteria for ballistic or diffusive energy dynamics. In the case of the XXZ chain, our results are consistent with ballistic behavior, both in the massless and the massive phase. For the massless regime, we compare our numerical results to predictions from bosonization for, e.g., the velocity that the initial perturbation spreads with. In the case of ladders, we find an involved dynamics whose qualitative interpretation is still under scrutiny.

[1] Langer et al. Phys. Rev. B 79, 214409 (2009)

5:06PM X18.00012 Nonmagnetic impurities in a frustrated spin ladder[1] , ERIK WULF, SEBASTIAN MÜHLBAUER, TATIANA YANKOVA, VASILY GLAZKOV, ANDREY ZHELUDEV, ETH Zürich, Schafmattstr. 16, 8093 Zürich, Switzerland — Sul-Cu_2Cl_4 is a representative of the spin S=1/2 4-leg ladders. Due to weak interladder interactions it shows almost perfect 1D character. The singlet ground state is separated from the excited triplet state by a gap of Δ=0.52meV which can be closed by a critical field of H_c=3.7T. At H_c the disordered spin liquid undergoes a phase transition to chiral helimagnetic order. By replacing nonmagnetic chlorine atoms by nonmagnetic bromine atoms random bond disorder is introduced in Sul-$Cu_2(Cl_{1-x}Br_x)_4$. Measurements of the magnetization and the specific heat show a drastically changed behavior in an applied field even at low bromine concentrations. At T>0 the material exhibits an intermediate phase between the spin liquid phase and the helimagnetic ordered phase for x=0.01, while the phase transition to the helimagnetic order is suppressed already for x=0.025. Nevertheless, the critical field H_c to overcome the excitation gap is independent from the impurity concentration.

[1]We gratefully acknowledge financial from the Swiss National Science Foundation under MaNEP and Division 6

5:18PM X18.00013 Exotic gapless Bose metals and insulators on multi-leg ladders , RYAN V. MISHMASH, MATT S. BLOCK, UCSB, RIBHU K. KAUL, UK, Lexington, DONNA N. SHENG, CSU, Northridge, OLEXEI I. MOTRUNICH, Caltech, MATTHEW P.A. FISHER, UCSB — We present recent work establishing compelling evidence for the existence of quasi-1D descendants of the d-wave Bose liquid (DBL), a novel 2D quantum phase of itinerant bosons first discussed in [1]. In particular, we study a model of hard-core bosons moving on the N-leg ladder square lattice with frustrating four-site ring exchange. In this talk, we focus on two novel phases: an incompressible gapless Mott insulator on the 3-leg ladder and a compressible gapless Bose metal on the 4-leg ladder. The former is a fundamentally quasi-1D phase that is insulating along the ladder but has two 1D gapless modes and power law transverse density-density correlations at incommensurate wave vectors; extensions of this phase to full 2D will be discussed. The latter, on the other hand, is conducting along the ladder and has five 1D gapless modes, one more than the number of legs; this represents a significant step forward in establishing the existence of the DBL in two dimensions. In both cases, we can understand the nature of the phase using slave-particle-inspired variational wave functions consisting of a product of two distinct Slater determinants, the properties of which compare impressively well to a DMRG solution of the model Hamiltonian. [1] O. I. Motrunich and M. P. A. Fisher, PRB **75**, 235116 (2007).

Thursday, March 24, 2011 2:30PM - 5:06PM –
Session X19 DCOMP: Classical and Quantum Molecular Dynamics D170

2:30PM X19.00001 Structure and Dynamics of Shock-Induced Nanobubble Collapse in Water , MOHAMMAD VEDADI, AMIT CHOUBEY, KEN-ICHI NOMURA, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, University of Southern California, ADRI VAN DUIN, Pennsylvania State University — Structure of water under shock and shock-induced collapse of nanobubbles in water are investigated with molecular dynamics simulations based on a reactive force field. Shock induces dramatic structural changes, including an ice-VII-like structural motif at a particle velocity of 1 km/s. The incipient ice VII formation and the calculated Hugoniot curve are in good agreement with experimental results. In the presence of a nanobubble, we observe a focused nanojet at the onset of nanobubble shrinkage and a secondary shock wave upon nanobubble collapse. The secondary shock wave propagates spherically backwards and induces high pressure as it propagates. Both the propagation velocity and the induced pressure are larger than those of the primary shock. We explored effects of nanobubble radius and shock amplitude on nanojet formation. The nanojet size increases by increasing particle velocity but the effect of increasing radius is more significant. The jet length scales linearly with the nanobubble radius, as observed in experiments on micron-to-millimeter size bubbles. Shock-induced collapse of a nanobubble in the vicinity of a cell membrane creates a transient nanopore when the nanojet impacts the membrane. Transient cell poration has potential applications in drug delivery.

2:42PM X19.00002 Thermal conductivity of ultra high temperature ceramics (UHTC) ZrB_2 and HfB_2 from atomistic simulations , JOHN LAWSON, NASA Ames Research Center, MURRAY DAW, Clemson University, CHARLES BAUSCHLICHER, NASA Ames Research Center — Ultra high temperature ceramics (UHTC) including ZrB_2 and HfB_2 are characterized by high melting point, good strength, and reasonable oxidation resistance. These materials are of interest for use as sharp leading edges for hypersonic vehicles among other applications. Progress in computational modeling of UHTCs has been limited in part due to the absence of suitable interatomic potentials. Recently, we developed Tersoff style parametrizations of such potentials for both ZrB_2 and HfB_2 appropriate for atomistic simulations. As an application, Green-Kubo molecular dynamics simulations were performed to evaluate the lattice thermal conductivity for single crystals of ZrB_2 and HfB_2. The atomic mass difference in these binary compounds leads to oscilations in the time correlation function of the heat current, in contrast to the more typical monotonic decay seen in monoatomic materials. Results at room temperature and at elevated temperatures will be reported.

2:54PM X19.00003 A robust and monotonically convergent iterative algorithm for solving the Kohn-Sham equations in metallic systems[1] , JEAN-LUC FATTEBERT, Lawrence Livermore National Laboratory — We propose a new iterative algorithm to efficiently calculate the electronic structure in Density Functional Theory calculations of metallic systems and warm dense matter with high electronic temperature. This parameter-free algorithm directly searches for a set of wave functions and a compatible single particle density that minimizes the Mermin finite temperature functional. It is particularly useful for simulating physical systems considered difficult to converge, such as large systems with variable occupancies and presenting charge sloshing. We demonstrate the effectiveness of the proposed algorithm and its implementation by applying it to challenging large scale problem in First-Principles Molecular Dynamics simulations.

[1]Prepared by LLNL under Contract DE-AC52-07NA27344

3:06PM X19.00004 Molecular Dynamics with Quantum Fluctuations , IONUT GEORGESCU, JASON DECKMAN, VLADIMIR MANDELSHTAM, University of California, Irvine — A new Quantum Dynamics approach, called Gaussian Molecular Dynamics (GMD), is introduced. As in the Centroid Molecular Dynamics (CMD), the N-body quantum system is mapped to an N-body classical system with an effective Hamiltonian arising within the Variational Gaussian Wave-packet approximation. The approach is exact for the harmonic oscillator and for the high-temperature limit, accurate in the short time limit and is computationally very efficient. GMD is furthermore used to estimate the diffusion constant and the spectrum of the velocity auto-correlation function of low pressure para-hydrogen at 14K and respectively 25K. The results are consistent with known experimental and theoretical results, such as CMD and RPMD.

3:18PM X19.00005 Biased Monte Carlo technique to accelerate Molecular Dynamics simulations of rare events , PRATYUSH TIWARY, AXEL VAN DE WALLE, Department of Applied Physics and Materials Science, Caltech — We propose a hybrid Monte Carlo (MC) -Molecular Dynamics (MD) technique to study temporally rare event dynamics. By using biased MC sampling (Metropolis-Hastings), we avoid actually visiting low energy states in the MD and instead carry out a quick estimate of the mean escape time to be added to the computer clock. The method does not assume anything about the nature of the transition surfaces separating basins in the energy surface. We then apply the method to the case of dislocation kink movement in BCC metals at low temperatures.

3:30PM X19.00006 Ab initio molecular dynamics simulations using a Chebyshev-filtered subspace iteration technique for modeling amorphous silicon dioxide[1] , MINJUNG KIM, KHOONGHONG KHOO, JAMES CHELIKOWSKY, University of Texas — Ab initio molecular dynamics simulations are a powerful tool for examining liquids and amorphous materials; however, such simulations are often computationally intensive. We present a molecular dynamics method that dramatically reduces the computational load using a new algorithm based on Chebyshev-filtered subspace iteration. We apply this method to amorphous silicon dioxide. Amorphous silicon dioxide has been intensively studied owing to its broad applications to electronic devices and photonics. We perform ab initio molecular dynamics simulations to obtain the amorphous structure of silicon dioxide. We employ implement several new procedures to investigate the effect of quenching rates and system sizes. The calculated structure factor for our amorphous structure is in good agreement with experimental data. We performed structural relaxations to calculate the hyperfine splitting constants. Our calculated hyperfine splitting constants of E'_γ oxygen defect centers show excellent agreement with electron paramagnetic resonance experiments. We will also discuss statistical results of oxygen-related defect centers.

[1]Department of Energy DE-FG02-06ER15760 oand DE-SC000187.

3:42PM X19.00007 Molecular Dynamics simulations of Carbon-Oxygen mixtures in the Core of White Dwarf Stars , ANDRE DA SILVA SCHNEIDER, JOE HUGHTO, CHARLES HOROWITZ, DON BERRY, Indiana University — A White Dwarf will be the final evolutionary state of most of the stars in our galaxy. The core of these faint and compact stars is a mixture of ions immersed in a degenerate electron gas. The latent heat of fusion of this mixture is important for White Dwarf cooling from which the age of stellar systems can be inferred. Assuming Carbon and Oxygen to be the most abundant elements we studied the phase diagram of the mixture using large classical molecular dynamics simulations. The ion interactions were modeled by a screened Coulomb potential and the system was kept in a half-solid half-liquid state. Understanding the chemical separation that takes place helps estimate the central abundance of these elements and is important for observations of White Dwarfs in globular star clusters [1].

[1] C.J. Horowitz, A.S. Schneider, and D.K. Berry, Physical Review Letters 104, 231101 (2010)

3:54PM X19.00008 Diffusion in Yukawa Crystals in White Dwarfs and Neutron Stars , JOSEPH HUGHTO, CHARLES HOROWITZ, ANDRE SCHNEIDER, Indiana University — Compact stars, white dwarfs and neutron stars, contain strongly interacting liquid and solid systems that we model using screened Yukawa interactions. Diffusion of impurities can release significant gravitational energy. We calculate diffusion constants using Molecular Dynamics (MD) simulations for both multicomponent liquid and single component solid systems. Diffusion in the solid depends strongly on the number and nature of crystal defects. We are not aware of previous direct calculations of diffusion in Yukawa crystals.

4:06PM X19.00009 MD Simulations of the Breaking Strain of Coulomb Crystals in Neutron Stars: Star mountains and gravitational waves[1] , CHARLES HOROWITZ, Indiana University, JOE HUGHTO, ANDRE SCHNEIDER, DON BERRY — Neutron stars — collapses stars half again as massive as the sun but with a 10-kilometer radius — have solid crusts made of dense coulomb crystals. We perform large-scale molecular dynamic simulations of the breaking strain (strength) of this crust including the effects of impurities, defects, and grain boundaries. We find neutron star crust to be the strongest material known, with a breaking stress 10 billion times stronger than steel [1]. This is because of the high density, high pressure, and the long-range nature of the coulomb interactions where each ion interacts with thousands of its neighbors. The crust can support massive mountains that, on a rapidly rotating neutron star, can radiate detectable gravitational waves. These oscillations of space and time, predicted by Einstein almost 100 years ago, should be detected in the next few years.

[1] C. J. Horowitz and Kai Kadau, Phys. Rev. Letters 102, 191102 (2009).

[1]This work was supported in part by DOE grant DE- FG02-87ER40365.

4:18PM X19.00010 Tracer Diffusion for Rough Hard Spheres , OLGA KRAVCHENKO, MARK THACHUK, UBC — We present a study of tracer diffusion in a rough sphere fluid. In such fluid collisions between particles exchange rotational and translational energy and momentum. As tracer particles grow in size, their diffusion constant is described by the Stokes-Einstein hydrodynamic result. In this limit, smooth hard spheres are shown to adopt "slip" boundary conditions. The current results show that rough hard spheres adopt boundary conditions proportional to their degree of roughness, defined by the radius of gyration. Spheres with maximum roughness adopt "stick" boundary conditions while those with intermediate roughness adopt values between the "slip" and "stick" limits. This dependence is found to be almost linear. Changes in the diffusion constants as a function of roughness are also examined and it is found that the dependence is stronger than suggested by the low-density, Boltzmann result. Rough hard spheres model the effect of inelasticity of a real collision and show that even without the presence of attractive forces, the boundary conditions for large particles can deviate from "slip" and approach "stick."

4:30PM X19.00011 Solvation and thermal effects on the optical properties of naturaldyes: a case study on the flavylium cyanin , ARRIGO CALZOLARI, CNR-IOM, BARIS MALCIOGLU, SISSA, Trieste IT, RALPH GEBAUER, ICTP, Trieste, IT, DANIELE VARSANO, Univ. "La Sapienza," Rome IT, STEFANO BARONI, SISSA, Trieste IT — We present a first-principles study of the effects of both hydration and thermal dynamics on the optical properties of a natural anthocyanin dye, namely, *cyanin* (Cya), in aqueous solution. We combine Car-Parrinello molecular dynamics and time-dependent density functional theory (TDDFT) [1] approaches to simulate the time evolution of UV-vis spectrum of the hydrated Cya molecule at room temperature [2,3]. The spectrum of the dye calculated in the gas phase [4] is characterized by two peaks in the red and in the blue, which would bring about a greenish hue incompatible with the dark purple coloration observed in nature. Describing the effect of the water solvent through a polarizable continuum model does not modify qualitatively the resulting picture. An explicit simulation of both solvent and thermal effects using ab-initio molecular dynamics results instead in a spectrum that is compatible with the observed coloration. This result is analyzed in terms of the spectroscopic effects of molecular distortions, induced by thermal fluctuations. [1] *turbo*-TDDFT, B. Walker, A. Saitta, R. Gebauer, S. Baroni, *Phys. Rev. Lett.* **2006**, 96, 113001. [2] A. Calzolari, et. al , *J. Chem. Phys.* **132**, 114304 (2010). [3] O.B. Malcioglu, A. Calzolari, R. Ghebauer, D. Varsano, and S. Baroni, preprint (2010). [4] A. Calzolari, et al, *J. Phys. Chem. A* **113** 8801 (2009).

4:42PM X19.00012 ABSTRACT WITHDRAWN –

4:54PM X19.00013 Model inter-atomic potential for Cu-Zr system generated using a multi-canonical simulation combined with a first-principles calculation , YOSHIHIDE YOSHIMOTO, Department of Applied Mathematics and Physics, Graduate School of Engineering, Tottori University — We can obtain an accurate force field for a molecular dynamics simulation from a first principles calculation. However, the available physical time for a direct first-principles molecular dynamics simulation is often limited to ~ 10 ps because of its high computational cost. If we want to achieve much longer physical time, a possible approach is to build a model inter-atomic potential from a first-principles calculation. As a kind of this approach, Yoshimoto has proposed the "thermodynamic downfolding" method[1,2] which generates an inter-atomic potential based on a multicanonical simulation combined with a first-principles calculation. With this method, we can expect that the thermodynamics of the system is conserved to a maximum extent. In this presentation, application of the method to Cu-Zr system will be reported. This system is interesting because at an composition this system become a bulk metallic glass which has several technologically attracting properties. The melting properties of the system will be covered.

[1] Y. Yoshimoto, J. Chem. Phys., 125, 184103 (2006)
[2] Y. Yoshimoto, J. Phys. Soc. Jpn., 79, 034602 (2010).

Thursday, March 24, 2011 2:30PM - 5:30PM –
Session X20 DMP FIAP GERA: Focus Session: Thermoelectric Materials: Theory D168

2:30PM X20.00001 Atomistic simulations of heat transport in nanostructures , DAVIDE DONADIO, Max Planck Institute for Polymer Research — Engineering materials at the nanoscale allows for tuning several of their properties over a broad range. These holds particularly for thermoelectric performances of group IV semiconductors, such as silicon and germanium. Experiments [1,2] suggest that improvements of the thermoelectric figure of merit in nanostructured silicon are mostly related to a drop in the thermal conductivity of about two orders of magnitude with respect to the bulk. In spite of success of macroscopic empirical approaches, we argue that atomistic simulations are necessary to provide the correct physical behavior and achieve significant understanding of a complex phenomenon such as thermal transport at the nanoscale (~ 10nm). By means of atomistic simulation methods, we address the issue of lattice thermal transport in silicon and SiGe nanostructures and nanostructured materials, e.g. nanowires, nanoporous and amorphous silicon thin films. We have reviewed and compared several simulation approaches (equilibrium and non-equilibrium molecular dynamics and anharmonic lattice dynamics), and developed a new method for large scale simulations, based on the scattering approach. We have identified strength, weaknesses and possible artifacts for each method, and established reliable simulation procedures to compute thermal transport properties. Our results shed light on the cooperative effects of dimensionality reduction, nanostructuring and disorder, in reducing the thermal conductivity of silicon-based nanostructured materials, stemming from prominent changes of lattice vibrational properties and enhancement of phonon scattering [3].

[1] A. I. Hochbaum, et al. Nature (London) **451**, 163 (2008).
[2] J.-K. Yu, et al. Nature Nanotech. **5**, 718 (2010).
[3] D. Donadio and G. Galli, Phys. Rev. Lett. **102**; 195901 (2009), Nano Lett. **10**, 847 (2010); M. K. Y. Chan, et al. Phys. Rev. B **81**, 174303 (2010).

3:06PM X20.00002 Thermoelectric performance of Si-Ge heterostructured nanowires from first-principles , ARASH MOSTOFI, MATTHEW SHELLEY, Imperial College London — We present calculations of the thermoelectric figure of merit ZT of both pristine and axially heterostructured Si/Ge nanowires as a function of their compositional disorder, growth direction and diameter. Our method is based on density-functional theory (DFT). Both charge and transport properties are calculated within the Landauer-Buttiker formalism. We compute ZT for realistic nanowires (ca. 10,000 atoms and 100 nm in length) by using maximally-localized Wannier functions to map large-scale DFT calculations onto short-ranged model Hamiltonians with negligible loss of accuracy. The approach is fully automated and robust, such that large numbers of configurations of the system can be explored with high throughput and efficiency. While we focus here on their application to thermoelectric nanowires, the algorithms we have developed are generally applicable to other classes of disordered quasi-one-dimensional nanostructures such as DNA, carbon nanotubes and graphene nanoribbons.

3:18PM X20.00003 Thermoelectric Properties of Ultra Narrow Silicon Nanowires from Atomistic Calculations , NEOPHYTOU NEOPHYTOS, HANS KOSINA, Institute for Microelectronics, Technical University of Vienna — The progress in nanomaterials' synthesis allows the realization of thermoelectric devices based on 1D nanowires (NWs). In these confined systems the electrical and thermal conductivities, and the Seebeck coefficient can be designed to some degree independently, providing enhanced ZT values as compared to the bulk material's value. We calculate the electrical conductivity, the Seebeck coefficient, and the electronic part of the thermal conductivity of scaled Si NWs. We use the atomistic sp3d5s*-spin-orbit-coupled tight-binding model and linearized Boltzmann transport. Our calculations include up to 5500 atoms, a task still computationally affordable within this model. We examine n-type and p-type NWs of diameters between 3nm and 12nm for [100], [110] and [111] transport orientations, at different doping levels. Using experimentally measured values for the lattice thermal conductivity, the expected ZT values of the nanowires are estimated. We further provide directions for power factor optimization with structure confinement.

3:30PM X20.00004 Interface scattering and thermal conductivity in Si/SiGe alloy superlattices[1] , ZLATAN AKSAMIJA, University of Wisconsin-Madison, IRENA KNEZEVIC, Univeristy of Wisconsin-Madison — $Si/Si_{1-x}Ge_x$ alloy superlattices (SLs) show promise for application as efficient thermoelectrics because of their low thermal conductivity, below that of the bulk $Si_{1-x}Ge_x$ alloy. Lattice thermal conductivity in these superlattices is dominated by scattering from the rough interfaces between layers, even at room temperature. Therefore, interface properties, such as roughness, orientation, and composition, are expected to play a significant role in thermal transport and offer additional degrees of freedom to control the thermal conductivity in semiconductor nanostructures based on superlattices. In this paper, we demonstrate the sensitivity of the lattice thermal conductivity in SLs to the interface properties, using a momentum-dependent model for scattering of phonons from rough material interfaces. Our results show excellent agreement with experimental data and explain the measured thickness and temperature dependence, as well as anisotropy of thermal conductivity in superlattices.

[1]This work has been supported by the Computing Innovation Fellows Project (NSF award No. 0937060 to the Computing Research Association, sub-award CIF-146 to the University of Wisconsin) and by the AFOSR YIP program (award No. FA9550-09-1-0230).

3:42PM X20.00005 Molecular dynamics simulation of the thermal transport across Si/Al interfaces , WOON IH CHOI, KWISEON KIM, SREEKANT NARUMANCHI, NREL — Efficient heat dissipation is critical for power electronics where the device package consists of several layers of different materials. Conventional thermal interface materials are bottlenecks in heat removal. Detailed understanding of interfacial heat resistance would benefit efforts to improve the device design. We have chosen Si/Al interfaces for this thermal transport study. We construct Si-Al MEAM interatomic potential parameters based on the density functional theory (DFT) calculations. We generate various interface structures using the first-principles molecular dynamics (MD) simulations. Using the direct method to compute the thermal conductance, we investigated various interface structures. We will discuss the effect of the inter-diffused layers and roughness of the interfaces on the thermal boundary conductance. We will also compare our result with limited data in the literature.

3:54PM X20.00006 Thermal Boundary Resistance at Ideal Gas Solid-Fluid Interfaces , SANG-HAMITRA NEOGI, GERALD MAHAN, Pennsylvania State University — We study the thermal boundary resistance at the interface between an ideal gas solid and another ideal gas fluid. In the solid side, heat is mostly carried by phonons, and thermal resistance occurs due to the partial reflection of phonons at the interface. In the fluid side, the sound waves can carry diffusive heat from the interface into the bulk of the liquid. We include both longitudinal and transverse sound modes of the fluid in the theory. The sound modes in the fluid and the reflected phonons in the solid have the same frequency as the phonon incident at the interface from the solid side. The wave vector for the sound modes is then calculated using the knowledge of the fluid pair distribution function in the bulk. The pair distribution function near the interface is modified due to the presence of the solid atoms. We solve coupled equations of motion for the atoms at the interface to obtain the phonon reflection coefficients. The Kapitza resistance is then obtained using the knowledge of these reflection coefficients. The calculation provides a method for extending the Young-Maris theory to the fluid-solid substances.

4:06PM X20.00007 Micro to Nano Scale Heat Conduction in Thermoelectric Materials , MARTIN MALDOVAN, MIT — Understanding and controlling heat transfer in solids is very important for increasing the efficiency of thermoelectric materials such as skutterudites, clatharates, superlattices, nanowires, and quantum dots. Although the mechanisms governing the thermal conductivity have been understood for years, a comprehensive theoretical method to calculate heat transfer, particularly at small scales, has not been available. This is mainly due to the complexity of anharmonic processes and phonon boundary scattering. We present a comprehensive theoretical model to calculate the thermal conductivity of thermoelectric materials at small length scales. The approach involves an exact calculation of the reduction of the phonon mean free paths due to boundary scattering and removes the need to solve the Boltzmann equation or to use adjustable terms as in the Callaway or Holland models. The analysis is based on the kinetic theory of transport processes and considers general expressions for dispersion relations, phonon mean free paths, and surface specularity parameters. The results show an excellent agreement with experiments for thin films, nanowires, and superlattices over a wide range of temperature and across multiple length scales. The theoretical approach can further be applied to a wide variety of problems involving the conduction of heat in micro/nanostructured thermoelectrics. This research was funded by the MIT Energy Initiative.

4:18PM X20.00008 Quantum Thermoelectric Effects on the Nanoscale , JUSTIN BERGFIELD, CHARLES STAFFORD, University of Arizona — An exact expression for the heat current in a nanostructure coupled to multiple metallic electrodes is derived, including both electron-electron and electron-phonon interactions. We use this formalism to investigate quantum effects on the flow of charge and entropy, and find an enormous quantum enhancement of thermoelectric effects in the vicinity of higher-order interferences in the transmission spectrum of a nanoscale junction. A nonequilibrium quantum analysis of a single-molecule junction based on 3,3'-biphenyldithiol demonstrates a maximum operating efficiency of 27% of the Carnot limit. Nonlocal quantum corrections to thermoelectric transport coefficients in multiterminal geometries are predicted.

4:30PM X20.00009 Thermal transport in Si-based disordered systems: amorphous silicon and silicon germanium alloys , YUPING HE, IVANA SAVIC, GIULIA GALLI, UC Davis, DAVIDE DONADIO, MPI for Polymer Research — Understanding and modeling heat transport in structurally and mass disordered semiconductors (e.g. amorphous silicon–a-Si and SiGe alloys) have long been a challenging problem in solid state physics. Using a combination of techniques (equilibrium and non- equilibrium molecular dynamics and lattice dynamics), we analyze the nature of vibrations and compute the thermal conductivities (k) of a-Si, bulk and nanoporous SiGe. We find that in amorphous and mass disordered systems, two types of modes are present, phonons and diffusive modes. In a-Si, phonons (who are only 3 % of the total vibrations) contribute to approximately half of k [1]. The value of k critically depends on the morphology of the system [2], for example it considerably dereases if thin films or samples with nano-holes are considered. A discussion of how mean free paths and lifetimes change as a function of morphology and disorder will be presented, together with results showing the effect,on k, of disorder at pores or film surfaces.Work supported by grant DOE DE-FC02-06ER25777.

[1] Y.He, D.Donadio and G.Galli (submitted, 2010).
[2] Y. He, D. Donadio, Joo-H. Lee, J. C. Grossman and G. Galli (submitted, 2010)

4:42PM X20.00010 Atomistic study of heat transport in SiGe alloys[1] , IVANA SAVIC, YUPING HE, Department of Chemistry, University of California at Davis, Davis, California, USA, DAVIDE DONADIO, Max Planck Institute for Polymer Research, Mainz, Germany, GIULIA GALLI, Department of Chemistry and Department of Physics, University of California at Davis, Davis, California, USA — Semiconductor alloys, e.g. SiGe, are considered as promising materials to build efficient thermoelectric devices [1], and atomistic modeling of heat transport in these systems may help complement and guide experiments in optimizing their efficiency. We analyze strengths and weaknesses of several atomistic approaches in modeling the thermal conductivity of SiGe alloys, and we analyze in detail their range of validity. In particular, we focus on equilibrium molecular dynamics [2], an approach based on the solution of the Boltzmann transport equation [3] and Green function techniques [4]. Applications to both bulk and nanostructured SiGe will be presented.

[1] A. J. Minnich, M. S. Dresselhaus, Z. F. Ren, and G. Chen, Energy Environ. Sci. 2, 466 (2009). [2] See e.g. D. Donadio and G. Galli, Phys. Rev. Lett. 102, 195901 (2009); Nano Lett. 10, 847 (2010). [3] See e.g. J. E. Turney, E. S. Landry, A. J. J. McGaughey, and C. H. Amon, Phys. Rev. B, 79, 064301 (2009). [4] See e.g. I. Savic, N. Mingo, and D. A. Stewart, Phys. Rev. Lett. 101, 165502 (2008).

[1]Work supported by DOE-SciDAC-e, DE-FC02-06ER25777.

4:54PM X20.00011 Scattering of charge carriers and phonons in thermoelectric devices , GIUSEPPE ROMANO, LEE JOO-HYOUNG, JEFFREY GROSSMAN, Massachusetts Institute of Technology — We investigate the effects of the scattering of charge carriers and phonons on the figure of merit of thermoelectric devices. Despite many efforts devoted to the optimization of the figure of merit ZT, the commercial diffusion of such systems is still limited due to their low efficiency. The main problem behind the engineering of ZT is the interdependency between the Seebeck coefficients, electrical conductivity and thermal conductivity. ZT could be maximized by either increasing the Seebeck coefficient or decreasing the thermal conductivity. While the first approach involves the distortion of the electronic density of states [1], the thermal conductivity can be lowered by inserting nonporous in the bulk materials [2]. Recent works have shown a detailed comparison between np-Ge and np-Si material and investigated the effect of the porosity on ZT [3]. Here we couple classical molecular dynamics and continuous simulation to study the phonon-phonon, phonon-pore, electron-phonon and phonon-boundary scattering and their effects on the electrical and thermal conductivities. The knowledge gained about material properties is then used to perform simulations of thermoelectric devices.

[1] PRL **104**, 016602 (2010)
[2] PRB **80**, 155327 (2009)
[3] APL **95**, 013106 (2009)

5:06PM X20.00012 Many-body effects in frequency-dependent charge and thermal transport[1] , JESUS CRUZ, JAMES FREERICKS, Georgetown University — Recently, Shastry has proposed that thermoelectric properties (thermopower, Lorenz number, and figure of merit) can be determined accurately in strongly correlated materials by examining their high frequency behavior. He also has derived a sum rule similar to the f-sum rule in optical conductivity, for the frequency dependent thermal conductivity. We examine these ideas within the context of an exactly solvable model (the Falicov-Kimball model) with dynamical mean-field theory. We see that the low-frequency and high-frequency limits are not so close in this system. We also discuss the thermal conductivity sum rule. These results are important in trying to understand strong electron correlation effects in thermoelectrics.

[1]Work supported by the National Science Foundation grants DMR-0705266 and DMR-1006605

5:18PM X20.00013 Effective medium theory for thermoelectrics , PAUL HANEY, National Institute of Standards and Technology — We report on the application of effective medium theory to binary compound thermoelectric materials. We find a range of parameters for the conductivity and thermopower of the constituent elements such that the compound has an enhanced power factor. The results of effective medium theory are compared to full numerical simulations of an ensemble of disordered systems, and good qualitative agreement is found between the two calculations. The effect of various tailored geometries are explored in the direct numerical solution of the compound thermoelectrics.

Thursday, March 24, 2011 2:30PM - 5:18PM –

Session X21 GIMS: Focus Session: Novel X-Ray Instrumentation and Measurement Techniques

D161

2:30PM X21.00001 Inelastic X-ray Scattering at Third Generation Synchrotron Sources: Present Activities and Future Plans[1] , JOHN HILL, Brookhaven National Laboratory — This talk will review present activities and future plans for utilizing inelastic x-ray scattering to study excitations in hard condensed matter systems. In particular, at current third generation sources it is now possible to observe the key elementary excitations in solids, including phonons, magnons, orbital excitations and electronic excitations such as plasmons and charge transfer excitations. The technique offers a number of advantages over existing methods for the study of these excitations, including especially, the ability to study very small sample volumes, the range of momentum and energy transfers available and the ability to work in disparate sample environments. A few recent illustrative examples are discussed. The first of these is a study of phonons in SmFeAs(O,F) which show an anomalous renormalization of certain phonons and for which momentum-dependent measurements of the electron-phonon coupling have been made. The second example will focus on work being performed at the Swiss Light Source in which spin waves in (La,Sr)CuO4 have been observed. Finally, the current and future state of inelastic x-ray scattering instrumentation in this country is discussed, including the upgrade plans at the Advanced Photon Source, and plans for new inelastic beamlines at the NSLS-II source currently under construction at Brookhaven National Laboratory

[1]Work at Brookhaven National Laboratory supported by the US Department of Energy, Division of Materials Science under contract number DE-AC02-98CH10886

3:06PM X21.00002 The new X-ray absorption spectroscopy beamline at Diamond: B18 , SILVIA RAMOS, GIANNANTONIO CIBIN, STEPHEN PARRY, ANDY J. DENT, Diamond Light Source Ltd., Harwell Science and Innovation Campus, Didcot OX11 0DE, United Kingdom — The new core XAS spectroscopy beamline at Diamond (B18) has been designed to provide a reliable spectrometer for a broad scientific community. The instrument first became operational in April 2010 and is currently combining further commissining with a rapidly growing user programme. The main goal of the optics design of B18 was to achieve high stability in an instrument that can operate over a wide energy range (2.05 to 35.0 keV). XAS measurements can be carried out using several detection methods: transmission, electron yield and fluorescence (with a Ge detector, a Si drift detector or a gas microstrip). It is also possible to carry out combined absorption and diffraction measurements. The instrument offers several sample environments: a liquid nitrogen cryostat capable of loading over 40 samples, a pulse tube cryostat with base temperature of 1.6 K and an infrared furnace with a maximum temperature of 800^{o}C and can integrate a variety of specialised set-ups designed by the users. In this talk we will present the beamline and selected examples to show its capabilities.

3:18PM X21.00003 The soft x-ray materials research (SXR) instrument at the Linac Coherent Light Source , JOSHUA J. TURNER, Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, CA, OLEG KRUPIN, European XFEL, Hamburg, Germany, WILLIAM SCHLOTTER, Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, CA — The soft x-ray materials science research (SXR) instrument completed commissioning in June 2010 and began experimental user operations shortly afterwards. This instrument delivers intense, ultra-short soft x-ray pulses from the Linac Coherent Light Source, the free-electron laser at the SLAC National Accelerator Laboratory. These are fully coherent and can contain up to 10^{13} photons per pulse (or about 3 mJ per pulse) with bunch lengths from 300 femtoseconds down to sub-10 femtoseconds. The instrument includes a monochromator whose energy range spans energies from 480 eV - 2000 eV and a Kirkpatrick-Baez mirror system to create a focal spot of a few microns in diameter. The SXR instrument has a diverse set of end stations available to conduct a large variety of experimental techniques such as coherent imaging, resonant x-ray diffraction, photoelectron spectroscopy, and x-ray emission and/or absorption. First studies include fields spanning liquid femtosecond chemistry and time-resolved resonant inelastic x-ray scattering to ordering in solids and ultrafast magnetization. An overview of the instrument and its capabilities will be given.

3:30PM X21.00004 Polarization Depend Soft X-ray Scattering of Anisotropic Organic Thin Films[1] , H. ADE, E. GANN, B. COLLINS, H. YAN, NCSU, J. COCHRAN, M. CHABINYC, UCSB — Crystalline, semi-crystalline and liquid-crystalline organic materials have locally large anisotropic bond orientation statistics. This strongly impacts the mechanical, optical and electronic properties. For example, charge transport in organic thin films is often highly anisotropic and overall transport depends upon domain size, degree of order within domains, domain correlations, and the domain boundaries. Knowing the relative impact of all parameters is necessary for a detailed understanding of organic thin film transistors. - We demonstrate a novel scattering method to characterize such films: Polarization Dependent Soft X-ray Scattering (P-SoXS). In scattering, the linear dichroic absorption often exploited in x-ray microscopy is accompanied by strong linear dichroic dispersion, leading to large contrast based on bond orientation. This can not be achieved with hard x-rays or neutrons. We demonstrate P-SoXS on devices based on prototypical materials such as pentacene, poly(2,5-bis(3-tetradecyllthiophen-2-yl)thieno[3,2-b]thiophene) (pBTTT) and poly(3-hexylthiophene) (P3HT). The use of linear or circularly polarized x-rays allows the bond orientation contrast to be switched on and off, respectively, which is very useful to characterize the correlated and individual domain size.

[1]NSF DMR-0906457 and DMR-0906224, DOE DE-FG02-98ER45737

3:42PM X21.00005 Probing buried interfaces by Index-Matched Soft X-ray Scattering[1] , E. GANN, J. SEOK, NCSU, J. COCHRAN, M. CHABINYC, UCSB, B. COLLINS, H. ADE, NCSU — Interfaces are often critical to function and performance in systems ranging from electronics to biology. Organic-organic interfaces are the location for charge transport in organic thin film transistors and exciton splitting in organic photovoltaics. Complete morphological characterization of buried interfaces is unfortunately difficult to achieve with conventional tools. We present a new method termed Index-Matched Soft X-ray Scattering (IM-SoXS). By matching the real part of the complex index of refraction of the top layer to that of vacuum through judicious choice of photon energy, we can minimize scatter from the top surface and substantially increase scatter from a buried interface, revealing both the spatial distribution and amplitude of the interfacial roughness. We demonstrate the method on samples with engineered and controlled interfacial roughness and provide examples of systems of scientific interest for which IM-SoXS should provide improved understanding of interface morphology and its relation to performance and function in systems.

[1]NSF DMR-0906457 and DMR-0906224

3:54PM X21.00006 Lensless x-ray imaging in reflection geometry , DANIEL PARKS, University of Oregon, SUJOY ROY, Lawrence Berkeley National Lab, KEOKI SEU, RUN SU, University of Oregon, JOSHUA TURNER, SLAC National Accelerator Laboratory, WEILUN CHAO, ERIK ANDERSON, Center for X-ray Optics Lawrence Berkeley National Laboratory, STEFANO CABRINI, Molecular Foundry Lawrence Berkeley National Laboratory, STEPHEN KEVAN, University of Oregon — We report on the development of a technique for lensless x-ray imaging in reflection geometry. In an approach similar to Fourier transform holography, we use a set of apertures to define object and reference waves from light which has already scattered from the sample. Back propagation from the apertures gives the image at the sample plane. This technique can be used with extended objects without additional masking, and can be used in reflection and transmission geometries. The extension of lensless x-ray imaging into reflection geometry opens the possibility of imaging surfaces in thin films, buried interfaces in multilayers, or Bragg planes in single crystals.

4:06PM X21.00007 Determination of Total X-ray Absorption Coefficient using Non-Resonant X-ray Emission , ANDREW ACHKAR, University of Waterloo, TOM REGIER, Canadian Light Source, ERIC MONKMAN, KYLE SHEN, Cornell University, DAVID HAWTHORN, University of Waterloo — Inverse partial fluorescence yield (IPFY) is a newly developed x-ray absorption spectroscopy (XAS) that utilizes non-resonant emission processes to measure the x- ray absorption of a material. Unlike XAS by traditional transmission, total electron yield and total fluorescence yield, IPFY is free of pinhole, saturation, and self-absorption effects. Moreover, IPFY exhibits a simple angle dependence that can be exploited to deduce the total x-ray absorption coefficient from a series of measurements performed with different experimental geometries. We quantitatively determine the total x-ray absorption coefficient of insulating NiO and $NdGaO_3$ single crystals at soft x-ray energies using this approach.

4:18PM X21.00008 Hard X-ray Microscopy with Multilayer Laue Lenses , HYON CHOL KANG, Chosun University — The possibility of imaging at near-atomic resolution using x-rays has been a dream ever since the short-wavelength nature of x-rays was demonstrated by von Laue and coworkers nearly a century ago. Even today the scientific impact of atomic-scale focusing of electromagnetic radiation would be deep and broad, because x-ray microscopy provides capabilities (ability to penetrate, sensitive and accurate elemental and structural information) that are complementary to other high-resolution microscopies. Although hard x-rays can in principle be focused to spot sizes on the order of their wavelength (0.1 nm), this limit has never been approached because of the difficulty in fabricating the optics. Multilayer Laue lens(MLL) is a novel diffractive optic for hard x-ray nano-focusing, which can be fabricated by sputter deposition of zone plate structure on flat substrate. According to the theoretical results, MLL is capable of focusing x-rays to well below 1 nm. We have demonstrated 2-dimensional focusing of hard x-rays with MLLs to a spot size of 25 nm x 27 nm with an efficiency of 2% at a photon energy of 12 keV, while 1-dimensional focus of 16 nm has been achieved. In this talk, we will present an overview of MLL microscopy and recent accomplishments for the determination of chemical composition in nanoscale systems. Lastly, we will give the capabilities of MLL microscopy that have the potential to significantly advance materials science, nanoscience, bio-medical science and environmental science.

4:54PM X21.00009 Dynamical diffraction effects on beam focusing for x-ray back reflection from curved multi-plate x-ray crystal cavity , YING-YI CHANG, SUNG-YU CHEN, Department of Physics, National Tsing Hua University, MAU-TSU TANG, National Synchrotron Radiation Research Center, M. YABASHI, Spring-8/RIKEN Mikazuki, Hyogo, Japan, YI-WEI TSAI, YU-HSIN WU, SHIH-CHANG WENG, CHIA-HUNG CHU, PO-YU LIAO, Department of Physics, National Tsing Hua University, SHIH-LIN CHANG, National Synchrotron Radiation Research Center — We have recently observed diffraction enhanced beam-focusing in curved multi-plate x-ray crystal cavities of silicon using (12 4 0) as the back reflection at 14.4388 keV. The measurement on the transmitted x-ray beam size through the crystal cavities shows a reduced focal length and an extremely long beam waist at the focal point. This effect could be understood according to the dynamical theory of x-ray diffraction. Based on the consideration of the excitation of the dispersion surface for each curved crystal surface involved in the crystal device, beam focusing and beam splitting occur, leading to the observed focusing feature. Detailed dynamical calculations on the transmitted intensities at different positions near the focal point will be discussed.

5:06PM X21.00010 High-Resolution Thermal Expansion Measurements of Single-Crystal Sapphire for Application as X-Ray Backscattering Monochromator[1] , JOHN J. NEUMEIER, Montana State University, I. SERGEEV, European Synchrotron Radiation Facility, D. BESSAS, R.P. HERMANN, Forschungszentrum Juelich — We report measurements of the thermal expansion of high-purity single crystal sapphire along the a and c directions. The data were acquired using a thermal expansion cell that is constructed of fused silica with a relative resolution of approximately $3x10^{-9}$. Comparison will be made to existing literature values determined from dilatometry and high-resolution x-ray diffraction. This project's main goal is the use of sapphire as x-ray backscattering monochromator for phonon spectroscopy using nuclear inelastic scattering. Tuning of the monochromator is done by varying the sapphire temperature, and the new thermal expansion values will improve the energy calibration.

[1]This material is based upon work supported by the National Science Foundation (Grant DMR-0907036).

Thursday, March 24, 2011 2:30PM - 5:18PM –
Session X22 DCMP: Metals: Bulk Properties and Nanostructures D163

2:30PM X22.00001 Phonon self energy in transition metals , LAURENT CHAPUT, IJL, UMR CNRS 7198, Nancy Universite, France, ATSUSHI TOGO, ISAO TANAKA, Department of Materials Science and Engineering, Kyoto University, Japan, GILLES HUG, LEM, UMR 104 ONERA-CNRS, ONERA, France — We present *ab initio* calculations of the phonon self energy of transition metals obtained using second order many body perturbation theory.[1] The code we have implemented[2] use the symmetry properties of the phonon-phonon interactions to express the self energy as a sum over irreducible triplets. It is analogous to the reduction of integration to the irreducible part of the Brillouin zone for one particle properties. The self energy of transition metals is then calculated. We show that the Peierls approximation[3] is in fact reasonable for *bcc* and *fcc* metals, but fails for the *hcp*. The decays paths of phonons producing the self energy is finally analyzed using surfaces of reciprocal space defined by conservation law.

[1]S. Narasimhan and D. Vanderbilt, Phys. Rev. B, 43, 4541 (1991)
[2]L. Chaput, A. Togo, I. Tanaka and G. Hug, submitted to Phys. Rev. B
[3]R. E. Peierls, Quantum Theory of Solids, Oxford University Press,1964

2:42PM X22.00002 Observation of phonon softening in Cr near its Neel transition , RUQING XU, Argonne National Laboratory, TAI-CHANG CHIANG, University of Illinois at Urbana-Champaign — Chromium is a classic antiferromagnetic spin-density-wave system, with many unique properties yet to be fully understood despite the extensive experimental and theoretical efforts in the past. For instance, near its two magnetic transitions at 311K and 123K, the elastic constants of Cr have been observed to soften abruptly by ultrasonic experiments, indicating a strong lattice-spin interaction. However, such softening has never been confirmed in previous measurements of Cr's phonon dispersion relations. To address this issue we have carried out studies with inelastic x-ray scattering (IXS) as well as x-ray thermal diffuse scattering (TDS) at temperatures around the Neel transition (311K). While the IXS measurements did not find obvious changes in the overall phonon dispersion relations of Cr, abrupt changes in TDS intensities were clearly observed across the transition at wavevectors close to the Brillouin zone centers, unveiling a softening in the long-wavelength lattice excitations in Cr at the Neel transition.

2:54PM X22.00003 First-principles study of phonon-phonon interaction in FCC metals at high temperatures , XIAOLI TANG, CHEN W. LI, Department of Material Science and Applied Physics, California Institute of Technology, BRENT FULTZ, Material Science and Applied Physics, California Institute of Technology — Third-order lattice anharmonicity induced phonon broadening of FCC metals (including Al and noble metals Cu, Ag, Au) were calculated from first-principles density functional theory (DFT) using the second-order perturbation theory, where anharmonic force constants were obtained from supercell finite displacement method combined with DFT calculations. For aluminum, the good agreement between our calculations and prior measurement of phonon linewidth at 300K and our new measurement of phonon density of states to 750K indicates the third-order phonon-phonon interactions can account for the lifetime broadenings of phonons in aluminum to at least 80% of its melting temperature. A systematic study of noble metals further suggests that, despite of the similarity among these systems, scattering kinematics play an important role in determining the relative anharmonicity between the modes, while potential anharmonicity modulates the absolute phonon decay rate.

3:06PM X22.00004 Dynamical behavior of coherent phonons in semimetals: Measuring fast electron decoherence rates with slow pulses , JIAN CHEN, Stanford PULSE Institute, SLAC National Accelerator Laboratory, JINGJING LI, Department of Physics, University of Michigan, STEPHEN FAHY, Department of Physics, University College Cork, Ireland, ROBERTO MERLIN, Department of Physics, University of Michigan, DAVID REIS, Stanford PULSE Institute, SLAC National Accelerator Laboratory — Coherent light illumination of solids above the band-gap leads not only to a population of photoexcited carriers, but also to the generation of coherent electronic states of particular symmetries which can drive vibrations of the same symmetry. For A1g and Eg symmetry phonons in Bi and Sb, there has been some controversy regarding the generation mechanism of coherent vibrations. Here, we use a combination of ultrafast stimulated Raman scattering (RS) and cw spontaneous RS to determine the lifetime of electronic coherences of A1g and Eg symmetry. Their lifetime can be inferred from a comparison between pump-probe measurements of the amplitude of the corresponding coherent phonons, and a determination of the spontaneous RS cross sections. Our results represent a new approach to probe extremely fast electron decoherence rates using much slower (50-100fs FWHM) laser pulses. The Eg electronic coherence, resulting from a fragile unequal distribution of carriers in three equivalent regions of the band structure, is extremely short lived. Its temperature-dependent lifetime is in the range 2-12 fs in Bi and 5-12 fs in Sb.

3:18PM X22.00005 First-principles calculations of lattice stabilities in Mo , WESTON NIELSON, VIDVUDS OZOLINS, University of California, Los Angeles — The determination of accurate lattice stabilities is of great importance in producing phase diagrams of metallic alloys using the CALPHAD approach. Ab-initio molecular dynamics simulations in combination with thermodynamic integration are used to determine the lattice stabilities of fcc and bcc phases in Molybdenum at a range of temperatures. We employ the so-called fixed-cell-shape molecular dynamics approach, which involves the calculation of free energies over varying lattice strains. Our results also predict that at high temperatures fcc Mo is harmonically unstable.

3:30PM X22.00006 Competing orders in the Dirac-like electronic structure and the non-linear sigma model with the topological terms , POUYAN GHAEMI, LBNL and Department of Physics UC Berkeley, SHINSEI RYU, Department of Physics UC Berkeley — The Dirac-like electronic structure can host a large number of competing orders in the form of mass terms. In particular, two different order parameters, can be said to be dual to each other, when a static defect in one of them traps a quantum number (or "charge") of the other. The complementary nature of the pair of the order parameters shows up in their dynamical properties (correlation functions) in the following sense: When a quantum phase transition is driven by one type of fluctuations in order parameter, approaching the transition from the disordered (paramagnetic) side, the order parameter correlation function at the critical point is reduced. On the other hand, such fluctuations enhances the correlation of the dual order parameter. Such complementary behaviors in the correlation function can be used to diagnose the nature of quantum fluctuations that is the driving force of the quantum phase transition.

3:42PM X22.00007 Concentration dependence of the electron-phonon coupling from metals to semiconductors , ANDREI SERGEEV, MICHAEL REIZER, VLADIMIR MITIN, SUNY at Buffalo — We study dependence of the deformation potential (DP) on concentration of carriers in the wide range from metals to semiconductors. DP in metals and semiconductors has a different nature. In metals, DP is due to electron gas compressibility, while in semiconductors this contribution is negligible due to small carrier concentrations. DP in semiconductors originates from a shift of the conduction band edge under the deformation, while in metals such contribution is small because of strong screening. We investigate DP in the transition region and found that the electron-phonon coupling has a significant minimum at intermediate concentrations. The effects of disorder on the coupling are also investigated. Theoretical conclusions are compared with available data on semi-metals and highly-doped semiconductors.

3:54PM X22.00008 Investigation of the electronic structure of $TiTe_2$ using ARPES , JIANQIAO MENG, GEY-HONG GWEON, ANDREW LAFORGE, SRIRAM SHASTRY, Department of Physics, UC Santa Cruz, ARTHUR PENN RAMIREZ, Baskin School of Engineering, UC Santa Cruz, ZACK SCHLESINGER, Department of Physics, UC Santa Cruz, KAI ROSSNAGEL, Institute for Experimental and Applied Physics, University of Kiel, DEPARTMENT OF PHYSICS, UC SANTA CRUZ TEAM, BASKIN SCHOOL OF ENGINEERING, UC SANTA CRUZ COLLABORATION, INSTITUTE FOR EXPERIMENTAL AND APPLIED PHYSICS, UNIVERSITY OF KIEL COLLABORATION — $TiTe_2$ is considered a model Fermi liquid material in the field of angle-resolved photoelectron spectroscopy (ARPES). Over the years, many groups have contributed to improving the quality of the ARPES data on $TiTe_2$, helping to understand the connection between the ARPES data and the transport properties. However, some key questions remain unanswered, the most outstanding one being the anomalous temperature dependence in the Hall coefficient R_H. Here, we present a detailed high resolution ARPES data set in a wide range of temperature and momentum. This reveals some new features: temperature dependence in the band width, temperature dependence of the Ti 3d and Te 5p occupancies, and subtle features in the line shapes as the peak crosses the Fermi level. We discuss these new features in comparison with previous ARPES studies and known transport properties.

4:06PM X22.00009 Anomalous Ordering in Inhomogeneously Strained Materials: Surface Critical Behavior in the Bulk[1] , KEVIN E. BASSLER, University of Houston, CHARO I. DEL GENIO, Max Plank Institute for Physics of Complex Systems, BO LI, University of Houston — We study a continuous quasi-two-dimensional order-disorder phase transition that occurs in a simple model of a material that is inhomogeneously strained due to the presence of dislocation lines. Performing Monte Carlo simulations of different system sizes and using finite size scaling, we measure critical exponents describing the transition of $\beta = 0.18 \pm 0.02$, $\gamma = 1.0 \pm 0.1$, and $\alpha = 0.10 \pm 0.02$. Comparable exponents have been reported in a variety of physical systems. These systems undergo a range of different types of phase transitions, including structural transitions, exciton percolation, and magnetic ordering. In particular, similar exponents have been found to describe the development of magnetic order at the onset of the pseudogap transition in hightemperature superconductors. Their common universal critical exponents suggest that the essential physics of the transition in all of these physical systems is the same as in our simple model. We argue that the nature of the transition in our model is related to surface transitions although our model has no free surface.

[1]This work is supported by the NSF through Grant No. DMR-0908286.

4:18PM X22.00010 Finding saddle points using Gentlest ascent dynamics , AMIT SAMANTA, XIANG ZHOU, Applied and Computational Mathematics, Princeton University, WEINAN E, Department of Mathematics and Program in Applied and Computational Mathematics, Princeton University — We present dynamical equations for determining transition states and escape paths from basins of attraction of a stable system on a potential energy landscape. It is shown that the stable fixed points of such dynamical systems are the index-1 saddle points. The method relies on determining the smallest eigenvalue of the Hessian matrix. The formalism is easy to extend to systems of higher dimensions and can be used to explore the free energy landscapes of systems whose large time scale separation makes the standard molecular dynamics inefficient. The utility of the algorithm is demonstrated by evaluating the activation parameters for homogeneous and heterogeneous dislocation nucleation.

4:30PM X22.00011 An efficient method to treat low barriers in kinetic ART simulations , PETER BROMMER, NORMAND MOUSSEAU, Département de physique, Université de Montréal, Québec, Canada — In kinetic Monte Carlo (KMC) the time scale of the simulation is dominated by the height of the lowest energy barrier separating two states. Rapid back-and-forth movements across very low barriers called flickers are a major limitation of the technique, as they can cost considerable CPU time without advancing the simulation. To accelerate KMC simulations, an energy basin finding algorithm has been presented [1]. In the kinetic Activation-Relaxation technique (kART) [2], KMC events are constructed during the simulation, taking full care of elastic deformations while avoiding the need for complete event search at every step. To account for low energy barriers located in this package, we implement a basin identification scheme that works on the fly as well. We apply this method to interstitial diffusion in bcc iron. There, rapid diffusion paths with low barriers for properly aligned interstitial clusters limit the simulated time. With our method, we can prevent unproductive oscillations in this diffusive basin while maintaining an appropriate distribution of exit states. This considerably extends the time scales accessible to simulation.
[1] Puchala *et al.*, *J. Chem. Phys.* **132**, 134104 (2010)
[2] El-Mellouhi *et al.*, *Phys. Rev. B*, **78**, 153202 (2008).

4:42PM X22.00012 ABSTRACT WITHDRAWN –

4:54PM X22.00013 Is the Debye-temperature a useful concept at the nanometer scale? Insights from *ab initio* free energy calculations of $Au_{13}$and $Au_{12}Fe$ nanoclusters , GHAZAL S. SHAFAI, MARISOL ALCANTARA ORTIGOZA, TALAT S. RAHMAN, University of Central Florida — We have calculated the phonon density of states, specific heat, and mean-square vibrational amplitudes of the five lowest-lying isomers of Au_{13} and two of $Au_{12}Fe$ nanoparticles, as dictated by their Helmholtz free energy. We find the vibrational entropic contributions to not affect the energy ordering of the isomers. We show that the highest phonon frequencies shift to slightly higher energies in the hybrid clusters: a signature of alloying. As expected the density of vibrational states differs significantly from the Debye model for bulk systems. The definition of the "Debye temperature" for the nanocrystal thus becomes ambiguous and depends very much on how it is calculated. In particular it neither correlates uniquely with atomic bond strengths nor does it relate to the maximum phonon frequency. The discrete phonon spectrum of nanoparticles is thus needed to describe the *exact* mean square displacement or the temperature dependency of the heat capacity. Work supported by DOE Grant DE-FG02-07ER46354

5:06PM X22.00014 Insights on the anomalously soft and stiff modes of metal nanoparticles , MARISOL ALCANTARA ORTIGOZA, TALAT S. RAHMAN, Department of Physics, University of Central Florida, Orlando FL, USA, ROLF HEID, KLAUS-PETER BOHNEN, Institut für Festkörperphysik, Karlsruher Institut für Technologie, Germany — The low- and high-energy tails of the phonon density of states (PDOS) of transition-metal nanoparticles is enhanced with respect to that of their bulk counterparts. For particles in the sub-nanometer scale, we propose a rationale for this fact based on ab initio calculations of their charge density and of the frequency and displacement pattern of their vibrational modes. We find that the radial breathing and non-radial vibrations – analogous to the pulsations observed in variable stars – correspond to the highest and lowest frequencies, respectively. This result is traced to the radial atomic distribution and the charge density distribution particular to the low-coordinated atoms, both of which give rise to modes that have no counterpart in the bulk. We find that the enhanced PDOS at low frequencies is at least partly due to the relatively small number of modes that nanoparticles can sustain and that clusters with bulk-like ordering render fewer and less stiff modes above the bulk limit.

Thursday, March 24, 2011 2:30PM - 5:30PM –

Session X23 DMP DCOMP: Focus Session: Iron Based Superconductors – Gap Symmetry D165

2:30PM X23.00001 Nodal and nodeless Superconductivity in Iron-Based Superconductors[1]

, RONNY THOMALE, Princeton University — The superconducting phase in Iron-based superconductors (pnictides) exhibits a variety of different properties depending on the doping regime and specific parameters such as band structure and interaction which describe the different compounds. The question of the symmetry of the superconducting order parameter combined with the role of interaction-induced anisotropies plays a decisive role to distinguish material-dependent effects from universal mechanisms in this family of compounds. In our talk we attempt to provide an overview of the superconducting phases currently discussed for different classes of pnictides. Specifically, we report on our work on functional renormalization group (FRG) calculations for the pnictides and how it can contribute to our understanding of the different compounds. We discuss from first principles why LaOFeAs shows nodeless while LaOFeP shows nodal anisotropic extended s-wave superconductivity, which we find to be dictated by the existence / non-existence of an additional hole pocket at $\mathrm{M} = (\pi, \pi)$ in the unfolded Brillouin zone. We also elaborate on the nodal phase in KFe_2As_2 as being of d-wave symmetry type and explain its microscopic origin related to the absence of electron pockets which are gapped out at large hole doping. In particular, we will draw a direct line from band structure and interaction parameter calculations to FRG which accomplishes to study Fermi surface instabilities from a truly ab initio starting point, and illustrate this approach for the LiFeAs compound.

[1]Support by a Feodor Lynen Scholarship of the Humboldt Foundation and DFG grant SPP 1458/1 is acknowledged.

3:06PM X23.00002 Do theoretical calculations really predict nodes in Fe-based superconductors?

, IGOR MAZIN, Naval Research Laboratory — It is well established that calculations based on the LDA band structure and the Hubbard model, with the parameters $U \sim 1.3 - 1.6$ eV, and $J \sim 0.2 - 0.3J$ (a "UJ" model), yield strongly anisotropic, and sometimes nodal gaps. The physical origin of this effect is well understood: the two leading terms in the model are $\sum U n_{i\uparrow} n_{i\downarrow}$ and $\sum{}' U n_i n_j$. The former ensures that the coupling to spin fluctuations proceeds only through the like orbitals, and the latter, not being renormalized by the standard Tolmachev-Morel-Anderson logarithm, tends to equalize the positive and the negative order parameters. Both these features are suspect on a general physics basis: the leading magnetic interaction in itinerant systems is the Hund-rule coupling, which couples every orbital with all the others, and the pnictides, with the order parameter less than 20 meV, should have nearly as strong renormalization of the Coulomb pseudopotential as the conventional superconductors. I will argue that, instead of the UJ model, in pnictides one should use the "I" model, derived from the density functional theory (which is supposed to describe the static susceptibility on the mean field level very accurately). The "I" here is simply the Stoner factor, the second variation of the LSDA magnetic energy. Unfortunately, this approach is very unlikely to produce gap nodes as easily as the UJ model, indicating that one has to look elsewhere for the nodes origin.

3:18PM X23.00003 Competing Pairing Symmetries in a Generalized Two-Orbital Model for the Pnictides

, A. NICHOLSON, W. GE, X. ZHANG, University of Tennessee and ORNL, J. RIERA, Universidad Nacional de Rosario, M. DAGHOFER, IFW Dresden, A. OLES, Max-Plank Institut fur Festkorperforchung, Heienberstrasse, G. MARTINS, Oakland University, A. MOREO, E. DAGOTTO, University of Tennessee and ORNL — An extended "t-U-J" two-orbital model [1] for the pnictides will be introduced that includes Heisenberg terms deduced from the strong coupling expansion of the Hubbard model. This extension allows us to enhance the strength of the $(\pi, 0)$-$(0, \pi)$ spin order and favors the presence of tightly bound pairing states even in the small clusters that are exactly diagonalized. The A_{1g} and B_{2g} pairing symmetries are found to compete in the realistic spin-ordered and metallic regime. The dynamical pairing susceptibility additionally unveils low-lying B_{1g} states, suggesting that small changes in parameters may render any of the three channels stable. These results contribute to understanding the puzzling results in pnictides where both nodeless and nodal states have been reported.

[1] A. Moreo *et. al.*, Phys. Rev. **B** 79, 134502 (2009)
[2] A. Nicholson *et. al.*, preprint

3:30PM X23.00004 What the magnitude of $2\Delta/T_c$ on the hole pockets can tell us about the structure of the gaps on electron pockets in Fe-based superconductors?

, SAURABH MAITI, ANDREY CHUBUKOV, University of Wisconsin — There is evidence from transport and penetration depth measurements that some Fe-based superconductors (pnictides) are nodal and some nodeless. Most notable example of nodal behavior is $BaFe_2(As_{1-x}P_x)_2$. But as of this date, there has been no direct probes of the gap structure in this material. ARPES is a direct probe to measure the gap evolution along the Fermi surfaces (FS), but in $BaFe_2(As_{1-x}P_x)_2$ accurate laser ARPES data are only available for hole FSs at Γ point, along which the gaps are nearly identical and are nearly angle-independent. We addressed the issue whether one can use ARPES data for $2\Delta_h/T_c$ on the hole FSs to predict the gap structure and magnitude along the two electron FSs. For this, we considered the non-linear gap equations in realistic 2D multi-pocket models. We found that, in the 4-pocket model, at least in certain limits, the electronic gaps have accidental nodes if $2\Delta_h/T_c$ is below a certain value close to the BCS result, and have no nodes if $2\Delta_h/T_c$ exceeds this value. This, combined with the experimental input on the $2\Delta_h/T_c$, allows us to predict the forms of the electronic gaps based on the ARPES data for the gaps on the hole pockets The verification of these results by the ARPES measurements along the electron FSs will be a crucial test for 2D itinerant multi-pocket models for Fe-pnictides.

3:42PM X23.00005 Observation of a ubiquitous three-dimensional superconducting gap function in optimally-doped $Ba_{0.6}K_{0.4}Fe_2As_2$

, Y.-M. XU, Lawrence Berkeley National Laboratory, Y.-B. HUANG, Chinese Academy of Sciences, X.-Y. CUI, E. RAZZOLI, M. RADOVIC, M. SHI, Swiss Light Source, G.-F. CHEN, Renmin University, P. ZHENG, N.-L. WANG, Chinese Academy of Sciences, C.-L. ZHANG, Oak Ridge National Laboratory, P.-C. DAI, The University of Tennessee, J.-P. HU, Purdue University, Z. WANG, Boston College, H. DING, Chinese Academy of Sciences — The knowledge of the quasi-three-dimensional (3D) superconducting (SC) gap is essential for understanding the superconducting mechanism of the iron-pnictides highlighted by their multiband and quasi-3D electronic structure. By using the k_z-capability of angle-resolved photoemission, we completely determined the SC gap on all five FSs in 3D on $Ba_{0.6}K_{0.4}Fe_2As_2$ samples. We found a significant k_z dispersion of the SC gap which can only derive from interlayer pairing. Remarkably, the SC energy gaps can be described by a single 3D gap function with two energy scales characterizing the strengths of intra-layer (Δ_1) and interlayer (Δ_2) pairing. The anisotropy ratio Δ_2/Δ_1, determined from the gap function, is close to the c-axis anisotropy ratio of the magnetic exchange coupling J_c/J_{ab} in the parent compound. The ubiquitous gap function for all the 3D FSs reveals that pairing is short-ranged and strongly constrain the possible pairing force in the pnictides.

3:54PM X23.00006 Field dependence of the zero energy density of states of an anisotropic $s_\pm$ superconductor

, YAN WANG, PETER HIRSCHFELD, Department of Physics, University of Florida, Gainesville, FL 32611, USA, SIEGFRIED GRASER, EKM, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — The pairing symmetry in iron-based superconductors (SC) is generally believed to be an $s_\pm$-wave state. Although ARPES suggests a mainly isotropic gap on all Fermi surface sheets, different thermodynamic and transport measurements are still inconclusive about the existence and orientation of gap nodes. Specific heat measurements in a magnetic field showing a square root like dependence of the Sommerfeld coefficient $\gamma(B)$ have been reported, contradicting the linear behavior expected for a fully gapped system. For a d-wave SC, $\gamma(B) \propto \sqrt{B}$ is well-known as Volovik effect. For a fully gapped $s_\pm$-wave SC with $\Delta_+ \neq \Delta_-$, a similar concave field dependence is expected. To distinguish these two effects we apply a two-band model using the Riccati parametrization of the Eilenberger equation to study the density of states around a single vortex and compare it with self-consistent calculations in the vortex lattice. Different models for the momentum dependence of the gap on each band relevant to the iron-based SC, ranging from isotropic to strongly anisotropic and nodal gaps are investigated. Partial support was provided by DOE DE-FG02-05ER46236 (PJH).

4:06PM X23.00007 Measurement of a sign-changing two-gap superconducting phase in $Ba(Fe_{1-x}Co_x)_2As_2$ single crystals using scanning tunneling spectroscopy (STS) , M.L. TEAGUE, G.K. DRAYNA, G.P. LOCKHART, T.P. WU, N.-C. YEH, Dept. of Physics, Caltech, Pasadena, CA 91125, USA, P. CHEN, B. SHEN, H.-H. WEN, Institute of Physics, Chinese Academy of Sciences, CHINA — We present STS studies of the iron pnictide superconductors $Ba(Fe_{1-x}Co_x)_2As_2$ (x=0.06, 0.08, 0.12). Studies on single crystals, cleaved at room temperature in a pure argon atmosphere, reveal direct spectroscopic evidence for predominantly two-gap superconductivity. These gaps decrease with increasing temperature and vanish immediately above the superconducting transition, T_C. Fourier transformation of the tunneling conductance demonstrates slight doping- and energy-dependent quasiparticle scattering interferences (QPI) near the nesting wave-vectors $(\pm\pi,0)/(0,\pm\pi)$ and also near $(\pm2\pi,0)/(0,\pm2\pi)$. The dominant QPI near $(\pm\pi,0)/(0,\pm\pi)$ and the two-gap nature are consistent with sign-changing s-wave superconductivity. The excess zero-bias conductance and the large gap-to-T_C ratios suggest significant unitary impurity scattering. Further studies of the magnetic field dependence will be discussed. This work was supported by NSF Grant DMR-0907251.

4:18PM X23.00008 Local measurement of the superfluid density in the pnictide superconductors $Ba(Fe_{1-x}Co_x)_2As_2$ across the superconducting dome , LAN LUAN, T.M. LIPPMAN, Stanford institute for materials and energy science, SLAC, C.W. HICKS, School of Physics and Astronomy, University of St Andrews, O.M. AUSLAENDER, Physics Department, Technion-Israel Institute of Technology, J.A. BERT, JIUN-HAW CHU, J.G. ANALYTIS, I.R. FISHER, K.A. MOLER, Stanford institute for materials and energy science, SLAC — We locally measure the superfluid density $\rho_s(T)$ in $Ba(Fe_{1-x}Co_x)_2As_2$ single crystals with magnetic force microscopy and scanning SQUID susceptometry. These high-precision, local-probe-based techniques enable us to measure both the zero temperature value of the superfluid density $\rho_s(0)$ and the temperature variation, to distinguish homogeneous from spatially varying responses, and to report systematic behavior as a function of Co doping across the superconducting dome. We find that $\rho_s(T)$ increases sharply with decreasing temperature below the superconducting transition temperature T_c of both optimally doped and underdoped compounds, and that $\rho_s(0)$ falls more quickly with T_c on the underdoped side of the dome than on the overdoped. These observations, as well as the increasing temperature induced change of $\rho_s(T)$ at low temperatures upon underdoping, are consistent with magnetic fluctuation mediated pairing and the coexistence of magnetism and superconductivity.

4:30PM X23.00009 A sign of change: pinning down the pairing symmetry of the iron-based superconductors , EREZ BERG, Harvard University, NETANEL LINDNER, TAMAR PEREG-BARNEA, California Institute of Technology — Understanding the structure of the order parameter of the iron-based superconductors is the key to unveil their pairing mechanism. Although there has been much theoretical and experimental indications that the order parameter changes its sign in momentum space, direct evidence is still lacking. The difficulty stems from the fact that the order parameter is likely to be of s-wave symmetry, and therefore designing a phase sensitive experiment that would clearly reveal the sign change is non-trivial. Here, we examine a contact between a sign-changing superconductor and an ordinary, uniform-sign superconductor. If the the barrier between the two superconductors is not too high, the frustration of the Josephson coupling between different portions of the Fermi surface across the contact can lead to surprising consequences, such as time-reversal symmetry breaking at the interface and unusual energy-phase relations with multiple local minima. We propose this mechanism as a possible explanation for the half-integer flux quantum transitions in niobium-iron pnictide loops, which were discovered in a recent experiment (C-T. Chen et. al., Nature Physics 6, 260 (2010)).

4:42PM X23.00010 Probing the Superconducting Order Parameter of $Ba(Fe_{1-x}Co_x)_2As_2$ by Josephson Interferometry[1] , J.M. ATKINSON, D.J. VAN HARLINGEN, University of Illinois at Urbana-Champaign, P. CANFIELD, N. NI, Iowa State University, J.D. STRAND, Syracuse University — Since the discovery of the first Fe-based superconductors in 2006, extensive effort has been directed toward characterizing and modeling the novel properties of these exotic materials, in particular, the symmetry of their superconducting order parameter. We probe the order parameter in Co-doped $BaFe_2As_2$ single crystals by fabricating Josephson junctions on polished faces orthogonal to the c-axis. It has been proposed that the Fe-pnictides form electron and hole pockets in the Fermi surface that have s-wave Cooper pair symmetry but opposite phases, the so-called s$\pm$ model. The modulation of the critical current I_C as a function of magnetic flux applied along the c-axis is different for junctions fabricated on a corner (between [100] and [110] faces) or on an edge (either [100] or [110]). In the same way, the product I_CR should be different for each type of junction. The combination of these effects may help us map the phase anisotropy and test for this pairing symmetry. We will present preliminary results of these studies and attempts to match them with existing theoretical models.

[1]Work supported by the Department of Energy grant BNL-150252 through the CES-EFRC.

4:54PM X23.00011 Robust nodal gap structure in $BaFe_2(As_{1-x}P_x)_2$ with P doping revealed by magnetic penetration depth measurements , KENICHIRO HASHIMOTO, RYO KATSUMATA, SHO TONEGAWA, SHIGERU KASAHARA, TAKAHITO TERASHIMA, TAKASADA SHIBAUCHI, YUJI MATSUDA, Kyoto University, ALESSANDRO SERAFIN, ANTONY CARRINGTON, University of Bristol — A number of experimental studies show that the non-universal superconducting gap structures with and without nodes is realized in iron pnictides, depending on the doping materials and its doping level. It has been suggested that in a framework of s++ wave symmetry, vertical nodal gap structure occurs during the crossover from s++ to s+- state due to the competition between the orbital and magnetic fluctuations as well as the impurity scattering effect. On the other hand, within the spin-fluctuation mediated pairing mechanism, three dimensional nodal structures is discussed. Therefore, it is important to uncover the doping dependence of the superconducting gap structure and its impurity effect. Here we report the magnetic penetration depth results measured down to 100 mK in the P-doped Ba122 system indicate robust nodal gap structure. We especially focus on doping evolution of the superfluid density with P doping. We also discuss the impurity effect introduced by Pb heavy ion beam respective to the in-plane.

5:06PM X23.00012 Two-Gap Paring of the Optimal Doped (M,K)Fe_2As_2 with M = Ba, Sr , FENGYAN WEI, Texas Center for Superconductivity at University of Houston and Department of Physics, BING LV, Texas Center for Superconductivity at University of Houston, FENG CHEN, YUYI XUE, Texas Center for Superconductivity at University of Houston and Department of Physics, CHINGWU CHU, Texas Center for Superconductivity at University of Houston and Department of Physics,Lawrence Berkeley National Laboratory — The gap structure revealed by the specific heat of iron pnictides remains unsettled. Not only do the reported characters vary for similar $Ba_{0.6}K_{0.4}Fe_2As_2$ and $Sr_{0.55}K_{0.45}Fe_2As_2$, single gap and two-gap pairings have also been suggested in the crystals with the same nominal composition of $Ba_{0.6}K_{0.4}Fe_2As_2$. It seems that either the gap structure is unusually sensitive to the sample details or some analysis procedures need to be refined Here we explored both the (Sr,K)Fe_2As_2 and (Ba,K)Fe_2As_2 systems, and different procedures were used to extract the phonon background. In the case of (Sr,K)Fe_2As_2, the phonon background seems to be insensitive to both the procedures and the potassium doping. For (Ba,K)Fe_2As_2, however, the data suggest a significant doping dependency of the soft phonons. The observations cast doubts on the previous procedures of using either $BaFe_2As_2$ or $Ba(Fe_{0.9}Co_{0.1})_2As_2$ to estimate the phonon background of $Ba_{0.6}K_{0.4}Fe_2As_2$. A new procedure, therefore, is developed. The result will be presented and discussed.

5:18PM X23.00013 Superconducting gap measurements on Co-doped SrFe2As2 single crystals by point contact spectroscopy[1] , CASSANDRA R. HUNT, H.Z. ARHAM, W.K. PARK, L.H. GREENE, University of Illinois at Urbana-Champaign, J. GILLETT, S. SEBASTIAN, University of Cambridge — We present point contact spectroscopy results on single crystal Co-doped $SrFe_2As_2$. Two sets of Andreev-like enhancements in conductance are seen with nominally c-axis contacts. For temperatures up to $T_c = 14.5$ K, the conductance is fit to a Blonder-Tinkham-Klapwijk (BTK) model extended to two independent bands with lifetime broadening [1]. We also consider recently proposed $s_{\pm}$-wave extensions to BTK [2,3]. Many recent reports claim multiple gaps in the 122 compounds, however care must be taken to distinguish the presence of Andreev peaks from other excitation modes. We find robust evidence of an SC gap at 6 meV and evidence of another conductance enhancement at 12 mV that tracks the inner gap. The origin of this feature, and of multi-gap features as measured by PCS, are discussed. [1] G. E. Blonder, M. Tinkham, and T. M. Klapwijk, PRB **25**, 45154532 (1982). [2] A. A. Golubov, *et al.* PRL **103**, 077003 (2009). [3] I. B. Sperstad, J. Linder, A. Sudbo, PRB **80**, 144507 (2009).

[1]Work at UIUC supported by U.S. DOE under Award No.DE-AC02-98CH10886. Work at Cambridge supported by the EPSRC, Trinity College, the Royal Society and the Commonwealth Trust.

Thursday, March 24, 2011 2:30PM - 5:30PM –

Session X24 DCOMP: Focus Session: Quantum Transport Simulations and Computational Electronics – Molecular Junctions D167

2:30PM X24.00001 Efficient k.p method for first-principles calculation of Seebeck coefficient in quantum transport[1] , DAVID A. STRUBBE, Department of Physics, University of California, Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory, SU YING QUEK, Molecular Foundry, LBNL, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University, J.B. NEATON, Molecular Foundry, LBNL, STEVEN G. LOUIE, Dept. of Physics, University of California, Berkeley; Molecular Foundry and Materials Sciences Division, LBNL — Thermoelectric properties of molecular junctions reveal fundamental aspects of nanoscale charge transport at interfaces and are relevant to potential organic/inorganic hybrid thermoelectric materials. Quantum transport calculations typically evaluate the Seebeck coefficient S by finite differences of the transmission as a function of energy. However, in ab initio calculations this quantity is difficult to converge for realistic systems and can require very large k-grids. We derive a new analytic-derivative method to evaluate S via k.p perturbation theory, implement it in a DFT-based scattering-state transport code, and apply it to calculations of molecular junctions. This technique improves k-point convergence by avoiding critical points in the lead bandstructure and allows more efficient calculations of Seebeck coefficients.

[1]Support from DOE (DE-AC02-05CH11231), NSF (DMR10-1006184 and GRFP Fellowship), NERSC, TeraGrid.

2:42PM X24.00002 First-Principles Studies of Charge Dynamics in Single-Molecule Junctions at Finite Bias[1] , PIERRE DARANCET, Molecular Foundry, LBNL, HYOUNG JOON CHOI, Physics, Yonsei University, JONATHAN R. WIDAWSKY, SCOTT BERKLEY, LATHA VENKATARAMAN, Columbia University, JEFFREY B. NEATON, Molecular Foundry, LBNL — Extending well-established measurements of low-bias conductance of single molecule junctions, new experiments report IV characteristics of organic molecules for biases as high as 1V [1]. Such measurements provide a unique probe of electronic properties of well-defined metal-organic nanointerfaces when driven out-of-equilibrium, and an opportunity to examine a still-missing quantitative theory of out-of-equilibrium charge dynamics at the nanoscale. Here we will present first-principles transport calculations for several amine-Au and pyridine-Au linked junctions at different levels of approximation: first mean-field, and then including electron-electron correlations at equilibrium and out-of-equilibrium. We show that incorporating electronic correlations at equilibrium already leads to a very good agreement with experiments [1], and discuss how these corrections might change out of equilibrium.

[1] Widawsky et al., Nanotechnology (2009).

[1]This work was supported by DOE via Helios SERC. Computational support is provided by NERSC.

2:54PM X24.00003 Understanding the Role of Direct Au-C Links to Electrodes in Single Molecule Junctions[1] , HECTOR VAZQUEZ, JONATHAN WIDAWSKY, ZHANG-LING CHENG, SEVERIN SCHNEEBELI, RACHID SKOUTA, RONALD BRESLOW, MARK S. HYBERTSEN, LATHA VENKATARAMAN — Recent experiments have shown that use of tri-methyl tin (SnMe3) link groups results in the formation of alkane single molecule junctions with measured conductance ∼100 times higher than found for any other link group previously used. Further evidence points to the in-situ formation of direct Au-C bonds to the electrode. In this work we use Density-Functional Theory based calculations to study the formation and structure of junctions based on direct Au-C link bonds. Transport calculations based on Non-Equilibrium Green's Functions for benzene and alkane molecules anchored through Au-C bonds show that the alkane backbone couples more strongly to the leads, resulting in a higher transmission as compared with other link groups. In the case of benzene, however, transport is primarily through the σ system, yielding a smaller conductance increase. Finally, we discuss corrections to the position of molecular resonances found in the DFT-based calculations and the implications for conductance.

[1]Primary funding provided by the NSEC program of the NSF under grant number 0641523.

3:06PM X24.00004 Phonon-assisted tunneling in two-level quantum dots or diatomic molecules[1] , KEVIN INGERSENT, U. Florida, EDSON VERNEK, GISELE IORIO, Fed. U. Uberlandia, Brazil — Electron-electron interactions in nanoscale systems can be significantly modified by coupling to bosonic modes (photons, phonons, and plasmons) that act as sources of dissipation and decoherence (dephasing). Photon-assisted tunneling can take place through ground and excited states of various types of quantum-dot system, while signatures of vibrational modes are seen in transport through single-molecule transistors in the Coulomb blockade and Kondo regimes. We report numerical renormalization-group results for a quantum dot or diatomic molecule that has two active levels, taking into account both intra-level and inter-level Coulomb interactions. We focus on how decoherence induced by phonon-assisted inter-level transitions affects the formation of the many-body Kondo singlet between the dot/molecule and the leads, and quantify the consequent modification of the zero-bias electrical conductance.

[1]Supported by NSF grant DMR-0710540

3:18PM X24.00005 Quantum current of a molecular photo-switch between two graphene sheets , G.P. BRIVIO, C. MOTTA, Università di Milano-Bicocca, Italy, M.I. TRIONI, CNR, ISTM, Milano (Italy), K.L. SEBASTIAN, Indian Institute of Science, Bangalore (India) — Light responsive materials that reversibly change shape under alternate UV and visible irradiation have attracted much interest because they can be used as optical switches, since the isomers show different features in the dimension, HOMO-LUMO gap and transmission spectrum. In view to integrate the photo-switch in the carbon based electronics devices, the conductance of a system constituted by a photochromic molecule between two graphene electrodes is investigated. In this work the conductance of the junction formed by diarylperfluorocyclopentene between two semi-infinite graphene sheets was computed using the non-equilibrium Green's function method combined with density functional theory via the TranSiesta code. The results emphasize the role of the graphene and the molecular electronic states in the switching behaviour of this hybrid system.

3:30PM X24.00006 Correlation between Raman scattering and conductance in a molecular junction , TAE-HO PARK, MICHAEL GALPERIN, Department of Chemistry and Biochemistry, University of California at San Diego — Raman spectroscopy of molecular junctions is a promising diagnostic and control tool. We present a model for non-resonant Raman spectroscopy, generalizing previous considerations to strong laser pulses of arbitrary time dependence. The model paves a way to realistic simulations of Raman spectroscopy experiments in molecular conduction junctions. We demonstrate within the model that the optical properties of molecular conduction junctions are strongly correlated with the electron transport properties. Feynman diagrams responsible for such similarity are analyzed for both processes, and possible explanation for observed (anti-)correlated behavior of Stokes signal and conductance is proposed.

3:42PM X24.00007 Towards *single-atom-controlled* device[1] , SUBHASISH MANDAL, RANJIT PATI, Dept. of Physics, Michigan Technological University — *Single-atom-controlled* device has been explored recently in the context of molecular junction. Here, by using a codoping model, where a cation and an anion are introduced simultaneously into the host to maintain charge neutrality, we have probed the electron transport characteristics in a strongly coupled single molecular junction. We have used 1, 12-dicarba-*closo*-dodecaborane inorganic molecule as a precursor and have replaced one of the vertex carbon atoms by a boron atom and simultaneously decorated it with an endohedrally doped alkali atom (Li/Na) to look into the role of dopant atoms on the conductivity. The commonly used thiolate anchoring groups are used to attach the molecule in between two gold electrodes, and a parameter free, first-principles, nonequilibrium Green's function approach is used to calculate the current-voltage characteristics. Charge transfer from the alkali atom to the host is found to have a profound effect on the electronic structure causing a dramatic change in the conductivity. Since the single alkali atom controls the behavior of electron flow in this circuit, we term this device as a *single-atom-controlled* device.

[1]NSF Grant No. 0643420

3:54PM X24.00008 Conformational and Voltage Gating in a Molecular Three Terminal Device , SAIKAT MUKHOPADHYAY, RAVINDRA PANDEY, Michigan Technological University, SHASHI KARNA, Army Research Laboratory — The effect of the conformational changes in the gate arm of a three terminal molecular device is investigated. The donor-acceptor molecular moieties connected through a ring describe the two arms, whereas a π-conjugated molecular wire is used as a gate in the proposed architecture. In the absence of the gate field, the device exhibits current switching between the non-planar and planar orientations of the π -electron moieties with respect to each other with maximum $I_{(ON)}/I_{(OFF)}$ =14. When the gate field is applied, $I_{(ON)}/I_{(OFF)}$ ratio decreases, thus suggesting that the effects of the conformational changes in the gate arm and the applied gate field oppose each other in the architecture considered. Furthermore, the tunneling current corresponding to conformational gating in two different directions appears to exhibit oscillatory nature with a phase factor of $\pi/2$ in presence of the gate field.

4:06PM X24.00009 Charge transport in strongly coupled molecular junctions: 'In-phase' and 'out of phase' contribution to electron tunneling[1] , PARTHA PRATIM PAL, RANJIT PATI, Michigan Technological University — We report a first principles study on the evolution of charge transport in a two-terminal molecular scale device with the increase in the length of the molecular wire build out of cubane oligomers. In particular, for wires of three different lengths, we look into the relative contribution of the 'in-phase' and the 'out-of-phase' components of the total electronic current under the influence of an external bias. In the low bias regime, the 'out-of-phase' contribution to total current is minimal and 'in-phase' or elastic tunneling of the electrons is responsible for the net electronic current. This is true irrespective of the length of the molecular spacer. In this regime, the I-V characteristics follow Ohm's law and the conductance of the wires is found to decrease exponentially with length which is in agreement with experimental results. However, after a certain 'off-set' voltage, the I-V characteristics become non-linear and the 'out-of-phase' tunneling starts to contribute substantially to the net current.

[1]This work is supported by NSF under grant no. 0643420.

4:18PM X24.00010 Negative Differential Resistance at Low Bias: C60-Based Molecular Devices , WENCHANG LU, North Carolina State University, Raleigh, NC and CSMD, ORNL, TN, XIAOHONG ZHENG, NC State University, Raleigh, NC, T.A. ABTEW, NC State University, VINCENT MEUNIER, CSMD, ORNL, TN, JERRY BERNHOLC, NC State University, Raleigh, nC and CSMD, ORNL, TN — Unlike single-C60-based devices, molecular assemblies based on two or more C60 can exhibit negative differential resistance (NDR). We evaluate electron transport properties of molecular devices built from two C60 connected by an alkane chain, using a non-equilibrium Green function technique implemented within the framework of linear-scaling DFT. We find that electronic conduction in these systems is mediated by C60's lowest unoccupied molecular orbitals (LUMOs), as in the case of a single-C60-based device. However, as the LUMOs' positions are pinned to the chemical potentials of their respective electrodes, their relative alignment shifts with applied bias and leads to an NDR at a very low bias. Furthermore, the position and magnitude of the NDR can be tuned by chemical modification of the C60s and by changing the length of the alkane linker. The flexibility and richness of C60-based molecular electronics components point to a potentially promising route for the design of molecular devices and chemical sensors.

4:30PM X24.00011 Charge injection and transport across metal-C60 and C60-petacene interfaces: A first-principles study[1] , YONG-HOON KIM, Korea Advanced Institute of Science and Technology — Recent experiments demonstrated that [60]fullerene (C_{60}) molecules adsorbed on metal surfaces provide favorable energy level alignment for both electron and hole injections in the context of light-emitting diode applications [1,2]. The efficient hole injection across C_{60} layers is rather surprising, since C_{60}s are highly electron-accepting molecules and should behave as a hole blocking (rather than hole injection) layer. To provide a microscopic understanding of these seemingly contradictory finding, we consider Au–C_{60}–pentacene–C_{60}–Au molecular junctions using a first-principles computational approach. We find the Fermi level pinning at the Au–C_{60} interfaces and the strongly configuration-dependent charge transport efficiency at the C_{60}–pentacene interfaces. The former finding is in agreement with a recent experimental report [2] and our earlier conclusion from the study of polymerized C_{60} wires [3]. We will explain the latter observation based on the nature of charge tunneling across π–π orbitals [1] Lee, J.Y., Appl. Phys. Lett. **88**, 073512 (2006) [2] Wang, Z.B *et al.*, Appl. Phys. Lett. **95**, 043302 (2009). [3] Lee, G.I., Kang, J.K., & Kim, Y.-H., J. Phys. Chem. C **112**, 7029 (2008).

[1]This work was supported by KOSEF (Grant No. 2008-02807) and NRF (Grant No. 2010-0006910).

4:42PM X24.00012 Electron correlation enhancement of the diode property of asymmetric molecule , YOSHIHIRO ASAI, HISAO NAKAMURA, National Institute of Advanced Industrial Science and Technology (AIST), JOSHUA HIHATH, NONGJIAN TAO, Arizona State University — Stimulated by the giant diode property found in tetraphenlydithiol derivative including dipyrimidinil-diphenly diblock [1], a possible mechanism of the giant diode property was investigated theoretically based on electron correlation. We found that the mean field theory (MFT) fails in describing the giant diode property, as it was confirmed by first principle calculation of ballistic electronic current through the diode molecule using GGA. Electron correlation effect on electric current taken into account within the self-consistent GW approximation using Keldysh Green's function theory was found to give the fair account of the giant diode property. We conclude that elastic electron collision beyond MFT enhances the diode property quite a lot.

[1] I.Díez-Pérez et al, Nature Chemistry, 635 (2009).

4:54PM X24.00013 First Principles Study and Theoretical Analysis of a Single Molecular Diode by $p-n$ di-block molecules , HISAO NAKAMURA, YOSHIHIRO ASAI, National Institute of Advanced Industrial Science and Technology, JOSH HIHATH, NONGJIAN TAO, Arizona State University — The concept of a single molecular diode was first proposed by Aviram and Ratner, and there have been many studies of synthesis D-σ-A or $p-n$ di-block molecules and measurements of the current-voltage $(I-V)$ characteristics for relating molecular junctions. Recently, the $I-V$measurement in a symmetric tetraphenyl junction and non-symmetric dipyrimidinyl -diphenyl diblock junction was performed, and clear rectification was found in the latter system, which resembles the $p-n$ junction by the covalent connection between electron-deficient bypyrimidinyl and electron-rich biphenyl moieties, though an applied bias is much lower than the resonant level. In this presentation, we performed the first principles calculations of electron transport for the above tetraphenyl and dipyrimidinyl -diphenyl diblock junctions by the self-consistent nonequilibrium Green's function theory with the use of our HiRUNE program module. We carried out the systematic analysis of the rectification behavior and identified the change of electron-pathway in the bridge molecule relating to $p-n$ junction based on the first principles data. The relation between the rectifying action and molecular conformation, particularly, the torsion of diblock, will be discussed.

5:06PM X24.00014 Temperature influence on a molecular switching under electric field: quantum transport ab initio calculation[1] , MAIA VERGNIORY, Donostia International Physics Center, JOSE GRANDINO-ROLDAN, University of Jaen, ARAN GARCÍA-LEKUE, Donostia International Physics Center, LIN-WANG WANG, Lawrence Berkeley National Labortaory, QUANTUM TRANSPORT TEAM — A molecular transistor based on torsion-angle conformation change driven by gate electric field is designed and studied using *ab initio* calculations. This transistor consists of a $\mathrm{SH-C_6H_2F(CH_3)C_6H_2(CH_3)F-SH}$ molecule sandwiched between two Au(111) electrodes, where the interaction between the molecular dipole and a gate voltage induced electric field will cause the molecule to twist along its c-axis. This twist changes the quantum conductivity of the molecule. The effect of thermal fluctuation on the molecular conformation is studied, so is the ability of the transistor to shut off its current. The advantages and challenges of using such molecular conformation change as a mechanism for transistor gating are discussed

[1]This work has been supported partially by the U.S. Department Of Energy BES/SC under contract No. DE-AC02-05CH11231 and and the Spanish MICINN (Grant No. FIS2010-19609-C02-02).

5:18PM X24.00015 Vibronic- and mechanical-spin control in spin-1 molecular devices[1] , DAVID RUIZ-TIJERINA, Ohio University, PABLO CORNAGLIA, CARLOS BALSEIRO, Centro Atomico Bariloche and Instituto Balseiro, Argentina, SERGIO ULLOA, Ohio University — Using numerical renormalization group calculations, we study the effect of a vibronic mode on the electronic transport through a deformable spin-1 molecular device. We analyze the experimental situation of Parks et. al. [Science 328 1370 (2010)], where it is observed that stretching the molecule introduces a static magnetic anisotropy. The device is modeled as an interacting two-level system with only one level coupled to metallic leads, in which the static anisotropy is modulated by a vibronic mode. We performed calculations of the local spectral density, which indicate that this dynamic magnetic anisotropy can counter the static effects and drive the ground state into a non Fermi-liquid phase with non-zero spectral density at the Fermi level. It also renormalizes the couplings between the molecule and the metallic leads in an anisotropic fashion, reducing the spin-1 Kondo temperature of the device.

[1]Supported by NSF-PIRE and MWN/CIAM

Thursday, March 24, 2011 2:30PM - 5:18PM –

Session X25 DCMP: Superconductivity: Optical, Raman and Other Spectroscopies D166

2:30PM X25.00001 How can we relate the critical temperature and the superconducting gap amplitude in cuprate superconductors? , ALAIN SACUTO, SEABSTIEN BLANC, YANN GALLAIS, MAXIMILIEN CAZAYOUS, MARIE AUDE MEASSON, Laboratoire Matériaux et Phénomènes Quantiques, CNRS Université Paris Diderot - Paris 7, Paris Cedex 13, France, J.S. WEN, Z.J. XU, GENDA GU, Matter Physics and Materials Science, Brookhaven National Laboratory (BNL), USA — We explore the superconducting state of hole-doped cuprates by electronic Raman scattering as a function of both temperature and doping level. We observe a loss of coherent quasi-particles in the anti-nodal region and show that coherent Bogoliubov quasiparticles are confined around the nodes. This contrasts to conventional superconductors where superconductivity develops uniformly along the normal-state Fermi surface. We define the fraction of coherent Fermi surface, f_c around the nodes for which quasi-particles are well defined and superconductivity sets in. We establish that $T_c \propto f_c \Delta_{max}$. Δ_{max} is the maximum amplitude of the d-wave superconducting gap. This new relation differs from the standard BCS theory and gives us some clues for increasing T_c in the cuprates. S. Blanc et al. Phys. Rev. B **82**, 144516 (2010); S. Blanc et al. Phys. Rev. B **80**, 140502 (2009).

2:42PM X25.00002 Raman response in density wave materials , ELIZABETH NOWADNICK, ALEXANDER KEMPER, BRIAN MORITZ, THOMAS DEVEREAUX, Stanford University and SLAC — Raman spectroscopy, which uses different incoming and outgoing light polarizations to measure different areas of the Brillouin zone, allows researchers to probe the nature of charge and spin density wave gaps. We present calculations of the Raman response for two density wave materials: rare earth tri-tellurides in the charge density wave state and the iron pnictides in the spin density wave state. Both of these materials have phase diagrams which can be further understood by clarifying the nature of the density wave state. For example, in the tri-tellurides, either one or two charge density wave gaps are present depending on the type of rare earth element in the compound. In the pnictides, which we treat with a multiband model, superconductivity coexists with or is in close proximity to a spin density wave state. We discuss what can be learned from our calculations and compare to experimental results.

2:54PM X25.00003 Far-infrared spectroscopy of magnetic-field-induced pairbreaking in superconducting thin films[1] , XIAOXIANG XI, University of Florida, J. HWANG, Pusan National University, C. MARTIN, D.B. TANNER, University of Florida, G.L. CARR, Brookhaven National Laboratory — A magnetic field will break the time-reversal symmetry of the superconducting condensate pairing, giving rise to a pair-breaking effect. This pairbreaking has been confirmed by our recent far-infrared transmission and reflection measurement of a superconducting NbTiN thin film in an in-plane magnetic field. The complex optical conductivity was extracted, and the optical gap was obtained from its real part. Comparison with the pair-breaking theory of Abrikosov and Gor'kov yields good quantitative agreement, confirming directly the theory's validity for the optical conductivity.

[1]Supported by the US DOE through contracts DE-FG02-02ER45984 at UF and DE-AC02-98CH10886 at the NSLS. Access to the high-field magnet is courtesy of J.J. Tu (CCNY).

3:06PM X25.00004 Optical properties of the pseudogap state in deeply underdoped cuprates , ADAM POUND, University of Guelph, JULES CARBOTTE, McMaster University, ELISABETH NICOL, University of Guelph — Recent optical measurements of deeply underdoped cuprates have revealed that a coherent Drude response persists well below the end of the superconducting dome in the phase diagram[1]. We show that this observation is consistent with the resonating valence bond spin-liquid model proposed by Yang, Rice, and Zhang[2]. Within this model, we analyze the three elements that cause the overall reduction in optical conductivity in the approach to the Mott insulating state: a Gutzwiller factor associated with increased correlations, which causes a reduction in the coherent part of the carrier Green's function; a shrinking of the Fermi surface defining the hole Luttinger contours; and an increase in optical effective mass. We show that each of these elements yields qualitative agreement with various experimental observations. Finally, we show how the increased magnitude of the pseudogap at low doping modifies the microwave conductivity and the Wiedemann-Franz law.

[1] W.J. Padilla et al., Phys. Rev. B 72, 060511 (2005)
[2] K.-Y. Yang, T.M. Rice, F.-C. Zhang, Phys. Rev. B 73, 174501 (2006)

3:18PM X25.00005 Point group sensitive probes of the pseudogap electronic structure in Bi2212 , J.P. HINTON, UC Berkeley, LBNL, J.D. KORALEK, LBNL, J. ORENSTEIN, UC Berkeley, LBNL, I. FIRMO, M. HAMIDIAN, K. FUJITA, LASSP Cornell U, CMPMS BNL, J.C. DAVIS, LASSP Cornell U, CMPMS BNL, SUPA U St. Andrews — We combine optical transient grating spectroscopy (TGS) and spectroscopic imaging scanning tunneling microscopy (SI-STM) to study the pseudogap electronic structure in the underdoped cuprate superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$. In TGS a pair of 50 fs pump pulses at 800 nm coincident on the sample surface generate a sinusoidal variation in the index of refraction. This index grating is phase sensitively probed, allowing us to clearly resolve two components in the optical response below Tc. We attribute one of the components to a coherent nonlinear optical process, whose properties are sensitive to the point group symmetry of the pseudogap electronic structure. We compare the results of these optical experiments with recent analysis of SI-STM data (M. J. Lawler *et al* **Nature 466**,347 (2010)) which measures the amplitude of peaks at various reciprocal lattice vectors in the Fourier transform of atomically resolved images of the pseudogap electronic structure. The symmetry properties of the SI-STM Bragg amplitudes provide additional evidence relevant to the point group of the pseudogap electronic structure.

3:30PM X25.00006 Evidence for symmetry breaking in the pseudogap phase of the single-layer Cuprate Pb-Bi2201 , J.D. KORALEK, J. HINTON, J. ORENSTEIN, LBNL/Berkeley, R.-H. HE, M. HASHIMOTO, Z.-X. SHEN, H. KARAPETYAN, A. KAPITULNIK, Stanford/SIMES, H. EISAKI, AIST — We use time-resolved optical spectroscopy, combined with angle resolved photoemission, and polar Kerr effect measurements, to study the single-layer Cuprate superconductor $Pb_{0.55}Bi_{1.5}Sr_{1.6}La_{0.4}CuO_{6+\delta}$ (Pb-Bi2201). Near optimal doping this material has convenient temperature scales with a T_c of 38K and T^* of 130K, allowing signals associated with the superconducting and pseudogap phases to be clearly separated in the raw data. The unusual time dependence of the pseudogap signal is suggestive of a coherent nonlinear optical process which is sensitive to changes in the electronic point group symmetry. This nonlinear signal turns on at T^* and persists to low temperature. Angle resolved photoemission and polar Kerr effect measurements performed on the same batch of samples reveal the opening of a particle-hole asymmetric gap and the onset of Kerr rotation, both with strikingly similar temperature dependence to the nonlinear optical signal.

3:42PM X25.00007 BCS-BEC Crossover Approach to the Optical Conductivity in high T_c Superconductors , DAN WULIN, HAO GUO, James Franck Institute and Department of Physics, University of Chicago, CHIH-CHUN CHIEN, Los Alamos National Laboratory, KATHRYN LEVIN, James Franck Institute and Department of Physics, University of Chicago — We address the finite frequency ω conductivity in the cuprates. We presume that the pseudogap arises from stronger-than-BCS attraction, which leads to non-condensed pairs above and below T_c. Our theoretical formalism, which is consistent with gauge invariance and the transverse f-sum rule, yields a mid infrared peak associated with the energy needed to break pairs. It also leads to a situation in which very high ω spectral weight participates in the formation of the condensate. These observations, along with others reported here are consistent with experiment.

3:54PM X25.00008 Kerr effect measurements in the pseudo-gap regime of LBCO and Pb-BSCO using high resolution Sagnac , HOVNATAN KARAPETYAN, VIKRAM NATHAN, RUIHUA HE, MAKOTO HASHIMOTO, ZHI-XUN SHEN, AHARON KAPITULNIK, Stanford University, HIROSHI EISAKI, Nanoelectronics Research Institute, AIST, Japan, JAKE KORALEK, JAMIE HINTON, JOE ORENSTEIN, Lawrence Berkeley National Laboratory, JOHN TRANQUADA, GENDA GU, MARKUS HUECKER, Brookhaven National Laboratory — Polar Kerr effect in several high-Tc superconductors systems was measured at zero magnetic field with high precision using a cryogenic Sagnac fiber interferometer with zero-area. We observed non-zero Kerr rotations of order $\sim 1\mu$rad appearing near the pseudogap temperature T^*, and marking what appears to be a true phase transition. In this talk we will review our work on $YBa_2Cu_3O_{6+x}$, $La_{1.875}Ba_{0.125}CuO_4$ and $Pb_{0.55}Bi_{1.5}Sr_{1.6}La_{0.4}CuO_{6+\delta}$. In particular, in Pb-BSCO we observe an emergence of Kerr signal that coincides with ARPES data showing an abrupt change at T^* from a relatively simple one- band metal into a state with profoundly-altered electronic structure.

4:06PM X25.00009 DC Transport in Pseudogapped Superconductors: The Role of the Fermi Arcs , HAO GUO, BENJAMIN M. FREGOSO, DAN WULIN, James Franck Institute and Department of Physics, University of Chicago, CHIH-CHUN CHIEN, Los Alamos National Laboratory, KATHRYN LEVIN, James Franck Institute and Department of Physics, University of Chicago — We examine the dc conductivity σ in a d-wave pseudogapped high T_c superconductor for a range of different hole doping concentrations and temperatures T. Our approach is based on treating the cuprates as mid-way between BCS and Bose Einstein condensation and our correlation functions are demonstrably consistent with gauge invariance and the transverse f-sum rule. Studies of the $\omega \to 0$ dc conductivity below T_c lead to a peak structure (observed experimentally) while above T_c we show that pseudogap effects manifest themselves in the resistivity primarily through a depression in the effective carrier number with decreasing T. We discuss related implications for resistivity vs $T > T_c$ experiments and demonstrate that the trends with hole doping are compatible with the data, while the role of the Fermi arcs appears overall to be secondary.

4:18PM X25.00010 Ultrafast transient grating and pump probe measurements in optimally doped $La_{2-x}Sr_xCuO_4$ thin films , DARIUS TORCHINSKY, FAHAD MAHMOOD, DAVID HSIEH, JAMES MCIVER, MIT, A. BOLLINGER, I. BOZOVIC, Brookhaven National Laboratory, NUH GEDIK, MIT — We have performed pump probe and transient grating measurements on high-T_c thin films of optimally doped $La_{2-x}Sr_xCuO_4$. In these experiments, a pair of femtosecond pulses are interfered on the sample generating a sinusoidal intensity modulation that in turn induces a density grating of photoexcitations. The resulting change in reflectivity allows time-resolved optical measurement of the separate effects of recombination and diffusion. We describe the temperature and excitation density dependence of these measurements and discuss their implications on the nature of superconductivity in the cuprates.

4:30PM X25.00011 Ultrafast quasiparticle dynamics of $La_{2-x}Sr_xCuO_4$ probed by time-resolved THz spectroscopy , ALEX FRENZEL, Massachusetts Institute of Technology / Harvard University, DANIEL PILON, Massachusetts Institute of Technology, ANTHONY BOLLINGER, IVAN BOZOVIC, Brookhaven National Laboratory, NUH GEDIK, Massachusetts Institute of Technology — We have studied picosecond quasiparticle recombination dynamics in the superconducting state of the cuprate superconductor $La_{2-x}Sr_xCuO_4$. After excitation by a 1.5 eV optical pulse, the optical conductivity in the range 0.5 - 2 THz is measured at varying time delays using coherent time-domain terahertz spectroscopy. We show that the conventional two-fluid model, which successfully describes the optical conductivity in YBCO, is unable to accurately reproduce our results. At optimal doping, we observe a weak dependence on excitation density in the recovery rate at low fluence. We comment on the recovery rate of the superconducting state in terms of the bimolecular recombination dynamics described by the phenomenological Rothwarf-Taylor model.

4:42PM X25.00012 Optical conductivity in dynamic Hubbard model , GIANG BACH, Department of Physics, University of Alberta, Edmonton, Alberta, Canada, T6G 2J1, JORGE HIRSCH, Department of Physics, University of California, San Diego, La Jolla, California, 92093-0319, FRANK MARSIGLIO, Department of Physics, University of Alberta, Edmonton, Alberta, Canada, T6G 2J1 — The Dynamic Hubbard model is a candidate to capture the physics of two-band Hubbard models, such as the enhancement of critical Hubbard U for the Mott transition. A pseudo-spin $1/2$ auxiliary field, which modifies the Coulomb U interaction based on the on-site occupancy of electrons, breaks the electron-hole symmetry normally associated with the Hubbard model. The dependence of optical conductivity on the number of particles also reveals the effect of the pseudo-spin on the spectral weight distribution as a function of frequency.

4:54PM X25.00013 Optical and DC conductivity in the two-dimensional $t-t'-t''$ Hubbard model near the antiferromagnetic quantum critical point[1] , DOMINIC BERGERON, ANDRÉ-MARIE S. TREMBLAY, Dept. de physique, RQMP, Universite de Sherbrooke — We calculate the conductivity of the two-dimensional Hubbard model with second and third nearest neighbor hoppings t' and t'' for dopings in the vicinity of the antiferromagnetic quantum critical point (QCP) using the two-particle self-consistent approach. This approach is non-perturbative and was benchmarked against quantum Monte Carlo calculations from weak to intermediate coupling. We include vertex corrections that are the analogs of the Maki-Thompson and the Aslamazov-Larkin terms in the theory of paraconductivity, but for antiferromagnetic fluctuations. With these corrections the f-sum rule is satisfied and important effects in DC and optical conductivity are obtained. In the pseudogap regime induced by antiferromagnetic correlations, the resistivity increases with vertex corrections. This effect is stronger on the hole-doped side where the system changes from metallic to insulating. This is opposite to what is observed when $t' = t'' = 0$. On the non-magnetic side of the QCP, the resistivity decreases with vertex corrections.

[1]NSERC (Canada), CRC (A.-M.T.), RQCHP and Compute Canada

5:06PM X25.00014 Exact nonequilibrium model for time-resolved photoemission spectroscopy of an electronic charge density wave insulator at zero temperature , WEN SHEN, JAMES FREERICKS, Georgetown University — We exactly solve the nonequilibrium problem of electrons moving in a lattice potential that corresponds to a checkerboard ordered charge density wave at zero temperature. The exact solution can be found in arbitrary dimensions by calculating a series of two-by-two evolution operators with the Trotter formula. We examine how the charge density wave responds to being excited into nonequilibrium by a large electric field femtosecond pulse. We find that the order parameter is rapidly reduced (but not to zero) and then rings with an oscillation frequency given by the potential scattering energy U. The density of states shows evidence of gap closing for short times, which then reforms for long times. We discuss the implications of the solution of this model for the nonequilibrium melting of charge density waves observed in recent experiments.

Thursday, March 24, 2011 2:30PM - 5:30PM –

Session X26 DMP DCOMP: Focus Session: Iron Based Superconductors – Fe(Se-Te) D162/164

2:30PM X26.00001 Evidence for local moment magnetism in superconducting $FeTe_{0.35}Se_{0.65}$, GUANGYONG XU, ZHIJUN XU, JINSHENG WEN, Brookhaven National Laboratory, SONGXUE CHI, NIST Center for Neutron Research, WEI KU, GENDA GU, JOHN TRANQUADA, Brookhaven National Laboratory — We investigate the temperature evolution (from 5 K to 300 K) of low energy spin fluctuations in Fe-based superconductor $FeTe_{0.35}Se_{0.65}$ ($T_c \sim 14$ K) via inelastic neutron scattering. The magnetic excitation spectrum in the superconducting phase appears qualitatively similar to those observed in other Fe-based superconductors, with a spin gap (at about 5 meV) and a resonance peak at $\hbar\omega \sim 6.5$ meV. At higher temperatures, the spectral weight of the low-temperature resonance is found to redistribute to lower energies below the spin gap. A significant moment ($\gtrsim 0.26\mu_B$/Fe) is found for the integrated spectral weight below merely $\hbar\omega \sim 12$ meV, with nearly no temperature dependence up to 300K, indicating existence of strong local moments.

2:42PM X26.00002 Low-energy magnetic excitations in the parent superconducting phases $Fe_{1+x}Te$ for $x = 0.07 - 0.18$, CHRIS STOCK, EFRAIN RODRIGUEZ, MARK GREEN, NIST Center for Neutron Research — We present inelastic neutron scattering measurements of the phases $Fe_{1+x}Te$ for varying amounts of interstitial iron in the lattice. The x in $Fe_{1+x}Te$ corresponds to interstitial iron located between the two-dimensional FeTe sheets, and the amount of x greatly affects the nature of the crystallographic transition and the magnetic ordering at lower temperatures in this system. The low energy spectrum of the magnetic excitations from 0.5 meV to 10 meV using the Multi-Axis Crystal Spectrometer (MACS) will be presented for both the incommensurate and commensurate phases. Neutron polarized diffraction experiments that detail the nature of the magnetic ordering will also be presented.

2:54PM X26.00003 Neutron Scattering Study of the Dependence of Magnetic Correlations on Se and Fe Content in the Fe(Te,Se) System , ZHIJUN XU, JINSHENG WEN, GUANGYONG XU, GENDA GU, JOHN TRANQUADA, Brookhaven National Laboratory — We have performed a series of neutron scattering and magnetization measurements on $Fe_{1+y}Te_{1-x}Se_x$ with different Fe and Se compositions to study the interplay between magnetism and superconductivity.[1] FeTeSe is rather unique for possessing two different types of spin configurations: one is a "bicollinear" or "E-type" structure that corresponds to the static order near (0.5,0), and the other is a "collinear" or "C-type" spin configuration that gives rise to spin excitations near (0.5,0.5). [2] Short-range static magnetic order near the (0.5,0) in-plane wave-vector (using the two-Fe unit cell) is found in all non-superconducting samples. The static order disappears and bulk superconductivity emerges, as the spectral weight of the magnetic excitations shift to the region of reciprocal space near the in-plane wave-vector (0.5,0.5) with Se doping. Besides Se doping, Fe also plays an essential role in superconductivity and the magnetic correlations. Our results suggest that spin fluctuations associated with the collinear magnetic structure appear to be universal in all Fe-based superconductors, and there is a strong correlation between superconductivity and the character of the magnetic order/fluctuations in this system. [1] Zhijun Xu *et al.*, Phys. Rev. **B** 82, 104525 (2010) [2] Wei-Guo Yin *et al.*, Phys. Rev. Lett. 105, 107004 (2010)

3:06PM X26.00004 Spin Excitations in Fe(Se,Te)[1] , MARK LUMSDEN, Oak Ridge National Laboratory — The full spectrum of magnetic excitations in both superconducting $FeTe_{0.51}Se_{0.49}$ (x=0.49) and non- superconducting $Fe_{1.04}Te_{0.73}Se_{0.27}$ (x=0.27) was studied using inelastic neutron scattering on single crystal samples. The magnetic excitations are two-dimensional in nature and are observed for energy transfers as high as 300 meV. The zero energy extrapolation of the measured dispersion shows incommensurate excitations emanating from a wavevector near (0.5,0.5), the location of the resonance in the superconducting material. For low energy transfers, the spectrum consists of a set of incommensurate spots, four-fold symmetric about the (1,0) (square lattice (π,π)) wavevector. At higher energies, these spots evolve into rings centered on Q=(1,0). These excitations are notably different than the cones of scattering expected from a long-range magnetically ordered material and likely reflect the itinerant nature of the magnetism. The qualitative evolution of the incommensurate excitation spectrum is similar that seen previously in the cuprates. Despite the incommensurate nature of the spectrum, the observed resonance in the x=0.49 sample remains peaked at the (0.5,0.5) wavevector as in other Fe-based superconductors. At low energies, the x=0.27 sample exhibits an additional feature in the excitation spectrum centered near Q=(0.5,0), the wavevector of magnetic order in $Fe_{1+y}Te$. This scattering persists for all energies below about 10 meV and forms the short range order observed for this concentration. This scattering is completely absent in the x=0.49 sample which contains no excess Fe.

[1]work supported by the Scientific User Facilities Division, Office of Basic Energy Sciences, DOE

3:42PM X26.00005 Chemical tuning of magnetism and superconductivity in Fe_{1+x}(Te,Se) , EFRAIN E. RODRIGUEZ, CHRIS STOCK, NIST Center for Neutron Research, NICHOLAS P. BUTCH, JOHNPIERRE PAGLIONE, Center for Nanophysics and Advanced Materials, U. of Maryland, MARK GREEN, NIST Center for Neutron Research — We present evidence demonstrating how the magnetism and superconductivity can be tuned for the phases $Fe_{1+x}Te$ and $Fe_{1+x}Te_{1+y}Se_{1+y}$. Through the use of iodine vapor as an oxidant, we can de-intercalate these materials to remove the interstitial iron, *i.e* the x in Fe_{1+x}(Te,Se). Our analysis of the neutron inelastic scattering indicates that paramagnetism from this interstitial iron is detrimental to superconducting properties, and magnetization measurements show that superconducting volume fraction is indeed increased as the amount of interstitial iron is removed. Diffraction results detailing changes in key structural parameters and magnetic ordering will also be presented.

3:54PM X26.00006 Local lattice dynamic correlation in $FeSe_xTe_{1-x}$, KEESEONG PARK, DESPINA LOUCA, University of Virginia, Charlottesville, Virginia 22904, USA., JON TAYLOR, ISIS Spallation Neutron Source, Rutherford Appleton Laboratory, Chilton, Didcot OX110QX, UK., JIAQIANG YAN, Division of Materials Science and Engineering, Ames Laboratory, Ames, IA 50011, USA. — With the use of inelastic neutron scattering, the local lattice dynamics were determined for the new Fe-based superconductors, $FeSe_xTe_{1-x}$ with x=0.1, 0.5 and 0.9. The nature of the dynamic pair correlations was characterized above and below the phase transitions. In the x=0.1 sample that is not superconducting(SC), the nearest Fe-Te and Fe-Fe pair correlations gradually disappear with increasing energy by 35 meV. The same energy dependence is observed above and below the magnetic transition. This energy corresponds to the cut-off frequency of the phonon vibrational modes. On the other hand, in the SC x=0.5 and 0.9, the Fe-Fe correlations gain weight just above the elastic, only to be quickly suppressed by 15 meV. This effect is stronger below the transition than above. The Fe-Te correlations that overlap with the Fe-Fe bonds persist in x=0.5 (possibly in x=0.9 as well but are too weak). On the other hand, the Fe-Se correlations persist beyond this energy, and eventually disappear by 30 meV. These differences in the local lattice dynamics between the non-SC and SC might provide a clue towards understanding the phonon contribution to the mechanism of superconductivity in this system.

4:06PM X26.00007 Magnetic field dependence of spin fluctuations in superconducting FeSe0.4Te0.6[1] , V. THAMPY, Institute of Quantum Matter, Dept. of Physics, Johns Hopkins Univ, Y. ZHAO, NIST Center for Neutron Reseach, W. BAO, Dept. of Physics, Renmin Univ. of China, Z. MAO, Dept. of Physics, Tulane Univ., J. RODRIGUEZ, NIST Center for Neutron Reseach, D. ARGYRIOU, Helmholtz-Zentrum Berlin für Materialen und Energy, Germany, A. SAVICI, G. GRANROTH, Oak Ridge National Lab, A. HIESS, Institut Max von Laue-Paul Langevin, France, C. BROHOLM, Institute of Quantum Matter, Dept. of Physics, Johns Hopkins Univ — Spin fluctuations may play a key role in metals where superconductivity appears as a magnetic phase is suppressed under pressure or with chemical substitution. The suppressed magnetism is manifested as a gap in the spin fluctuation spectrum and a spin resonance to which the spectral weight is shifted. We have studied the effect of high magnetic fields on this resonance. While fine structure is observed, these features do not shift with field and persist in zero field and in the normal state. Temperature difference spectra are however, significantly broadened in high fields.

[1]Work at JHU supported by DoE through DE-FG02-08ER46544.

4:18PM X26.00008 Neutron study of spin fluctuations in iron chalcogenide , SONGXUE CHI, Oak Ridge National Lab, TANER YILDIRIM, JEFFREY LYNN, NIST Center for Neutron Research, CHENGLIN ZHANG, University of Tennessee, Knoxville, JOSE RODRIGUES, NIST Center for Neutron Research, PENGCHENG DAI, University of Tennessee, Knoxville, DANIEL PHELAN, DEEPAK SINGH, RICK PAUL, NIST Center for Neutron Research — The incommensurate spin excitations in the nonsuperconducting $FeTe_{0.72}Se_{0.28}$ have been studied using both cold and thermal neutron spectroscopy. At low energies spectrum weight shifts from (1/2,0) commensurate excitations to the incommensurate quartets about the (1,0) point, which disperse outward before the inward dispersion at higher energies. The steep dispersion is disturbed in the energy range between 20 meV and 32 meV, resulting in abnormal excitations that are also observed in the superconducting $FeTe_{0.62}Se_{0.38}$. Polarized neutron measurements were carried out and the origin of these abnormal excitations is discussed.

4:30PM X26.00009 ARPES study of FeTe single crystal and $FeTeO_x$ films[1] , YUEFENG NIE, Department of Physics, University of Connecticut, Storrs, CT 06269, MARTIN MANSSON[2], YASMINE SASSA, CHRISTOF NIEDERMAYER, Laboratory for Neutron Scattering, ETH Zäurich and Paul Scherrer Institute, PSI, Switzerland, GENDA GU, Condensed Matter Physics and Materials Science, Brookhaven National Laboratory (BNL), Upton, NY 11973, JOSEPH BUDNICK, BARRETT WELLS, Department of Physics, University of Connecticut, Storrs, CT 06269 — We have performed an ARPES investigation of FeTe single crystals, films, as well as the novel superconducting film FeTeOx. Our results from the single crystals reflect the previously reported Fermi surface pocket around the X-point [(π,0)], possibly connected to a spin-density wave (SDW) order [Y. Xia, PRL 103, 037002 (2009)] . Unlike this previous report, our results also reveal the presence of an energy gap which would be expected from the SDW order. The temperature dependence shows that the gap closes in the rough vicinity of the magnetic transition temperature, supporting it's interpretation as reflecting the SDW state. We were able to produce an ARPES quality surface by cleaving films of FeTe and $FeTeO_x$, with the FeTe films showing similar features as the bulk.

[1]Funded by the DOE-BES through contract # DE-FG02-00ER45801.

[2]2nd affiliation: LSNS, EPFL, Lausanne, Switzerland

4:42PM X26.00010 ARPES Study of the Phase Diagram of $Fe_{1+y}Te_{1-x}Se_x$, ZHONGKAI LIU, MING YI, Stanford University, YULIN CHEN, SLAC National Laboratory, RUIHUA HE, Stanford University, DONGHUI LU, ROB MOORE, SLAC National Laboratory, JIN HU, TIJIANG LIU, ZHIQIANG MAO, Tulane University, ZHI-XUN SHEN, Stanford University, STANFORD UNIVERSITY TEAM, SLAC NATIONAL LABORATORY COLLABORATION, TULANE UNIVERSITY COLLABORATION — Iron chalcogenide $Fe_{1+y}Te_{1-x}Se_x$ is a unique member among the iron-based superconductor family due to its simplicity in structure and richness in physics. The end member $Fe_{1+y}Te$ has an antiferromagnetic order with Neel temperature $\sim$72K. Substitution of Se for Te suppresses this long-range magnetic order and enters a "spin-glass" phase where (π,0) short-range magnetic order contributes to weak charge carrier localization. Superconductivity emerges by further substitution of Se and suppression of the short-range magnetic order. Here we present ARPES study on this system, providing evidence of the underlying physics in the phase diagram by analyzing electronic structure information. The comparison of iron chalcogenide and other iron-based systems help us identify the governing physics in this new family of superconductors.

4:54PM X26.00011 ARPES studies on $FeTe_{1-x}Se_x$ iron chalcogenides epitaxial thin films , DAVIDE INNOCENTI, Advanced Light Source and University of Rome "Tor Vergata", LUCA MORESCHINI, ALS, YOUNG JUN CHANG, ANDREW WALTER, ALS and Fritz-Haber-Institut, AARON BOSTWICK, ALS, DANIELE DI CASTRO, ANTONELLO TEBANO, PIER GIANNI MEDAGLIA, University of Rome "Tor Vergata", EMILIO BELLINGERI, ILARIA PALLECCHI, CARLO FERDEGHINI, CNR-SPIN Genova, GIUSEPPE BALESTRINO, University of Rome "Tor Vergata", ELI ROTENBERG, ALS — The physics of iron-based chalcogenides raises fundamental questions on the interplay of magnetic order and electron pairing at the origin of the superconducting state. We have performed angle-resolved photemission spectroscopy (ARPES) studies on high-quality epitaxial thin films of $FeTe_{1-x}Se_x$, grown by *in situ* pulsed laser deposition (PLD) on beamline 7.0.1 at the ALS. Specifically, we are able to show the evolution of the band structure as a function of x. We discuss our experimental results in comparison to the available theoretical band calculations.

5:06PM X26.00012 ARPES Studies on $FeTe_{1-x}Se_x$[1] , HONGBO YANG, ZHIHUI PAN, GENDA GU, PETER JOHNSON, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, MICHAEL WEINERT, Department of Physics, University of Wisconsin - Milwaukee — Angle-resolved Photoelctron Spectoscopy (ARPES) is used to study the electronic structure of Fe based superconductor, $FeTe_{1-x}Se_x$. Detailed comparisons are made between the measured Fermi surfaces and first principles FLAPW calculations. In particular we explore the origin of a Dirac like cone at the center of the Brillouin zone.

[1]The work at Brookhaven is supported by the Department of Energy, that at the University of Wisconsin - Milwaukee by the National Science Foundation.

5:18PM X26.00013 ABSTRACT WITHDRAWN –

Thursday, March 24, 2011 2:30PM - 5:30PM –

Session X27 GQI: Quantum Computing and Simulation II C155

2:30PM X27.00001 Analysis of quantum Monte Carlo dynamics for quantum adiabatic evolution in infinite-range spin systems[1] , JUN-ICHI INOUE, Hokkaido University — We analytically derive deterministic equations of order parameters such as spontaneous magnetization in infinite-range quantum spin systems obeying quantum Monte Carlo dynamics. By means of the Trotter decomposition, we consider the transition probability of Glauber-type dynamics of microscopic states for the corresponding classical system. Under the static approximation, differential equations with respect to macroscopic order parameters are explicitly obtained from the master equation that describes the microscopic-law. We discuss several possible applications of our approach to disordered spin systems for statistical-mechanical informatics. Especially, we argue the ground state searching for infinite-range random spin systems via quantum adiabatic evolution.

[1]We were financially supported by Grant-in-Aid for Scientific Research (C) of Japan Society for the Promotion of Science, No. 22500195.

2:42PM X27.00002 Ramsey numbers and adiabatic quantum computing , FRANK GAITAN, Laboratory for Physical Sciences, LANE CLARK, Southern Illinois University — The graph-theoretic Ramsey numbers are notoriously difficult to calculate. In fact, only nine Ramsey numbers are currently known, with knowledge of other Ramsey numbers limited to bounds on their possible value. We describe a quantum algorithm for the computation of Ramsey numbers. We show how the problem of computing a Ramsey number can be mapped to a combinatorial optimization problem whose solution can be found using adiabatic quantum evolution (AQE). We numerically simulate this adiabatic quantum algorithm and show that it correctly determines the Ramsey numbers R(3,3) and R(2,s) for s $\leq$ 6. We also discuss experimental implementation of an adiabatic quantum computation of R(3,3).

2:54PM X27.00003 Two-particle quantum walks applied to the graph isomorphism problem[1] , JOHN KING GAMBLE, MARK FRIESEN, DONG ZHOU, ROBERT JOYNT, S.N. COPPERSMITH, University of Wisconsin-Madison — We show that an algorithm based on the dynamics of interacting quantum particles is more powerful than the corresponding algorithm for non-interacting particles. Specifically, our algorithm attempts to determine whether two graphs are isomorphic. We focus on strongly regular graphs (SRGs), a class of graphs with particularly high symmetry. By studying the dynamical evolution of two-particle quantum walks on pairs of non-isomorphic SRG's, we show that interacting particles can distinguish non-isomorphic graphs that noninteracting particles cannot. First, we prove that quantum walks of two noninteracting particles cannot distinguish pairs of non-isomorphic SRG's. Next, we demonstrate numerically that two interacting bosons are more powerful, in that their quantum walks distinguish all non-isomorphic pairs of SRGs we tried, including those with up to 64 vertices. Finally, we find a set of operators that determine these evolutions.

[1]This work was supported in part by ARO and DOD (W911NF-09-1-0439). J.K.G. acknowledges support from the NSF.

3:06PM X27.00004 Quantum Walks on Trees with Disorder , STEVEN JACKSON[1], TENG JIAN KHOO[2], FREDERICK STRAUCH, Williams College — Quantum walks on trees have the potential for exponential speedup compared to classical algorithms. It has been argued that disorder may limit this potential, due to Anderson localization. We report on an extensive numerical analysis of quantum walks with disorder and find evidence of a localization transition for large disorder, but a quantum-to-classical transition for intermediate disorder. These results suggest that quantum walks may yet retain their speedup for high-dimensional graphs with weak disorder.

[1](now at Princeton University)
[2](now at Cambridge University)

3:18PM X27.00005 Numerical investigations of quantum walks with hard-core bosons and the graph isomorphism problem[1] , MARK WELLONS, JOHN GAMBLE, ERIC BACH, MARK FRIESEN, ROBERT JOYNT, KENNETH RUDINGER, DONG ZHOU, SUSAN COPPERSMITH, University of Wisconsin-Madison — Gamble et al. investigated quantum walks of two hard-core bosons on a class of highly symmetric graphs called strongly regular graphs (SRGs) and showed that these walks will distinguish nonisomorphic graphs from the same family. However, J. Smith (arXiv:1004.0206) has shown that pairs of nonisomorphic graphs exist that cannot be distinguished by such quantum walks. Here we construct explicit counterexample graph pairs for 2 and 3-particle interacting and non-interacting walks. We also describe an algorithm that, given k particles, generates two graphs indistinguishable by a k-boson quantum walk. We find that these indistinguishable graph pairs generated by our algorithm scale in size quadratically with the number of particles. It follows that distinguishing graphs via simulating quantum walks with classical computers will likely require exponential time in the size of the graph, while leaving open the possibility that a quantum computer could distinguish the graphs in polynomial time.

[1]This work was supported by ARO and DOD (W911NF-09-1-0439) and NSF (CCF-0635355). J.K.G. acknowledges support from the NSF.

3:30PM X27.00006 Simulating Quantum Dynamics On A Quantum Computer , NATHAN WIEBE, University of Calgary, DOMINIC BERRY, IQC, PETER HOYER, BARRY SANDERS, University of Calgary — We develop an efficient quantum algorithm for simulating time-dependent Hamiltonian evolution of general input states on a quantum computer. Given conditions on the smoothness of the Hamiltonian, the complexity of the algorithm is close to linear in the evolution time, and therefore is comparable to algorithms for time-independent Hamiltonians. In addition, we show how the complexity can be reduced by optimizing the time steps. The complexity of the algorithm is quantified by calls to an oracle, which yields information about the Hamiltonian, and accounts for all computational resources. In contrast to previous work, which allowed an oracle query to yield an arbitrary number of bits or qubits, we assign a cost for each bit or qubit accessed. This per-bit or per-qubit costing of oracle calls reveals hitherto unnoticed simulation costs. We also account for discretization errors in the time and the representation of the Hamiltonian. We generalize the requirement of sparse Hamiltonians to being a sum of sparse Hamiltonians in various bases for which the transformation to a sparse Hamiltonian may be performed efficiently.

3:42PM X27.00007 Preparing Ground States of Many-Body Systems by Simulated Cooling , DVIR KAFRI, University of Maryland, College Park, Department of Physics, JACOB TAYLOR, University of Maryland, College Park, Department of Physics; National Institute of Standards and Technology, Gaithersburg, MD — Computational problems, such as satisfiability, can be rephrased in terms of the preparation of the ground state of a many-body Hamiltonian. More generally, a quantum simulator could provide information on many-body systems if the ground state can be appropriately prepared. Adiabatic preparation is a common technique for obtaining the ground state of a quantum mechanical system, by slowly varying the system Hamiltonian. A principle disadvantage is that its timing scales with the gap energy of the intermediate Hamiltonian, for which a gap may not be promised, rather than the final Hamiltonian which may be known to be gapped. We present an alternative approach, in which an arbitrary system of qubits is cooled to an effective many-body ground state, through the algorithmic interaction with a small number of "bath" qubits. We specify bounds for the parameters of the algorithm, show that cooling time scales with the system's gap, and present simulated results on a frustrated few-spin system. We further discuss possible experimental applications.

3:54PM X27.00008 An Open-System Quantum Simulator with Trapped Ions , JULIO T. BARREIRO, MARKUS MUELLER, PHILIPP SCHINDLER, DANIEL NIGG, THOMAS MONZ, MICHAEL CHWALLA, MARKUS HENNRICH, CHRISTIAN F. ROOS, PETER ZOLLER, Universitaet Innsbruck, RAINER BLATT — The control of quantum systems is of fundamental scientific interest and promises powerful applications and technologies. Impressive progress has been achieved in isolating the systems from the environment and coherently controlling their dynamics, as demonstrated by the creation and manipulation of entanglement in various physical systems. However, for open quantum systems, engineering the dynamics of many particles by a controlled coupling to an environment remains largely unexplored. Here we report the first realization of a toolbox for simulating an open quantum system with up to five qubits. Using a quantum computing architecture with trapped ions, we combine multi-qubit gates with optical pumping to implement coherent operations and dissipative processes. We illustrate this engineering by the dissipative preparation of entangled states, the simulation of coherent many-body spin interactions and the quantum non-demolition measurement of multi-qubit observables. By adding controlled dissipation to coherent operations, this work offers novel prospects for open-system quantum simulation and computation.

4:06PM X27.00009 Discrete quantum walk on a binary tree , ZLATKO DIMCOVIC, IAN MILLIGAN, DAN ROCKWELL, ROBERT M. BURTON, THINH NGUYEN, YEVGENIY KOVCHEGOV, Oregon State University — We have recently constructed a framework for quantum walks, based on classical walks with memory. This framework reproduces known walks, while it can be used to build walks in systems that are difficult for current approaches. As our first example of its utility, we study a symmetric discrete quantum walk on the infinite binary tree. For a walk starting from a pure state at a given level in the tree, we compute the amplitude at the root, as a function of time and starting level. The result is strikingly different from the classical case, as its amplitude spans an order of magnitude, with a power law tail, while the classical one decays exponentially. (For example, for a delayed walk this property yields a polynomial vs. exponential speed up over the classical walk, in delay time.) The breadth of the probability peak indicates that any restriction of the extent of the tree, such as a matching tree, sinks or boundaries, would likely yield algorithms superior to classical. The calculation utilizes a variety of analytical techniques (memoried stochastic processes, combinatorics and path counting, transforms, steepest descent, orthogonal polynomials). This study also brings up interesting general questions about quantum processes on such structures.

4:18PM X27.00010 Quantum Random Walks of Non-Interacting Bosons on Strongly Regular Graphs[1] , KENNETH RUDINGER, JOHN KING GAMBLE, MARK WELLONS, MARK FRIESEN, DONG ZHOU, ERIC BACH, ROBERT JOYNT, S.N. COPPERSMITH, University of Wisconsin- Madison — We investigate the quantum dynamics of particles on graphs ("quantum walks"), with the aim of developing quantum algorithms for determining if two graphs are isomorphic and show that there are fundamental differences between the distinguishing power of two-particle and three-particle non-interacting quantum walks. We investigate quantum walks on strongly regular graphs (SRGs), a class of graphs with high symmetry. We show analytically that the two-particle walk always fails to distinguish non-isomorphic members of the same SRG family. We show numerically that the three-boson walk is able to distinguish 99.6% of 70,712 SRG comparisons made and that this distinguishing power comes from different multiplicities of certain graph substructures in non-isomorphic graphs. We identify certain distinguishing substructures and examine ones that appear in the four-boson walk, discovering they are able to distinguish almost all of the graphs that the three-boson walk failed on. This indicates a positive correlation between number of bosons in the walk and distinguishing power.

[1]This work was supported by ARO and DOD (W911NF-09-1-0439) and NSF (CCF-0635355). J.K.G. acknowledges support from the NSF.

4:30PM X27.00011 Real-time Simulations of Quantum Spin $\frac{1}{2}$ Particles Coupled to Multiple Spin Baths , MARTA L. GUERRA, M.A. NOVOTNY, Mississippi State University, HANS DE RAEDT, University Groningen — We present simulations in real time for one and two spin $\frac{1}{2}$ particles coupled to one or more baths of $\frac{1}{2}$-integer quantum spins. The simulations were performed using the algorithm and code of Prof. De Raedt [1,2]. We first simulated one spin coupled to one or two spin-baths with no interactions between the bath spins, as has been calculated theoretically [3]. We find in agreement with [3], that the quantum purity $\mathcal{P}(t)$ decays in both cases, exponentially for a single bath and algebraically for two baths. We extend these simulations by introducing random interactions between the bath spins in an attempt to reach the asymptotic decay rate at earlier times and for fewer spins in the baths. We also have performed similar studies for two spin $\frac{1}{2}$ quantum particles coupled to one, two, or more spin baths. The time- dependent quantum density matrix and $\mathcal{P}(t)$, as well as other quantities, are calculated in these simulations.
[1] V.V. Dobrovitski and H.A. De Raedt, Phys. Rev. E **67** 056702 (2003).
[2] S. Yuan, M.I. Katsnelson, and H. De Raedt, Phys. Rev. A **75** 052109 (2007).
[3] D.D. B. Rao, H. Kohler and F. Sols, New J. Physicis **10** 115017 (2008).

4:42PM X27.00012 Effects of Decoherence in Quantum Simulations , NAYELI ZUNIGA-HANSEN, MARK S. BYRD, YU-CHIEH CHI — We investigate the effects of decoherence in quantum simulations by observing the evolution of the system when the Quantum Information Processor is coupled to the environment. We simulate the noise as the interactions between the particles of the processor itself and observe the effects of varying the strength of the couplings. We perform these calculations for different quantum systems and compare the results of those that interact with the environment to the same system when it's completely isolated from it to observe the effects of the noise on the simulation and investigate ways to prevent the adverse effects of the noise.

4:54PM X27.00013 Computational codes for simulating the Schrödinger equation and the Master equation[1] , NAGENDRA DHAKAL, MICHAEL LEUENBERGER, University of Central Florida — We developed new codes for simulating the Schrödinger equation. We compared the codes with the FDTD codes and codes based on Quantum Monte Carlo method in 1, 2 and 3 dimensions. In addition, we simulated the Master equation for the purpose of studying the spatial and time evolution of the decoherence. Our main focus is to investigate the scalability of the codes and we found the Quantum Monte Carlo method is the most suitable for the simulation of the Master equation because it reduces the dimension of the problem to the dimension of Hilbert space, with the benefits of speeding up the process of calculation and at the same time reducing the memory. Our results are important for the implementation of quantum computing, quantum communication, and spintronics.

[1]We acknowledge support from NSF Grant No. ECCS-0901784 and AFOSR Grant No. FA9550-09-1-0450.

5:06PM X27.00014 Experimental photonic quantum simulation of frustrated Heisenberg spins , PHILIP WALTHER, University of Vienna, XIAO-SONG MA, Austrian Academy of Sciences, BORIVOJE DAKIC, University of VIenna, WILLIAM NAYLOR, ANTON ZEILINGER, Austrian Academy of Sciences — Quantum simulators are controllable quantum systems that can reproduce the dynamics of the system of interest, which are typically unfeasible for classical computers. The recent developments of quantum technology enable the precise control of individual quantum particles as required for studying complex quantum systems. In particular, quantum simulators capable of simulating frustrated Heisenberg spin systems provide a platform for understanding exotic matter such as high-temperature superconductors. Here we report the analog quantum simulation of arbitrary Heisenberg-type interactions among four spin-1/2 particles. This spin-1/2 tetramer is the two-dimensional archetype system whose ground state belongs to the class of valence-bond states. Depending on the interaction strength, frustration within the system emerges such that the ground state evolves from a localized to a resonating valence-bond state. This spin-1/2 tetramer is created using the polarization states of four photons. The precise single-particle addressability and a tunable measurement-induced interaction allows us to obtain fundamental insights into entanglement dynamics among individual particles by observing the frustration of entanglement, governed by quantum monogamy.

5:18PM X27.00015 A realistic topological quantum computation platform using hole-doped semiconductor nanowires and s-wave superconductors , MING GONG, LI MAO, Department of Physics and Astronomy, Washington State University, Pullman, Washington, 99164 USA, SUMANTA TEWARI, Department of Physics and Astronomy, Clemson University, Clemson, South Carolina, 29634, USA, CHUANWEI ZHANG, Department of Physics and Astronomy, Washington State University, Pullman, Washington, 99164 USA, ZHANG TEAM, TEWARI TEAM — We show that two majorana fermions exist at the two ends of a hole-doped semiconductor nanowire that is in proximity contact with an s-wave superconductor. The required experimental parameters (carrier density, g-factor, spin-orbit coupling effect, magnetic field, etc.) for the observation of the Majorana fermions are within the experimentally reachable regime of InSb and InAs nanowires and the mini gap that provides the topological protection for the Majorana zero energy states is of the order of the s-wave superconducting gap. The Majorana zero energy states can be observed through the zero bias peak in the STM signal. The Josephson effects between two nanowire are studied. The proposed model provides a realistic experimental platform for observing non-Abelian statistics and performing topological quantum computation. This work is supported by DARP-MTO (FA955-10-1-0497), and DARPA-YFA (N66001-10-1-4025).

Thursday, March 24, 2011 2:30PM - 5:30PM –

Session X28 DCMP: Carbon Nanotubes and Related Materials: Theoretical and Computational Studies C156

2:30PM X28.00001 Electron-phonon renormalization of the electronic structure of diamond , FELICIANO GIUSTINO, Department of Materials, University of Oxford, STEVEN G. LOUIE, MARVIN L. COHEN, University of California at Berkeley and Lawrence Berkeley National Laboratory — The calculation of band structures from first-principles has reached a high level of accuracy. Calculations combining density-functional theory with many-body perturbation theory often are in good agreement with measurements by photoemission, tunneling, and other spectroscopic probes. While significant efforts have been devoted to improving the description of electron-electron interactions in these calculations, the effect of lattice vibrations has largely been overlooked so far. In this work we study from first principles the electron-phonon renormalization of the band gap of diamond. The calculated temperature dependence of the gap and the broadening of the absorption edge are in excellent agreement with spectroscopic ellipsometry data. Interestingly we find a gap renormalization due to zero-point vibrations as large as 0.6 eV. We discuss the implications of our findings for the electronic structure of other carbon-based bulk materials and nanostructures.

2:42PM X28.00002 Intrinsic Twisting and Electronic Properties of Carbon Nanotubes : A First-Principles Study , KOICHIRO KATO, TAKASHI KORETSUNE, SUSUMU SAITO, Department of Physics, Tokyo Institute of Technology — We report the energetics and electronic structures of twisted single-walled CNTs in the framework of the density functional theory (DFT) with the local density approximation. As for very thin CNTs, we use conventional plane-wave DFT computational code. In order to utilize the periodic boundary condition implemented in the plane-wave DFT code, we study CNTs under several discretized twisting conditions. On the other hand, in the case of thicker nanotubes including experimentally abundant nanotube sizes, we use a real-space DFT computational code which can deal with twisted CNTs with only two atoms per "helical" unit cell. As a result, it is found that chiral CNTs become more stable in slightly twisted geometry. Our results suggest that chiral nanotubes would possess the intrinsic twisting. We also report the twisting-level dependence of the electronic structures. It is found that the fundamental gaps of most kinds of CNTs sensitively depend on twisting level. Importantly, the directions of the intrinsic twisting are the same as the directions of enlarging the fundamental gap except for very thin CNTs.

2:54PM X28.00003 Excitonic Hierarchies in Gapped Carbon Nanotubes , ROBERT KONIK, Brookhaven National Lab — We present evidence that the strong electron-electron interactions in gapped carbon nanotubes lead to a hierarchy of excitons within a given nanotube subband. We study these hierarchies by employing a field theoretic reduction of the gapped carbon nanotube permitting electron-electron interactions to be treated exactly. We analyze this reduction by employing a Wilsonian-like numerical renormalization group. We are so able to determine the gap ratios of the one-photon excitons as a function of the effective strength of interactions. We also determine within the same subband the gaps of the two-photon excitons, the single particle gaps, as well as a subset of the dark excitons. The strong electron-electron interactions in addition lead to strongly renormalized dispersion relations where the consequences of spin-charge separation can be readily observed.

3:06PM X28.00004 Biexcitonic Non-Linearities in Semiconducting Carbon Nanotubes[1] , TOROS TOROSYAN, IGOR BONDAREV, North Carolina Central University — We obtained an analytical expression for the biexciton binding energy as a function of the inter-exciton distance and binding energy of constituent quasi-one-dimensional excitons in single-wall semiconducting carbon nanotubes. This allows one to trace biexciton energy variation and relevant non-linear absorption under external conditions whereby the exciton binding energy varies. In particular, we show the biexciton-plasmon coupling tunability by means of the quantum confined Stark effect, both for the ground-ground state and for the ground-excited state biexcitonic configurations. The non-linear absorption lineshapes calculated exhibit characteristic asymmetric Rabi splitting as the exciton energy is tuned to the nearest interband plasmon resonance. These results are useful for tunable optoelectronic device applications of optically excited semiconducting carbon nanotubes, including the strong excitation regime with optical non-linearities.

[1]NSF (ECCS-1045661, HRD-0833184), NASA (NNX09AV07A), and ARO (W911NF-10-1-0105) support acknowledged.

3:18PM X28.00005 Spin manipulation in carbon nanotubes: All electrical spin filtering through spin-orbit interactions[1] , G. S. DINIZ, Ohio University, Athens-OH - USA, A. LATGÉ, Instituto de Fisica, Universidade Federal Fluminense, Niteroi - Brazil, S. E. ULLOA, Ohio University, Athens-OH - USA — Carbon nanotubes (CNTs) are known to exhibit interesting physical properties, such as metallic or insulating behavior for different chiral vectors. Application of external electric fields and the presence of spin-orbit interaction (SOI) result in modification of the energy level structure of CNTs and their conductance profiles. SOI couples spin and orbital degrees of freedom in these nanostructures, and we explore this effect in this work. We present calculations of the electronic transport of different single-wall CNTs in the presence of SOI. Our calculation uses a single-orbital tight-binding Hamiltonian representation and the equilibrium surface Green's function formalism [1] to calculate electronic transport. We consider the effects of both Rashba and intrinsic SOIs. Our results show possible implementations of carbon nanotubes as spin filtering devices for spatially asymmetric electric fields. We further discuss the spin polarization for different CNT size, chirality, field strength, and the spatially varying fields induced by the adsorption of DNA on their surface.
[1] M. B. Nardelli, Phys. Rev. B **60**, 7828 (1999).

[1]Supported by NSF and CAPES/Fulbright

3:30PM X28.00006 Substantial reduction of thermal conductivity of defected carbon nanotubes , CEM SEVIK, Artie McFerrin Dept of Chemical Engineering, Laboratory of Computational Engineering of Nanomaterials Texas A&M University, College Station, TX , HALDUN SEVINCLI, Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany, JUSTIN B. HASKIN, ALPER KINACI, Artie McFerrin Dept of Chemical Engineering, Laboratory of Computational Engineering of Nanomaterials Texas A&M University, College Station, TX , GIANAURELIO CUNIBERTI, Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany, TAHIR CAGIN, Artie McFerrin Dept of Chemical Engineering, Laboratory of Computational Engineering of Nanomaterials Texas A&M University, College Station, TX , TEXAS A&M UNIVERSITY TEAM, DRESDEN UNIVERSITY OF TECHNOLOGY TEAM — The influence of the structural details and defects on the thermal transport properties of carbon nanotubes (CNTs) are explored by molecular dynamics and real-space Kubo methodologies. A variety of randomly oriented and distributed defects, (mono- and di-vacancies, Stone Wales defects) on lattice thermal conductivity and anharmonic phonon mean free paths are studied for model systems in sizes up to 1000 nm. Substantial reduction in thermal conductivity, up to $\sim$80% reduction compared to the pristine CNTs, is observed for $\sim$0.5\% defect concentrations. Additionally, nearly the same saturation value of lattice thermal conductivity for CNTs with different type of defects is predicted.

3:42PM X28.00007 All About Chlorinated Carbon Nanotubes[1] , DOGAN ERBAHAR, SAVAS BERBER, Gebze Institute of Technology — The halogens are viable alternatives to harsher chemicals in the post-process of purification of carbon nanotube production. However the chlorine is known to bind less agresively to carbon nanotubes than fluorine and hydrogen. Therefore, in principle the residual Cl left after the halogen gas treatment of the nanotubes can be removed without damaging the nanotube walls easier. We report ab initio density functional calculation results about pure and defective carbon nanotubes of various diameters interacting with single and multiple chlorine atoms. We first focus on pure nanotubes and investigate the adsorption of additional Cl atoms near the first adsorbtion site, investigate the clustering tendency and most favourable configurations. We report the energetics results as well as the alteration of electronic properties. We then focus on monovacancy and divacancy defects on carbon nanotubes. It is a known fact that the defective site to be more active in this case. We apply the same procedure as in the pure nanotubes but also investigate the effect of chlorination on reconstruction process and also electronic transport properties.

[1]Supported by TUBITAK Grant No 108T740

3:54PM X28.00008 The origins of nanotube chirality: Is the edge-catalyst in control? , EVGENI PENEV, YUANYUE LIU, BORIS YAKOBSON, Rice University — The chance for a nanotube of a chiral angle c to emerge from the "primordial soup" of carbon atoms on the catalyst is determined by their relative energies. Massive computations allow one to evaluate the "elastic" energies of the caps, and the energies of their edges [1], G(c+C), which appears to be dominating. Importantly, the latter contains a "chemical phase shift" C, so that the probability of different chiralities is determined by the chemical conditions at the edge. Preference for specific chirality can be achieved by tuning chemical potential of edge terminating chemical. This offers a rational way to control the tube chiral symmetry, a tantalizing yet so far elusive goal.

[1] Y. Liu, A. Dobrinsky, and B.I. Yakobson, Phys. Rev. Lett. in press (Dec 10 2010 issue).

4:06PM X28.00009 Laser-Shot-Induced Chemical Reactions inside Nanotubes: a TDDFT investigation , HONG ZHANG, Sichuan University, China, YOSHIYUKI MIYAMOTO, NEC, Japan, ANGEL RUBIO, University of the Basque Country, Spain — We present the application of the time-dependent density functional theory (TDDFT) on ultrafast laser pulse which induces dynamics in molecules encapsulated by a nanotube. A strong laser pulse polarized perpendicular to the tube axis induces a giant bond-stretch of an HCl molecule inside both C and BN nanotubes. Depending on the initial orientation of the HCl molecule, the subsequent laser-induced dynamics is different [1]. We also observed a radial motion of the nanotube and vacancies appear on the tube wall when the HCl is perpendicular to tube axis. Furthermore, the disintegration of HCl molecules took place when their molecular axis tilted to tube axis. These simulations are important to analyze light-induced nanochemistry and manipulation of nanostructures encapsulated in organic and inorganic nanotubes. The computational scheme used in present work was a combination of the molecular dynamics and real-time propagation of electron wave functions under presence of strong optical field [2,3]. The energy conservation rule was checked to monitor the numerical stability. [1] Y. Miyamoto, H. Zhang, and A, Rubio, submitted., [2] O. Sugino and Y. Miyamoto, Phys. Rev. B59, 2579 (1999). [3] A. Castro, E. Rasanen, A. Rubio and E. K. U. Gross, Eur. Phys. Lett. 87, 53001 (2009).

4:18PM X28.00010 Ab initio study of the dependence of the reactivity upon carbon nanotube diameter , JONATHAN LAFLAMME JANSSEN, JASON BEAUDIN, MICHEL CÔTÉ, Département de physique, Université de Montréal, Canada, NICHOLAS D.M. HINE, PETER D. HAYNES, Imperial College, London, United Kingdom — One of the main research efforts of the recent years has been the development of an efficient way to select desired carbon nanotubes according to their size and their electronic properties. This selectivity would allow easier fabrication of field effect transistor and light-emitting diode devices with appropriate nanotubes. An appealing approach to assess this problem is to use the dependence of chemical functionalization thermodynamics on the material's properties. In this talk, ab initio studies of carbon nanotubes functionalized with bromophenyl will be presented. The radius dependence of the binding and activation energies of this functionalization will be reported. The purpose of this presentation is also to demonstrate the performance of linear-scaling density-functional theory code ONETEP, which provides the possibility carrying out large system simulations (up to several tens of thousands of atoms). Furthermore, the diameter dependence of the oxidation of carbon nanotubes by carbon dioxide will be presented.

4:30PM X28.00011 Electric field response on hybrid C/BN nanostructures , MIGUEL ALONSO-PRUNEDA, CIN2 (CSIC) — Synthesis of hybrid C/BN nanotubes [1] and nanosheets [2] offer a unique route for material engineering, by combination of the exciting properties of graphene with those of insulating polar BN. First principles (DFT) calculations of the zigzag-terminated edges between C and BN nanodomains will be presented, proving that unconventional physical effects similar to those observed at insulating oxide interfaces [3], can also exist in lower dimensions, opening alternative routes for tuning electronic properties at nanointerfaces. In particular, it will be shown that the magnetic character of the edge states in zigzag shaped graphene nanoribbons, and the polar BN edge, team up to give a spin asymmetric screening that induces half-semimetallicity at the interface [4]. This property is also observed in tubular geometries, where potential magnetoelectric effects will be discussed.

[1] Suenaga et. al. *Science* **278** 5338 (1997); Enouz et. al. *Nano Lett.* **7**, 1856 (2007).
[2] Ci et. al. *Nat. Materials* **9**, 430 (2010).
[3] Ohtomo & Hwang *Nature* **427**, 423 (2004); Brinkman et. al. *Nat. Mater.* **6**, 493 (2007); Reyren et. al. *Science* **317**, 5842 (2007).
[4] Pruneda *Phys. Rev. B* **81**, 161409(R) (2010).

4:42PM X28.00012 Study of Singlet-Triplet Gaps in π-Conjugated Polymers versus Graphene Nanoribbons and Single-Walled Carbon Nanotubes. The Effect of Dimensionality[1] , KARAN ARYANPOUR, SUMIT MAZUMDAR, Department of Physics, University of Arizona, HONGBO ZHAO, School of Physics and Telecommunication Engineering, South China Normal University — We compute and compare the gap between the optical singlet and lowest triplet excitons in poly (para-phenylenevinylene) (PPV) with semiconducting graphene nanoribbons (GNRs) and single-walled carbon nanotubes (SWCNTs) within Coulomb correlated model Hamiltonian. The singlet-triplet gaps in semiconducting GNRs and SWCNTs are more than one order of magnitude smaller that in PPV. We ascribe this to two-dimensionality. Spatial distribution of the electron-hole separation in excitons reveals significant localization of the triplet state wave function compared to singlet state in PPV. In GNRs and SWCNTs however, singlet and triplet wave functions exhibit comparably extended spatial distributions. Singlet-triplet gap size is an indicator of the effective Coulomb interaction strength which in turn controls the exciton binding energies of these systems. Exciton binding energy plays a deciding role in light emission and device performance in photovoltaics.

[1]Supported by NSF-DMR-0705163.

4:54PM X28.00013 Carbon-Based Zero-Bandgap Tunnel Transistors[1] , YOUNGKI YOON, SAYEEF SALAHUDDIN, University of California, Berkeley — Tunnel field-effect transistors (TFET) have been proposed as a means of breaking the classical limit of voltage requirement and energy dissipation in electronic devices. However, a tunnel barrier severely reduces the current and hence the speed at which the transistor can be operated. In this work, by performing an atomistic quantum simulation, we propose a novel transistor involving a unique interface between a graphene nanoribbon (GNR) and a metallic carbon nanotube (CNT), such that (i) at low voltages it acts exactly like a tunnel transistor reducing voltage requirement below the classical limit and (ii) at a larger voltage the tunnel barrier is dramatically diminished, resulting in a large flow of current [Appl. Phys. Lett. **97**, 033102 (2010)]. Indeed, experimental fabrication of such an interface could be possible using recently demonstrated methods where carbon nanotubes are unzipped to open up narrow graphene ribbons. Our results show that orders of magnitude improvement in ON current can be obtained in this structure.

[1]This work was supported in part by FCRP center on Functional Engineered and Nano Architectonics (FENA) and NSF.

5:06PM X28.00014 Josephson current in carbon nanotube quantum dots , RAMON AGUADO, CSIC, JONG SOO LIM, ROSA LOPEZ, Universitat de les Illes Balears, Spain, MAHN-SOO CHOI, Korea University — We study theoretically the Josephson current through a carbon nanotube quantum dot coupled to superconducting leads. Due to the interplay between the curvature-induced spin-orbit effect and external magnetic fields, we find a rich $0-\pi$ phase diagram in various transport regimes ranging from noninteracting to Coulomb Blockade, cotunneling and the Kondo limit.

5:18PM X28.00015 Kinetics of Gas Adsorption in Nanopores: A Computer Simulation Study , CHRISTOPHER E. PUEBLO, Southern Illinois University Carbondale, M. MERCEDES CALBI, University of Denver — Motivated by a variety of experimental results concerning gas adsorption in open-ended carbon nanotubes, we present a series of results for the kinetics of adsorption of a gas inside a nanopore. The study is based on a Kinetic Monte Carlo simulation in combination with a lattice model of adsorption. This allows us to monitor the change in coverage with time and extract corresponding adsorption rates or equilibration times. Adsorption in nanopores presents several distinctive features when compared to open surfaces. The adsorption process is mainly controlled by the energy states close to the ends of the pore; we analyze the consequences of this effect on the equilibration times of the system and also on temperature programmed desorption spectra.

Thursday, March 24, 2011 2:30PM - 5:18PM –

Session X29 GQI: Focus Session: Quantum Information for Quantum Foundations - Information Measures, Entanglement, and Entropies C148

2:30PM X29.00001 ABSTRACT WITHDRAWN –

2:42PM X29.00002 Uncertainty Relation for Smooth Entropies

, MARCO TOMAMICHEL, RENATO RENNER, ETH Zurich — Uncertainty relations give upper bounds on the accuracy by which the outcomes of two incompatible measurements can be predicted. While the established uncertainty relations apply to cases where the predictions are based on purely classical data (e.g., a description of the system's state before the measurement), an extended relation which remains valid in the presence of quantum information has been proposed recently [Berta et al., Nature Physics 6, 659 (2010)]. Here we generalize this uncertainty relation to one formulated in terms of smooth entropies. Since these entropy measures are related to operational quantities, our uncertainty relation has various applications. As an example, we show that it directly implies security of quantum key distribution protocols.

2:54PM X29.00003 Inadequacy of von Neumann entropy for characterising extractable work

, OSCAR DAHLSTEN, Singapore Centre for Quantum Technology, National University of Singapore, and Clarendon Laboratory, University of Oxford, RENATO RENNER, ETH Zurich, ELISABETH RIEPER, Singapore Centre for Quantum Technology, National University of Singapore, VLATKO VEDRAL, Singapore Centre for Quantum Technology, National University of Singapore, and Clarendon Laboratory, University of Oxford — The lack of knowledge an observer has about a system limits the amount of work it can extract. This lack of knowledge is normally quantified using the Shannon/von Neumann entropy. We show that this standard approach is, surprisingly, only correct in very specific circumstances. In general one should use the recently developed smooth entropy approach. For many common physical situations, including large but internally correlated systems, the resulting values for the extractable work can deviate arbitrarily from those suggested by the standard approach. (For details see arXiv:0908.0424)

3:06PM X29.00004 Interpreting quantum discord through quantum state merging[1]

, VAIBHAV MADHOK, University of New Mexico, ANIMESH DATTA, Clarendon Laborartory, University of Oxford — We present an operational interpretation of quantum discord based on the quantum state merging protocol. Quantum discord is the markup in the cost of quantum communication in the process of quantum state merging, if one discards relevant prior information. Our interpretation has an intuitive explanation based on the strong subadditivity of von Neumann entropy. We use our result to provide operational interpretations of other quantities like the local purity and quantum deficit. Finally, we discuss in brief some instances where our interpretation is valid in the single copy scenario.

[1]NSF Grant Nos. 0903953 and 0903692

3:18PM X29.00005 The thermodynamic meaning of negative entropy

, LIDIA DEL RIO, RENATO RENNER, JOHAN AABERG, ETH Zurich, OSCAR DAHLSTEN, VLATKO VEDRAL, entre for Quantum Technologies, National University of Singapore — Landauer's erasure principle states that all irreversible operations, like the erasure of data stored in a system, have an inherent work cost. This work cost depends on our knowledge of the system: the less we know about its state, the more it costs to erase it. Here, we analyse erasure in a general setting, where our information about a system can be quantum mechanical. We show that the work cost of erasure is bounded by the entropy of the system conditioned on that quantum information. Our result implies that conditional entropies, originally introduced in the context of information theory, have a direct thermodynamic significance. Since these entropies can become negative, a particular consequence is that an observer who is strongly correlated to a system may gain work while erasing it.

3:30PM X29.00006 Operational interpretations of quantum discord[1]

, MARCO PIANI, University of Waterloo, DANIEL CAVALCANTI, National University of Singapore, LEANDRO AOLITA, ICFO-Institut de Ciencies Fotoniques, SERGIO BOIXO, California Institute of Technology, KAVAN MODI, National University of Singapore, ANDREAS WINTER, University of Bristol — Quantum discord quantifies non-classical correlations going beyond the standard classification of quantum states into entangled and unentangled ones. Although it has received considerable attention, it still lacks any precise interpretation in terms of some protocol in which quantum features are relevant. Here we give quantum discord its first information-theoretic operational meaning in terms of entanglement consumption in an *extended quantum state merging* protocol. We further relate the asymmetry of quantum discord with the performance imbalance in quantum state merging and dense coding.

[1]National Research Foundation, the Ministry of Education of Singapore, the Spanish "Juan de la Cierva" Programme, NSERC, QuantumWorks, Ontario Centres of Excellence, the Royal Society, U.K. EPSRC and the European Commission

3:42PM X29.00007 Measures of non classical correlations

, MATTHIAS LANG, Center for Quantum Information and Control, University of New Mexico, ANIL SHAJI, School of Physics, Indian Institute of Science Education and Research, CARLTON CAVES, Center for Quantum Information and Control, University of New Mexico — To quantify non classical correlations in a quantum state, much effort has been put into the investigation of entanglement and its properties. It is known, however, that entanglement does not capture all quantum correlations. Several entropic measures of non-classical correlations beyond entanglement have been proposed, quantum discord being the most popular amongst them. We have developed an entropic framework for formulating such measures. We discuss new measures that emerge from this framework, and relations among the various measures, and we present numerical results for the measures for two-qubit states.

3:54PM X29.00008 Redundant imprinting of information in non-ideal environments: Quantum Darwinism via a noisy channel[1]

, MICHAEL ZWOLAK[2], Los Alamos National Laboratory, HAITAO QUAN, University of Maryland, College Park, WOJCIECH ZUREK, Los Alamos National Laboratory — Quantum Darwinism provides an information-theoretic framework for the emergence of the classical world from the quantum substrate. It recognizes that we - the observers - acquire our information about the "systems of interest" indirectly from their imprints on the environment. Objectivity, a key property of the classical world, arises via the proliferation of redundant information into the environment where many observers can then intercept it and independently determine the state of the system. While causing a system to decohere, environments that remain nearly invariant under the Hamiltonian dynamics, such as very mixed states, have a diminished ability to transmit information about the system, yet can still acquire redundant information about the system [1,2]. Our results show that Quantum Darwinism is robust with respect to non-ideal initial states of the environment.

[1] M. Z., H. T. Q., W. H. Z., Phys. Rev. Lett. 103, 110402 (2009)
[2] M. Z., H. T. Q., W. H. Z., Phys. Rev. A 81, 062110 (2010)

[1]This research is supported by the U.S. Department of Energy through the LANL/LDRD Program.
[2]http://mike.zwolak.org

4:06PM X29.00009 Quantum Darwinism in an Everyday Environment: Huge Redundancy in Scattered Photons[1] , CHARLES RIEDEL, University of California, Santa Barbara, WOJCIECH ZUREK, Los Alamos National Laboratory — We study quantum Darwinism—the redundant recording of information about the preferred states of a decohering system by its environment—for an object illuminated by a blackbody. In the cases of point-source, small disk, and isotropic illumination, we calculate the quantum mutual information between the object and its photon environment. We demonstrate that this realistic model exhibits fast and extensive proliferation of information about the object into the environment and results in redundancies orders of magnitude larger than the exactly soluble models considered to date. We also demonstrate a reduced ability to create records as initial environmental mixedness increases, in agreement with previous studies.

[1]This research is supported by the U.S. Department of Energy through the LANL/LDRD program and, in part, by the Foundational Questions Institute (FQXi).

4:18PM X29.00010 Quantum systems as embarrassed colleagues: what do tax evasion and state tomography have in common? , CHRIS FERRIE, Institute for Quantum Computing, University of Waterloo, ROBIN BLUME-KOHOUT, Theoretical Division, Los Alamos National Laboratory — Quantum state estimation (a.k.a. "tomography") plays a key role in designing quantum information processors. As a problem, it resembles probability estimation – e.g. for classical coins or dice – but with some subtle and important discrepancies. We demonstrate an improved classical analogue that captures many of these differences: the "noisy coin." Observations on noisy coins are unreliable – much like soliciting sensitive information such as ones tax preparation habits. So, like a quantum system, it cannot be sampled directly. Unlike standard coins or dice, whose worst-case estimation *risk* scales as $1/N$ for all states, noisy coins (and quantum states) have a worst-case risk that scales as $1/\sqrt{N}$ and is overwhelmingly dominated by nearly-pure states. The resulting optimal estimation strategies for noisy coins are surprising and counterintuitive. We demonstrate some important consequences for quantum state estimation – in particular, that adaptive tomography can recover the $1/N$ risk scaling of classical probability estimation.

4:30PM X29.00011 Quantum networks reveal quantum nonlocality , DANIEL CAVALCANTI, CQT-Centre for Quantum Technologies, MAFALDA ALMEIDA, VALERIO SCARANI, ANTONIO ACIN, CQT-ICFO COLLABORATION — The results of local measurements on some composite quantum systems cannot be reproduced classically. This impossibility, known as quantum nonlocality, represents a milestone in the foundations of quantum theory. Quantum nonlocality is also a valuable resource for information processing tasks, e.g. quantum communication, quantum key distribution, quantum state estimation, or randomness extraction. Still, deciding if a quantum state is nonlocal remains a challenging problem. Here we introduce a novel approach to this question: we study the nonlocal properties of quantum states when distributed and measured in networks. Using our framework, we show how any one-way entanglement distillable state leads to nonlocal correlations. Then, we prove that nonlocality is a non-additive resource, which can be activated. There exist states, local at the single-copy level, that become nonlocal when taking several copies of it. Our results imply that the nonlocality of quantum states strongly depends on the measurement context.

4:42PM X29.00012 A generalization of Noether's theorem and the information-theoretic approach to the study of symmetric dynamics[1] , IMAN MARVIAN, Perimeter Institute, IQC, ROBERT SPEKKENS, Perimeter Institute — Information theory provides a novel approach to study of the consequences of symmetry of dynamics which goes far beyond the traditional conservation laws and Noether's theorem. The conservation laws are not applicable to the dissipative and open systems. In fact, as we will show, even in the case of closed system dynamics if the state of system is not pure the conservation laws do not capture all the consequences of symmetry. Using information theoretic approach to this problem we introduce new quantities called asymmetry monotones, that if the system is closed they are constant of motion and otherwise, if the system is open, they are always non-increasing. We also explain how different results in quantum information theory can have non-trivial consequences about the symmetric dynamics of quantum systems.

[1]I.M. is supported by Mike and Ophelia Lazaridis scholarship.

4:54PM X29.00013 Closed Systems that Measure Particles , MICHAEL STEINER, RONALD RENDELL, Inspire Institute — The Measurement Problem has been of fundamental concern since the discovery of Schrödinger's equation. We have been developing a framework for which this problem can be considered under the assumption that the particle and detector are jointly considered a closed system. The framework is based on imposing conditions on quantum state evolution that such a closed system meet, including conservation of energy and momentum, no-cloning and no-signaling, gauge invariance, and relativity constraints. Another requirement will be presented, which is a quantum mechanical generalization of Newton's first law. Based on these conditions, we will derive and present several new results.

5:06PM X29.00014 Quantum Theory for a Total System with One Internal Measuring Apparatus , WEN-GE WANG, Univ of Sci & Tech of China — We propose a quantum theory for a total system including one internal measuring apparatus. The theory is based on three basic assumptions and a principle termed the principle of compatible description (PCD). The assumptions are: (i) Physical states of the total system can be associated with vectors in the Hilbert space. (ii) Dynamical evolution of a state vector obeys Schrö dinger equation. (iii) For a physical state of the total system described by a pure vector, in which a subsystem may play the role of an internal measuring apparatus, when certain stable condition is satisfied, the pure-vector description may be given a Born-type ensemble interpretation. The PCD states that different descriptions for the same state of the total system must give consistent predictions for results of measurements performed by the internal measuring apparatus. The proposed theory lies at a meeting point of Copenhagen, Everett's relative-state, and consistent-histories interpretations of quantum mechanics. While, it provides something new: For example, the PCD imposes a restriction to vectors that can be associated with physical states, which may effectively break the time-reversal symmetry of Schrödinger equation. As an application of the theory, we derive a condition under which a two-level quantum system may have definite properties, such that it may play the essential role of a measuring apparatus.

Thursday, March 24, 2011 2:30PM - 5:30PM –
Session X30 DCMP: Nanowires: Electronic Transport, Experimental C147/154

2:30PM X30.00001 Resistivity of Endotaxial Silicide Nanowires Measured with UHV-STM Nanoprobe[1] , SAM TOBLER, PETER BENNETT, Arizona State University — We have measured the resistivity of endotaxial silicide nanowires on silicon using a UHV STM nanoprobe in a 2-point configuration, which allows separation of intrinsic resistivity from contact resistance using a variable probe spacing. A fixed contact is provided by a thin metal film deposited by shadow evaporation with an edge profile 100nm wide and sheet resistance 500 ohms, while the second contact is provided by the STM tip. A controlled approach with 15 Ang displacement beyond the tunneling position allows for reliable and repeatable electrical contact without damage to the tungsten STM tip. Using this method, we have obtained resistivity values of 30 micro-ohm-cm and 120 micro-ohm-cm for CoSi2 nanowires of width 40nm and 20nm, respectively, on Si(110). The increase of resistivity with decreasing width is attributed to boundary scattering along the sidewalls of the nanowires.

[1]Supported by NSF Grant DMR0503705

2:42PM X30.00002 Field Effect Transistor based on Single Crystalline InSb Nanowire[1] , JIA LU, YENNAI WANG, KARAN BANERJEE, USC, HUIJUN YAO, Juelich Intitute, THOMAS SCHAEPERS, Juelich Institute, NAMI COLLABORATION, IBN COLLABORATION — Semiconductor nanowires have attracted substantial scientific and technological interests due to their unique properties arising from the size confinement effects. Among III-V group, indium antimonide (InSb) has the smallest bandgap energy (170 meV) at room temperature and possess an extremely high bulk electron mobility. It has been widely used in infrared optoelectronics and high-speed devices, and has inspired significant interest for fundamental studies in their nanostructure form. In this work, InSb nanowires with precise stoichiometry and zincblende crystal structure are synthesized via pulsed-laser chemical vapor deposition. Raman spectroscopy shows stoke and anti-stoke peaks of transverse-optical mode with asymmetric broadening. The nanowire demonstrates n-type semiconductor behavior. Enhanced surface scattering due to size confinement leads to reduced electron mobility.

[1]DAAD

2:54PM X30.00003 Realizing lateral wrap-gated nanowire FETs: Controlling gate length with chemistry rather than lithography , ADAM MICOLICH, School of Physics, University of New South Wales, Sydney NSW 2052, Australia, KRISTIAN STORM, GUSTAV NYLUND, LARS SAMUELSON, Solid State Physics/Nanometer Structure Consortium, Lund University S-211 00 Lund, Sweden — An important consideration in miniaturizing transistors is maximizing the coupling between the gate and the semiconductor channel. A semiconductor nanowire with a coaxial metal gate represents the optimum in gate-channel coupling, but has only been realized for vertically-oriented nanowire transistors. We report a method for producing laterally oriented fully wrap-gated nanowire field-effect transistors that provides exquisite control over the gate length via a single wet etch step, eliminating the need for additional lithography beyond that required to define the source/drain contacts and gate lead. Our design allows the contacts and nanowire segments extending beyond the wrap-gate to be controlled independently by biasing the doped substrate, significantly improving the sub-threshold electrical characteristics. Our devices provide stronger, more symmetric gating of the nanowire, operate at temperatures between 300 to 4 Kelvin, and offer new opportunities in applications ranging from studies of one-dimensional quantum transport through to chemical and biological sensing.

3:06PM X30.00004 Transport studies of ultrathin YSi_2 nanowires , SABAN M. HUS, HAO HU, VIOLETA IANCU, HANNO H. WEITERING, The University of Tennessee, AN-PING LI, Center for Nanophase Material Sciences, Oak Ridge National Laboratory — Extremely long YSi_2 nanowires have been fabricated via self-assembly during epitaxial growth of Y on the Si (100) 2x1 surface. The thinnest YSi_2 nanowires have a cross section of $\sim$0.4 x1.1 nm^2 and can grow up to 2 μm long. They are among the closest realizations of a one-dimensional conductor. Their electrical transport properties have been investigated with a variable-temperature four-tip scanning tunneling microscope (STM) using ex-situ fabricated contact pads. These ex-situ investigations indicated that the electrical conductivity of single nanowires is thermally activated, following an inverse Arrhenius law. In-situ contact fabrication has been accomplished via a field-induced atomic emission process from a gold STM tip. Details of the in-situ fabrication method and preliminary transport results will be presented. The research at Oak Ridge National Laboratory's Center for Nanophase Materials Sciences was sponsored by the Division of Scientific User Facilities, US Department of Energy.

3:18PM X30.00005 Experimental observation of very large magnetoconductance in microbial nanowires[1] , NIKHIL MALVANKAR, Depts. of Physics and Microbiology, University of Massachusetts, Amherst MA 01003, MADELINE VARGAS, DEREK LOVLEY, Dept. of Microbiology, University of Massachusetts, Amherst MA 01003, MARK TUOMINEN, Dept. of Physics, University of Massachusetts, Amherst MA 01003 — Microbial nanowires are 2-5 nm-wide conductive proteinous pili filaments secreted by some bacteria, which can grow tens of micrometers long and may serve as a conduit for long-distance electron transport. Our previous studies demonstrated that pili of Geobacter sulfurreducens exhibit properties akin to disordered metals, and indicated a temperature-driven crossover from the regime of weak localization (WL) to strong localization (SL). Here we report a very large positive magnetoconductance (MC), up to 10,000 %, at 300K. MC increased exponentially with magnetic field. A crossover from positive MC (WL regime) to negative MC (SL) was observed at $\sim$ 280K when the localization and the phase-breaking lengths are expected to become comparable. We attribute positive MC to destruction of the quantum interference of delocalized electron wavefunctions and negative MC to shrinkage of the localized electron wavefunctions due to applied magnetic field, which is consistent with the temperature dependence of conductivity.

[1]Funded by U.S. DOE Genomic Sciences and Office of Naval Research

3:30PM X30.00006 Electron Transport in Gold Nanowires: Stable 1-, 2- and 3-Dimensional Atomic Structures and Non-Integer Conduction States , DOUGLAS SMITH, FRANCESCA TAVAZZA, LYLE LEVINE, JON PRATT, ANNE CHAKA, National Institute of Standards and Technology — We report experimental conductivity measurements made during highly stable tensile deformation of Au nanowires showing a rich variety of behaviors, including non-integer quantum conductance plateaus, transitions and slopes. Using tight binding conductance calculations on simulated nanowires previously deformed using density functional theory calculations, we demonstrate that all of these phenomena can arise from structural transitions between highly stable ordered atomic configurations that self-organize during tensile deformation.

3:42PM X30.00007 Gate-induced Fermi level tuning and ambipolar conduction control in InP nanowires , KRISTIAN STORM, GUSTAV NYLUND, MAGNUS BORGSTRÖM, JESPER WALLENTIN, CARINA FASTH, CLAES THELANDER, LARS SAMUELSON, Lund University — Semiconducting nanowires are an interesting platform for studies of fundamental material transport properties in one dimension as well as for building blocks for various types of devices. Most conventional semiconductor devices are based upon doping for its operation, but as device dimensions are decreased, the random position of a few incorporated impurity atoms may come to dominate device characteristics. We present measurements of InP nanowires in which the Fermi level is tuned at efficiency close to the theoretical limit using semi-wrapped gates. Furthermore, we present ambipolar devices in which the Fermi level can be tuned across the entire bandgap of the semiconductor. We believe this will be of considerable importance and serve as a foundation for producing nanowire devices where the device behavior is induced by sequential gates wrapped around the nanowire channel, replacing the need for doping in certain types of devices. This way, the properties can be dynamically tuned using wrapgates, as opposed to statically set using the doping level.

3:54PM X30.00008 Transport Measurements on Sb doped Silicon Nanowires , PRATHYUSHA NUKALA, Dept. of Electrical Eng. University of North Texas, MARZIEH ZARE, GOPAL SAPKOTA, Dept. of Physics University of North Texas, PRADEEP GALI, USHA PHILIPOSE, Dept. of Electrical Eng. University of North Texas — Semiconductor nanowires (NWs) present an alternative approach for device scaling. N-type Si NWs are generally grown with silane as source with phosphine and arsenic as dopants, all of which are toxic in nature. We present a safe, cost-effective approach for synthesis of n- doped Si NWs using Sb. Structural and compositional characterization using electron microscopy and X-ray spectroscopy will be presented for crystallographic information on the quality and morphology. Ohmic contacts established to a single and on an array of doped and undoped NWs in an FET type of device configuration will provide information on several parameters such as type of majority carriers, mobility and concentration. We will highlight the promise of Sb doped Si NWs for electronic applications such as nano-scale field effect transistors and sensors.

4:06PM X30.00009 Role of defect states in charge transport in semiconductor nanowires[1] , DONGKYUN KO, XIANWEI ZHAO, KONGARA REDDY, WOLFGANG WINDL, NITIN PADTURE, NANDINI TRIVEDI, FENGYUAN YANG, EZEKIEL JOHNSTON-HALPERIN — Charge transport characteristics are investigated in Se-doped InP nanowires in order to determine the nature of the defect states. I-V curves indicate that transport is limited by trapped space charges rather than by Schottky at high bias. In addition, mobility calculations show that hopping between defect states plays an important role at low bias. A transition between hopping mechanisms as a function of temperature can be determined from the behavior of the temperature-dependent resistance R(T). Nearest neighbor hopping (NNH) is dominant in the high temperature regime (>158K) , $R \sim exp(T_0/T)^{1.03}$, and Efros-Shklovskii variable range hopping (ES-VRH) is dominant in the low temperature regime (<158K), $R \sim exp(T_{ES}/T)^{0.49}$. Gate-bias dependence of the transition temperature and hopping parameters are also investigated: these results suggest that applying positive gate-bias changes the strength of electron correlations in these quasi-1D systems.

[1]Funding for this research was provided by the Center for Emergent Materials at the Ohio State University, a NSF MRSEC (Award Number DMR-0820414).

4:18PM X30.00010 InAs Nanowire Transistors as Gas Sensor: the Role of Surface States[1] , DONG LIANG, JUAN DU, HAO TANG, XUAN P.A. GAO, Department of Physics, Case Western Reserve University — Utilizing the large surface-to-volume ratio, sensors of quasi one-dimensional semiconductor nanowires based electronic devices have been shown high sensitivity to the adsorption gaseous molecules or the binding of biomolecules in liquid, enabling a label-free sensing modality with high sensitivity and direct electrical readout. We report a study of the response of InAs nanowire field-effect transistor sensor devices to various gases and alcoholic vapors. It is concluded that the change in conductance of the device in response to chemical vapors is a combined result of both the charge transfer and modified electron mobility effects. In particular, we found that surface adsorption of most chemical molecules can reduce electron density in nanowires from $\sim 10^4$ to $\sim 10^3/\mu$m and enhance the electron mobility greatly (from tens to a few hundred of $cm^2/(V\ s)$) at the same time. These effects are attributed to the interactions between adsorbed molecules and the electron accumulation layer and rich surface states on the InAs nanowire surface. Journal reference: Nano Letters 9, 4348 (2009).

[1]Supported by ACS PRF #48800-DNI10.

4:30PM X30.00011 Surface passivated pure Indium Oxide nanowires for gas sensors , PRADEEP GALI, Department of Electrical Electrical Engineering, University of North Texas, KIRAN SHRESTHA, Department of Physics, University of North Texas, FANG LINGKUO, NIGEL SHEPHERD, Department of Materials science, University of North Texas, USHA PHILIPOSE, Department of Physics, University of North Texas — Indium oxide (In_2O_3) nanowires have applications in semiconductor electronics and gas sensing. We report on growth of stoichiometric In_2O_3 nanowires with diameter ranging from 40 to 80nm and lengths over 10 μm. Structural characterization done with SEM, XRD and TEM shows that the nanowires exhibits BCC structure and grow along the (100) direction. Energy Dispersive X-ray spectroscopy shows stoichiometric composition. Transport measurements on a single nanowire shows ohmic behavior and a resistance of about 100 KΩ. Photoluminescence spectrum at room temperature shows strong emission peaks at 370nm and 415nm, corresponding to near band edge and defect related emission respectively. We present a technique of post-growth annealing of these nanowires to eliminate the defect induced emission and enhance band edge emission. Passivating the surface of these nanowires enhances their gas sensing abilities.

4:42PM X30.00012 Synthesis and Characterization of InAs / InSb Nanowire Heterojunctions[1] , MINKYUNG JUNG, MICHAEL SCHROER, JASON PETTA, Princeton University — InSb is a very promising material for both electronic and optoelectronic devices due to its unique features, including a very small band gap, large bulk mobility, enormous electronic g- factor and strong spin-orbit interaction. In particular, the small effective mass of InSb makes it straightforward to fabricate devices that display effects due to quantum confinement [1,2]. Here InAs/InSb nanowire heterostructures were grown by metal-organic vapor-phase epitaxy on InAs (111)B substrates. We investigated morphology changes of InAs/InSb nanowires with varying growth temperature and V/III ratio. The samples were characterized using scanning electron microscopy and high resolution transmission electron microscopy. In order to study the transport properties of InAs/InSb nanowires, field effect transistors were fabricated on SiO_2/Si substrates and characterized at room temperature and 4.2 K.

[1] H. A. Nilsson *et al.*, Nano Lett. **9**, 3151 (2009)
[2] P. Caroff *et al.*, Small **4**, 878 (2008)

[1]Funded by the Sloan and Packard Foundations, and the Army Research Office.

4:54PM X30.00013 Measurement of minority carrier diffusion length in individual silicon nanowires with an in-situ grown p-n junction , A.D. MOHITE, D.E. PEREA, S. SINGH, S.A. DAYEH, S.T. PICRAUX, H. HTOON, LANL, CENTER FOR INTEGRATED NANOTECHNOLOGIES TEAM, CHEMISTRY DIVISION, LOS ALAMOS NATIONAL LABORATORY TEAM — We report a scanning photocurrent microscopy study across a p-n junction of individual in-situ doped Si nanowires (NWs). The measured photocurrent decreases exponentially as the laser spot is scanned away from the p-n junction in both directions. The photocurrent peak widens with increasing reverse bias, indicating the increase of depletion width. For a 40nm diameter NW, the fit of photocurrent decay to an exponential function gives minority carrier diffusion lengths of L_n=1.842 μm and L_p=1.45 μm for electrons and holes, respectively. Such relatively long minority carrier diffusion lengths are consistent with the low dopant incorporation we expected for our growth condition. This result further suggests that the diffusion length scales with doping concentration despite the impact of surface states of a 1D system. We will further discuss the dependence of the minority carrier diffusion length on diameter, doping concentrations, and back-gating.

5:06PM X30.00014 Andreev tunneling enhanced by Coulomb oscillations in superconductor-semiconductor hybrid Ge/Si nanowire devices , XIAOJIE HAO[1], Key Laboratory of Quantum Information, CAS, University of Science and Technology of China, Hefei, China; University of Michigan, USA, TAO TU, HAI-OU LI, CHENG ZHOU, GANG CAO, GUANG-CAN GUO, GUO-PING GUO, Key Laboratory of Quantum Information, CAS, University of Science and Technology of China, Hefei, China, WAYNE FUNG, ZHONGQING JI, WEI LU, Department of Electrical Engineering and Computer Science, The University of Michigan, Ann Arbor, USA — We explore the magneto-conductance of Ge/Si core/shell nanowire quantum dot devices contacted by superconducting leads. Significant magneto-conductance peaks around zero field are observed and show a periodic modulation with gate voltage as discrete states of the quantum dot are turned on- and off-resonance with the Fermi energy in the superconducting electrodes. The ability to create and control coherent transport in superconductor-semiconductor hybrid nanostructures allows for new opportunities in the study of various fundamental competing effects such as superconductivity and electron-electron interactions.

[1]Now at University of California, Los Angeles

5:18PM X30.00015 Minority Carrier Lifetimes and Surface Effects in VLS-Grown pn Junction Silicon Nanowires , YEONWOONG JUNG, ALEKSANDAR VACIC, Yale University, DANIEL PEREA, TOM PICRAUX, Los Alamos National Laboratory, MARK REED, Yale University, YALE UNIVERSITY COLLABORATION, LOS ALAMOS NATIONAL LABORATORY COLLABORATION — We study the minority carrier lifetimes and surface effects of pn junction Si nanowires. Axial pn junction Si nanowires with alternating p-n doped segments are grown based on the Au-catalyzed VLS process by an in-situ exchange of gas-phase dopants. As-grown nanowires display strong current rectification only after surface etching processes. By utilizing the reverse recovery transient of minority carriers, we directly characterize the minority carrier lifetimes and observe the decrease of the lifetimes with a decrease of nanowire diameters. Investigation of the diameter-dependent device ideality factor and current density strongly suggests that the surface recombination with an enhanced surface-to-volume ratio significantly governs the carrier transport. We also characterize the carrier lifetimes of nanowires with and without surface passivation layers, and observe an enhancement of the lifetimes in the surface-passivated ones. These studies elucidate the carrier transport mechanism in VLS pn junction Si nanowires and emphasize the importance of the surface passivation for efficient photovoltaic applications.

Thursday, March 24, 2011 2:30PM - 5:18PM –
Session X31 DCMP: Amorphous Solids, Glasses & Liquids I C145

2:30PM X31.00001 Evidence of Fatigue Damage in the Local Structure of Zr-based Bulk Metallic Glasses , DESPINA LOUCA, PENG TONG, University of Virginia, PETER LIAW, GONGYAO WANG, The University of Tennessee, YOSHIHIKO YOKOYAMA, Tohoku University, ANNA LLOBET, Los Alamos National Laboratory, RICK SPENCE, Argonne National Laboratory — Bulk metallic glasses (BMG) are particularly vulnerable to fatigue damage, where catastrophic failure may occur without observable macroscopic changes. The local atomic structure of two BMGs with compositions of $Zr_{50}Cu_{40}Al_{10}$ and $Zr_{60}Cu_{30}Al_{10}$was investigated by synchrotron X-ray and neutron diffraction via the pair density function analysis. Under a load of 1600 MPa, the number of compression cycles ranged from 0 – 10^7 at 10 Hz. At room temperature, a subtle but irreversible change is observed in the local structure due to fatigue. Upon cooling down to 10 K, however, a significant structural re-organization is observed especially in the short range that is proportional to the number of fatigue cycles. The effect becomes more pronounced with increasing the number of loading cycles. The changes are beyond the usual narrowing from reducing thermal vibrations. The results indicate that hardening occurs after fatigue.

2:42PM X31.00002 Analysis of Amorphous Iron Surface Energies and Bulk Properties using DFT[1] , CHARLES NEWNAM, U.S. Naval Academy, MICHAEL MEHL, U.S. Naval Research Laboratory, DANIEL FINKENSTADT, U.S. Naval Academy — From Ab Initio calculations, we compare the energy of amorphous Iron to bcc and fcc Iron structures, both at zero pressure and high pressure. From these calculations we draw conclusions on the properties of metallic glass structures over a range of pressure. Additionally, we address the adsorption energy of Oxygen on amorphous surfaces versus the structure's cell size and compared against bcc and fcc Iron structures. The adsorption energies allow us to evaluate the corrosion potential of an amorphous structure versus a typical crystalline surface.

[1]We gratefully acknowledge the financial support of ONR.

2:54PM X31.00003 Super-localization of atomic dynamics in liquid Iron[1] , MADHUSUDAN OJHA, DAVID J. KEFFER, The University of Tennessee, DON M. NICHOLSON, Oak Ridge National Laboratory, TAKESHI EGAMI, The University of Tennessee and Oak Ridge National Laboratory — Lattice dynamics in crystals is well described in terms of phonons. However, phonons cannot give precise description of the atomic dynamics in liquids because they are highly damped. We carried out MD simulations of liquid iron at high temperatures. The results are presented in terms of the dynamic pair-density function (DPDF), which describes the atomic correlation, or the distribution of atomic distances over time, at the angular frequency ω. Our analysis shows that the atomic dynamics in liquid iron above the boson mode (BM) is confined to only the nearest neighbors, resulting in super-localization of atomic dynamics. The dynamics of nearest neighbor shells is well described in terms of atomic level stresses. This super-localization of atomic dynamics in liquid iron implies that the dynamics of the local atomic level stresses represents the normal modes in liquids at high temperatures, and justifies the equipartition law observed for the atomic level stresses [1].

[1] V. Levashov, et al. Phys. Rev. B 78,064205 (2008)

[1]This work is supported by BES-DOE

3:06PM X31.00004 Data-mining for hidden order in metallic liquids and glasses , XIAOWEI FANG, Ames Laboratory - USDOE and University of Science and Technology of China, C.Z. WANG, Y.X. YAO, Ames Laboratory - USDOE, Iowa State University, Z.J. DING, University of Science and Technology of China, K.M. HO, Ames Laboratory - USDOE, Iowa State University — Although metallic liquids and glasses look quite homogenous macroscopically, most of them exhibit structural and chemical orders at the atomic scale. This short-range (SRO) or medium-range order (MRO) occurs on a length scale of 5-20 Å. However, they are generally difficult to discern at the macroscopic scale due to random orientations of the ordered units. In this paper, we develop an efficient computational algorithm to align the neighborhood cluster around each atom to reveal the hidden symmetry and order contained in the system. In our alignment algorithm, we put the center atoms into a common origin and rigidly rotate the clusters to maximize their common registry to reveal any existing SRO or MRO. The results determine what are the major competing orders and the strengths of various orders in the system. Such atomic scale information are very difficult to acquire by experiments and are critical for understanding the mechanism of glass formation and phase selections during the rapid solidification from the metallic liquids.

3:18PM X31.00005 Metallic States of Multicomponent Glasses , TERRENCE JACH, NIST, Gaithersburg, MD — The $K\alpha_3$ and $K\alpha_4$ satellite lines in x-ray fluorescence result from two-electron shake-up transitions. The ratio of these lines in some solids is known to be highly sensitive to the valence band of the material and a well-defined indicator of metallic vs. oxide states. The good energy resolution of a microcalorimeter x-ray detector allows us to determine the ratio in the fluorescence x-ray spectrum of glasses. An investigation of the satellite ratios of Mg and Al $K\alpha$ lines in a multi-component glass used as a NIST Standard Reference Material shows that these elements appear to be in a metallic state, despite the original constituents of the glass. This result would be hard to determine by x-ray photoemission spectroscopy because of charging effects in the glass. It remains to be determined whether the effect is due merely to incomplete oxidation of the atoms or actual nanoparticle-sized metallic phases in the glass.

3:30PM X31.00006 An NMR study of homogenous deformation-induced ordering in $La_{50}Ni_{15}Al_{35}$, MAGDALENA SANDOR, YUE WU, HAIBO KE, WEI HUA WANG — The mechanism of mechanical deformation is currently an unresolved issue of fundamental importance. ^{27}Al NMR nutation experiments in $La_{50}Ni_{15}$ Al_{35} bulk metallic glasses (BMG) were carried out to probe local structural changes induced by elastostatic compression at room temperature. It was observed that compression enhances local symmetry at Al sites with compression time. Modulated differential calorimetry studies were also performed to understand how free volume changes with compression time. Results provide insight into the nature of homogenous deformation and the interplay of free volume with local structural changes.

3:42PM X31.00007 Understanding intrinsic ductility from Poisson's ratio for amorphous solids through force-field tuning , YUNFENG SHI, JIAN LUO, Rensselaer Polytechnic Institute — This work is motivated by recently observed empirical relationship between the Poisson's ratio and the fracture energy for a range of metallic glasses and oxide glasses. Glassy solids with low Poisson's ratio are brittle and vice versa, with a critical Poisson's ratio of about 0.31. Here we used a force-field tuning scheme to investigate how a near-equilibrium elastic constant determines far-from-equilibrium fracture behavior. By modifying a well-studied binary Lennard-Jones system, we obtained a family of glassy systems with different Poisson's ratio ranging from 0.2 to 0.4. Interestingly, the model glasses with low Poisson's ratio exhibit brittle fracture in tension and vice versa, which agrees with experimental observations. Finally, we will discuss how ductility of amorphous solids can be comprehended in terms of the structure and bonding of the amorphous solids, both of which also dictate the Poisson's ratio.

3:54PM X31.00008 Universal Sound Attenuation in Amorphous Solids , DERVIS CAN VURAL, University of Illinois at Urbana Champaign — A large class of amorphous materials, including glasses, polymers, disordered crystals and in some cases quasi-crystals and proteins, show a striking degree of universality in their low temperature acoustic and thermal properties. Among the least understood is the dimensionless acoustic mean path $l/\lambda \sim 150$. Although many theories have been proposed to explain the universality of this constant, they rely on detailed phenomenological assumptions, such as the existence of tunneling two-state systems. In this talk, I present the many-body acoustic response of elastically coupled random matrices to demonstrate that the universality is a property of a general class of theories, and emerges regardless of the detailed assumptions regarding the constituents of the amorphous solid.

4:06PM X31.00009 Finite-temperature critical point of a glass transition , YAEL ELMATAD, University of California, Berkeley, ROBERT JACK, University of Bath, JUAN GARRAHAN, University of Nottingham, DAVID CHANDLER, University of California, Berkeley — We generalize the simplest kinetically constrained models of a glass-forming liquid by softening kinetic constraints, allowing them to be violated with a small rate. We demonstrate that these models support a first-order dynamical (space-time) phase transition between active (fluid) and inactive (glass) phases. The first-order phase boundary in these softened model ends in a finite-temperature dynamical critical point, which may be present in natural systems. In this case, the glass phase has a very large but finite relaxation time. We discuss links between the dynamical critical point and quantum phase transitions, showing that dynamical phase transitions in d dimensions map to quantum transitions in the same dimension, and hence to classical thermodynamic phase transitions in $d+1$ dimensions.

4:18PM X31.00010 Nonequilibrium relaxation and aging scaling properties of the Coulomb glass[1] , MATTHEW T. SHIMER, UWE C. TÄUBER, MICHEL PLEIMLING, Department of Physics, Virginia Tech — Using Monte Carlo simulations, we analyze the two-time density autocorrelation function for the two- and three-dimensional Coulomb glass with various long-range interaction potentials. A full aging scaling ansatz is sufficient to describe the nonequilibrium relaxation properties of these highly correlated disordered systems. By investigating the trends of the scaling exponents, we find that they are non-universal, and depend on temperature, charge density, and interaction strength.
Reference: EPL **91**, 67005 (2010).

[1]Research supported through the US Department of Energy (DOE-BES), grant no. DE-FG02-09ER46613.

4:30PM X31.00011 Vibrational excitations and elastic phases in Sodium Borate Glasses[1] , K. VIGNAROOBAN, P. BOOLCHAND, University of Cincinnati, M. MICOULAUT, University of Paris VI — Glass Transition temperatures (T_gs) and non-reversing enthalpy (ΔH_{nr}) at T_g of dry $(Na_2O)_x(B_2O_3)_{100-x}$ glasses across the $0\% < x < 44\%$ soda range are measured. Trends in $\Delta H_{nr}(x)$ show a reversibility window in the $20\% < x < 40\%$ range, and fix the Intermediate Phase (IP). IR and Raman vibrational modes including Boson modes are also examined. At low x ($< 20\%$), the Raman active 808 cm^{-1} mode of boroxyl rings steadily lowers in scattering strength and red-shifts with increasing x, suggesting that the stressed-rigid quasi 2D network of B_2O_3 glass at $x = 0$, steadily softens with a characteristic optical elastic power-law ($p_1 = 0.85(2)$). In the $26\% < x < 40\%$ range, a mode near 770 cm^{-1} rapidly grows in strength and red shifts with increasing x with a power- law of $p_2 = 1.05(5)$ characteristic of IPs observed earlier[a] in other 3D covalent and ionic networks. In addition, many other modes are observed, some blue-shift, some red-shift and some remain unchanged with x. These data will be discussed in relation to glass structure evolution with composition.

D.Novita et al. J. Phys. Condens. Matter 21, 205106 (2009)

[1]This work is supported by DMR- 08-53957

4:42PM X31.00012 Accelerated kinetics of amorphous silicon using an on-the-fly off-lattice kinetic Monte-Carlo method , JEAN-FRANCOIS JOLY, Universite de Montreal, FEDWA EL-MELLOUHI, Texas A&M University at Qatar, LAURENT KARIM BELAND, NORMAND MOUSSEAU, Universite de Montreal — The time evolution of a series of well relaxed amorphous silicon models was simulated using the kinetic Activation-RelaxationTechnique (kART), an on-the-fly off-lattice kinetic Monte Carlo method [1]. This novel algorithm uses the ART nouveau algorithm to generate activated events and links them with local topologies. It was shown to work well for crystals with few defects but this is the first time it is used to study an amorphous material. A parallel implementation allows us to increase the speed of the event generation phase. After each KMC step, new searches are initiated for each new topology encountered. Well relaxed amorphous silicon models of 1000 atoms described by a modified version of the empirical Stillinger-Weber potential [2] were used as a starting point for the simulations. Initial results show that the method is faster by orders of magnitude compared to conventional MD simulations up to temperatures of 500 K. Vacancy-type defects were also introduced in this system and their stability and lifetimes are calculated.

[1] El-Mellouhi et al., ,Phys Rev. B, 78, 153202 (2008)
[2] Vink et al., J. Non-Cryst. Sol. 282, 248 (2001)

4:54PM X31.00013 ABSTRACT WITHDRAWN –

5:06PM X31.00014 Properties of fluids under strong confinement: a mode coupling approach , SAROJ NANDI, Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore - 560012, India, SARIKA BHATTACHARYA, Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore - 560012, India, SRIRAM RAMASWAMY, Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore - 560012, India — We extend the mode coupling theory (MCT) of glass transition in bulk fluids to the case of confinement, which enhances the feedback mechanism to drive the system to a glassy state. Confinement enters the theory in terms of an external potential that produces an inhomogeneous density background, which in turn forces the fluid to relax diffusively. Below a certain density, the MCT transition becomes continuous and the critical density of continuous to discontinuous transition depends on the nature of the external potential. If the control parameters are in the proper region of phase space, the fluid shows a three-step relaxation scenario. We also incorporate shear in our theory and thereby show that the fluid, when confined, shows shear thinning at much lower shear rate compared to a bulk fluid.

Thursday, March 24, 2011 2:30PM - 4:30PM –

Session X32 FIAP DCOMP: Focus Session: Frontiers in Computational Thermodynamics of Materials II C144

2:30PM X32.00001 Low temperature phase transition predicted in the compound B13C2/B4C[1] , MICHAEL WIDOM, Carnegie Mellon University — The experimental phase diagram of boron-carbon exhibits the compound boron-carbide over a broad composition range that extends to low temperatures, in seeming contradiction to the third law of thermodynamics. First principles total energy calculations suggest the presence of two energy-minimizing structures in the boron-carbon phase diagram, B13C2 and B4C. Both distribute boron and carbon atoms on the same 15-atom rhombohedral unit cell (hR15), consisting of 12-atom icosahedra at cell vertices plus three-atom chains at cell centers. However, only B13C2 respects the rhombohedral symmetry, while B4C breaks the symmetry by replacing one of the icosahedral boron atoms with carbon. Because B4C is incompatible with the experimentally observed rhombohedral symmetry, it must lose thermodynamic stability at elevated temperatures. We report a study of the configurational ensemble obtained by substitution of boron or carbon on different sites using a semi-grand canonical ensemble. Varying chemical potential at low temperature, we find sharp transitions from beta-rhombohedral boron to B13C2 then to B4C and finally to graphitic carbon. Only the rhombohedral-symmetry phase B13C2 survives at high temperature while the symmetry-broken phase B4C loses stability around room temperature.

[1]In collaboration with Will Huhn

3:06PM X32.00002 Thermodynamic modeling of Pt-Al and Pd-Al , DEREK CARR, Brigham Young University — Pure platinum and pure palladium are too soft for typical jewelry applications. Adding small amounts of other metals can significantly increase their performance. However, international hallmarking standards require the alloys to be 95% pure by weight. How does one achieve significant improvements in performance adding only small amounts (5 wt-%) of other metals? Significant improvements are possible even with small additions if precipitate hardening can be induced. Using a combination of first-principles, cluster expansion, and Monte Carlo modeling, we have identified new Pt-rich/Pd-rich phases in Pt-Al and Pd-Al that should be useful in precipitate hardening. Thermodynamical modeling indicates that the phases are experimentally feasible (not kinetically inhibited).

3:18PM X32.00003 Equation of State and Viscosity of Tantalum and Iron from First Principles , LJUBOMIR MILJACIC, STEVEN DEMERS, AXEL VAN DE WALLE, California Institute of Technology — To understand and model at continuum level the high-energy-density dynamic response in transition metals like Tantalum and Iron, as it arises in hypervelocity impact experiments, an accurate prediction of the underlying thermodynamic and kinetic properties for a range of temperatures and pressures is of critical importance. The relevant time scale of atomic motion in a dense gas, liquid, and solid is accessible with *ab-initio* Molecular Dynamics (MD) simulations. We calculate EoS for Ta and Fe via Thermodynamical Integration in 2D (V,T) phase space throughout different single and two-component phases. To reduce the *ab-initio* demand in selected regions of the space, we fit available gas-liquid data to the Peng-Robinson model [1] and treat the solid phase within the Boxed-quasi-harmonic approximation [2]. In the fluid part of the 2D phase space, we calculate shear viscosity via Green-Kubo relations, as time integration of the stress autocorrelation function.

[1] Ind. Eng. Chem., Fundam **15**, 59 (1976)
[2] A. van de Walle and G. Ceder, *Rev. Mod. Phys.* **74** 11 (2002)

3:30PM X32.00004 Binary Magnesium Alloys: Searching for Novel Compounds by Computational Thermodynamics , RICHARD TAYLOR, STEFANO CURTAROLO, Duke University, GUS HART, Brigham Young University — Magnesium alloys are among the lightest structural materials and are of considerable technical interest. We use the high-throughput framework AFLOW to make T = 0 K ground state predictions by scanning a large set of known candidate structures for thermodynamic minima. The study presented here encompasses 34 Mg-X systems of interest (X=Al, Au, Ca, Cd, Cu, Fe, Ge, Hg, Ir, K, La, Pb, Pd, Pt, Mo, Na, Nb, Os, Rb, Re, Rh, Ru, Sc, Si, Sn, Sr, Ta, Tc, Ti, V, W, Y, Zn, Zr). Avenues for further investigation revealed by this study include stable phases found in addition to experimental phases and compound forming systems thought to be either immiscible or non-compound forming. The existence of potentially novel ordered phases presents new opportunities for materials design.

3:42PM X32.00005 High-throughput combinatorial search of novel topological insulators , KESONG YANG, WAHYU SETYAWAN, SHIDONG WANG, Department of Mechanical Engineering and Materials Science and Department of Physics, Duke University, JEFFREY MULLLEN, MARCO BUONGIORNO-NARDELLI, Department of Physics, North Carolina State University, STEFANO CURTAROLO, Department of Mechanical Engineering and Materials Science and Department of Physics, Duke University, CURTAROLO GROUP @ DUKE: COMPUTATIONAL MATERIALS SCIENCE TEAM, BUONGIORNO-NARDELLI GROUP @NCSU: ERMES GROUP TEAM — In recent years, topological insulators (TIs) have attracted lots of attentions not only because of their interesting electronic characteristics induced by spin-orbit coupling but also their potential applications. So far, experimentally observed topological insulators mainly include HgTe/CdTe quantum well structure, semiconducting alloy $Bi_{1-x}Sb_x$, and so-called second-generation TI materials, i.e., the family of Bi_2Se_3, Bi_2Te_3, and Sb_2Te_3. Later theoretical simulations predict more TIs such as $TlBiQ_2$ and $TlSbQ_2$ (Q=Te, Se, and S), $LaBiTe_3$ as well as half-Heusler alloys, LuPtSb and ScPtBi. Numerous attempts are being made to look for more TIs. In this presentation, we will introduce our high-throughput combinatorial approach to find novel TI materials based on the AFLOW framework and distributed libraries.

3:54PM X32.00006 Classification of the ICSD by crystal Prototype , JUNKAI XUE, WAHYU SETYAWAN, STEFANO CURTAROLO, Duke University — An efficient way to determine the prototypes of the ICSD database has been implemented within our high-throughput formalism. This presentation illustrates how we use this tool to search for structure/properties correlations in an automatic fashion.

4:06PM X32.00007 Novel Occurences of $L1_1$ and $L1_3$ found using the synnergy between High Throughput and Cluster Expansion , LANCE NELSON, GUS HART, Brigham Young University, STEFANO CURTAROLO, Duke University — Despite their geometric simplicity, $L1_1$(CuPt) and $L1_3$ ($CdPt_3$) fail to appear as groundstates in experimental systems. ($L1_1$ appears in CuPt only) Are these crystal structures actually energetically unfavorable, or have they simply been overlooked in experimental studies? Here we investigate, using computational methods, the energetic stability of these phases in all binary inter-metallic systems. We combine the results of two techniques,namely High Throughput (HT) and Cluster Expansion (CE), to maximize efficiency and ensure thoroughness. HT results show $L1_1$($L1_3$) to be stable in the following systems: AgPd, AgPt, CuPt, PdPt(CdPt,CuPt,PdPt,LiPd,LiPt). Cluster expansions constructed for these systems verify the HT findings in all cases, with the exception of the HT groundstate PdPt-$L1_1$.(D_4 is found to be energetically more favorable) Monte Carlo simulations, which are used to identify order-disorder transition temperatures, were performed for all occurences of these two phases. While the transition temperatures for some systems are found to be extremely low, others appear to be physically realizable.

4:18PM X32.00008 Ab Initio Insights on the Shapes of Nanocrystals[1] , ROMAN CHEPULSKYY, STEFANO CURTAROLO, Duke University — Catalytic, chemical, optical and electronic properties of nanocrystals are strongly influenced by their faceting. A variational approach based on quantum mechanical energies is introduced to evaluate stable and metastable shapes of nanocrystals. The method leads to a nanoscale equation of state, which is solved self-consistently. Using platinum as example, it is found that the surface energy dependence on the lattice parameter is the key factor controlling the equilibrium stability of the crystal shapes. The energies of different surfaces versus lattice parameter are calculated from first principles in high-throughput fashion. Considering several crystal shapes and using Wulff's construction, the transitions between stable and metastable shapes are predicted below 3 nm in diameter. Our variational approach explains experimental results and establishes a direction to search for better catalysts.

[1]Research supported by ONR and NSF.

Thursday, March 24, 2011 2:30PM - 5:18PM –
Session X33 DCMP: Quantum Fluids and Solids I C143/149

2:30PM X33.00001 Characterization of MEMS Devices for the Study of Superfluid Helium Films[1] , MIGUEL GONZALEZ, BYOUNG HEE MOON, PRADEEP BHUPATHI, PAN ZHENG, GEORGE LING, ERIK GARCELL, Department of Physics, University of Florida, Gainesville, FL 32611, USA, HO BUN CHAN, Department of Physics, The Hong Kong University of Science and Technology, Hong Kong, China, YOONSEOK LEE, Department of Physics, University of Florida, Gainesville, FL 32611, USA — Measurements on the mechanical attributes of MEMS resonators were performed at room and low temperatures. Specially devised resonators which can be actuated for shear motion were designed and fabricated using a state-of the-art multi-user MEMS process. The devices consist of a pair of parallel plates with a well-defined gap whose size can be controlled with high accuracy down to the sub-micron range. A full study of resonance properties at various pressures was performed at room temperature. Details of design, fabrication, and operation will be presented along with results from a preliminary study of a resonator immersed in liquid ^{4}He. The devices show potential for use in low temperature experiments and to investigate novel phenomena in quantum fluids at the micro/nano scale such as superfluid ^{3}He films.

[1]Supported by NSF through DMR- 0803516 (YL)

2:42PM X33.00002 Interplay of Aerogel Anisotropy and Textures in Superfluid ^{3}He , JIA LI, JOHANNES POLLANEN, CHARLES COLLETT, WILLIAM J. GANNON, WILLIAM P. HALPERIN, Department of Physics and Astronomy, Northwestern University — We have performed pulsed NMR on ^{3}He-B in 98.1% porosity aerogel with different anisotropy. The aerogel anisotropy was characterized with an optical, cross-polarization technique [1]. In the isotropic aerogel sample at P = 26 bar and $T < 1.2mK$, we find a single peak with a positive frequency shift relative to the Lamor frequency indicating an n-texture that is predominately perpendicular to the field. Upon warming, we find a crossover at $T \approx 1.2mK$ from $n \perp \mathbf{H}$ to a texture where n is predominately parallel to the field. Near the crossover the NMR intensity is distributed among two components indicating an inhomogeneous texture. We have also studied an anisotropic aerogel which was compressed along its cylinder axis by 22.5%. At the same pressure, we find a homogeneous texture for all T and a similar textural crossover from $n \perp \mathbf{H}$ to $n \parallel \mathbf{H}$, but for this sample the textural crossover happens near $T_{caerogel}$. We have introduced a model to account for the interplay of aerogel anisotropy and n-textures. Currently we are studying the tip angle dependence of NMR frequency shifts in these aerogels. This work was supported by the National Science Foundation, DMR-0703656.
[1] J. Pollanen et al. *J. of Non-Crystalline Solids* **354**, 4668 (2008).

2:54PM X33.00003 Equal-Spin Pairing Superfluid State of ^{3}He in Radially Compressed Aerogel , J. POLLANEN, J. LI, C. COLLETT, W.J. GANNON, W. P. HALPERIN, Northwestern University — Anisotropic quasiparticle scattering has been predicted to stabilize anisotropic superfluid states of ^{3}He [1,2]. We have performed pulsed nuclear magnetic resonance (NMR) experiments on ^{3}He in a homogeneously anisotropic 97.5% porosity aerogel. From the NMR frequency shifts on warming at P = 26 bar we find a single superfluid state exists between $0.7mK$ and $T_{caero} = 1.67mK$. Susceptibility measurements indicate this phase is an equal-spin pairing (ESP) state. The anisotropy of our cylindrical aerogel sample was induced during the growth and drying stages in the form of 14.3% radial compression. The sample was characterized with an optical, cross-polarization technique [3] to confirm the presence of a homogeneous optical axis aligned with the cylinder axis. Similar experiments and characterization have been performed on a homogeneously isotropic 98.1% aerogel and, in this case, we find the non-ESP aerogel B-phase is the stable state. We are currently studying the tip angle dependence of the NMR frequency shift to identify which of the ESP states we have observed and to explore the full P-T phase diagram of superfluid ^{3}He in these aerogels. This work was supported by the National Science Foundation, DMR-0703656. [1] C.L. Vicente, et al., PRB 72, 094519 (2005). [2] K. Aoyama and R. Ikeda, PRB 73, 060504(R) (2006). [3] J. Pollanen et al., JNCS 354, 4668 (2008).

3:06PM X33.00004 Moderate Magnetic Field Transverse Acoustics in Superfluid ^{3}He-B , C. COLLETT, S. SASAKI, J.P. DAVIS, J. POLLANEN, W.J. GANNON, J. LI, W.P. HALPERIN — We present the results of transverse acoustics studies in superfluid ^{3}He-B at fields up to 0.1 T. Using acoustic cavity interferometry, we observe the acoustic Faraday effect[1,2] for a transverse sound wave propagating along the magnetic field, and we measure Faraday rotations of the polarization of the sound up to 990°, significantly more extensive than has been previously reported. We use these results to extend previous calculations of the Landé g factor. We also find the field dependence of cavity interference oscillations resulting from coupling to the imaginary squashing mode (ISQ), a collective mode of the order parameter with total angular momentum $J = 2$. Measurements in large magnetic fields were performed at frequencies up to the pair breaking threshold, where there has been a recent report[3] of a new collective mode with $J = 4$. The discovery of Faraday rotations coming from this new mode is reported, along with their intersection with rotations from the ISQ. Support for this work from the NSF, grant DMR-0703656, is gratefully acknowledged.

[1]G.F. Moores and J.A. Sauls, J. Low Temp. Phys. **91**, 13 (1993).
[2]Y. Lee *et al.*, Nature **400**, 431 (1999).
[3]J.P. Davis *et al.*, Nature Physics **4**, 571 (2008).

3:18PM X33.00005 Lévy Flights and Anomalous Diffusion in Liquid ^{3}He-Aerogel[1] , JAMES SAULS, Northwestern University — The transport of heat by liquid ^{3}He impregated into silica aerogel is limited at low temperatures by elastic scattering of quasiparticles by the aerogel. The gossamer structure of silica aerogel is a realization of a random fractal - a solid with no long-range order, but power-law scaling of the density correlation function. Complementary to fractal scaling of the particle-particle correlation function is the appearance of a power law distribution of *free flight paths*. The open structure shown in the DLCA simulations of low-density aerogel leads to a distribution of exceedingly long flight paths governed by a Lévy distribution. I describe a theory for anomalous diffusion of quasiparticles in which the Lévy distribution of long free paths is interrupted by inelastic collisions between quasiparticles. These rare events lead to finite temperature corrections to the thermal diffusion coefficient of the form, $\kappa/T = K_0 - K_1\,(T/T^\star)^\beta$, where $T^\star$ is the temperature at which the elastic and inelastic mean free paths are equal and β is related to the fractal dimension of the Lévy distribution.

[1]Supported by National Science Foundation Grant DMR-0805277.

3:30PM X33.00006 Signatures of Crystalline Phases and Domain Walls in Superfluid ^{3}He Thin Films[1] , ANTON VORONTSOV, Montana State University, JAMES SAULS, Northwestern University — Thin films of superfluid ^{3}He may spontaneously break translation symmetry in the plane of the film.[2] Near a critical film thickness, $D_{c_1} \approx 13\,\xi_0$, a one-dimensional "stripe phase" develops as a periodic array of domain walls separating degenerate, but inequivalent B-phases, $(\Delta_{||}, \Delta_{||}, +\Delta_\perp)$ and $(\Delta_{||}, \Delta_{||}, -\Delta_\perp)$. These defects have a unique spectrum of topological excitations bound to the domain wall. We present results for the order parameter and Fermionic spectrum, and their observable signatures, for a single domain wall and for the stripe phase. The combination of particle-hole asymmetry and broken translational symmetry of the order parameter leads to a weak modulation of the density, $\delta n \sim \ln\left(E_f/k_BT_c\right)\left(k_BT_c/E_f\right)^2\,\bar{n}$, where $\bar{n}$ is the mean particle density. This leads to a modulation of the van der Walls attraction, and thus a small, static modulation of the film thickness. We report theoretical results for the density modulation, film thickness profile and optical reflectivity for the crystalline phases of superfluid ^{3}He.

[1]Supported by NSF Grants: DMR-0805277 and 0954342.
[2]Phys. Rev. Lett. 98,045301 (2007).

3:42PM X33.00007 Visualization of counterflow dynamics using frozen nanoparticles[1] , ENRICO FONDA, University of Trieste - University of Maryland, College Park, MATTHEW S. PAOLETTI, University of Texas at Austin, KATEPALLI R. SREENIVASAN, New York University, DANIEL P. LATHROP, University of Maryland, College Park — We study the dynamics of quantized vortices and quantum turbulence utilizing a particle tracking visualization technique. This is accomplished by using sub-micron and micron-sized hydrogen or atmospheric ice particles injected into He^4 flows that get trapped on the vortices. This technique has been used to observe and characterize reconnection of quantized vortices and thermal counterflow. We present the latest results using nano-sized ice particles. These sub-micron particles are superior to larger particles in a number of ways. In particular, being less affected by Stokes drag, they stay trapped on faster moving vortices and remain trapped closer to the lambda transition. Using these particles, we have made additional observations of counterflows at higher heat fluxes to shed light on the particle-vortex interaction mechanism. The technique has also been extended for visualization for fluid dynamics experiments using liquid nitrogen.

[1]This research was supported by the NSF-DMR.

3:54PM X33.00008 Numerical Real Space Renormalization of a 2D Random Boson Model , SHANKAR IYER, GIL REFAEL, California Institute of Technology — Interest in the random boson problem originated in experiments on Helium adsorbed in Vycor, but the problem arises in many contexts, including Josephson junction arrays and disordered cold atom systems. Recently, Altman, Kafri, Polkovnikov, and Refael have studied a rotor model description of interacting bosons subjected to quenched disorder in one dimension. Using a real space renormalization approach, they have identified a random fixed point that marks the transition between superfluid and Mott-glass phases. Here, we describe work that numerically extends their approach to the random boson problem in two dimensions. We first test the validity of the real space renormalization by comparison to exact diagonalization of small systems. Then, we move to larger systems and explore what the renormalization scheme can tell us about the nature of the insulating and superfluid phases.

4:06PM X33.00009 Third Sound in Superfluid ^{4}He Films Adsorbed on Packed Multiwall Carbon Nanotubes[1] , EMIN MENACHEKANIAN, GARY A. WILLIAMS, University of California, Los Angeles — An investigation of third-sound propagation is carried out with thin ^{4}He films adsorbed on multiwall carbon nanotubes. At an average diameter of 12 nm and a length of several microns, the powder of nanotubes is lightly packed into a cylindrical resonator, with a resistor bolometer at the cylinder end to detect the temperature oscillations accompanying the waves. The lowest standing-wave mode in the cavity is excited by mechanical vibrations, with FFT analysis allowing measurement of the sound speed as well as the dissipation. The Kosterlitz-Thouless onset transition is observed with increasing film thickness for temperatures between 1.3 and 1.7 K. At higher thicknesses capillary condensation becomes important, probably at connection points where the nanotubes touch. Layering effects in the third-sound velocity, associated with the relatively strong van der Waals coupling between helium and carbon, are not observed, and measurements below 1 K may be necessary to see this. There is also no indication of any effect of superfluidity attributable to the adsorption of helium on the inner surfaces of the nanotubes.

[1]This research has been supported by the National Science Foundation, Grant No. DMR 09-06467.

4:18PM X33.00010 ABSTRACT WITHDRAWN –

4:30PM X33.00011 Vortex-Loop Thermodynamics of Superfluid ^{4}He Under Pressure[1] , ANDREW FORRESTER, GARY A. WILLIAMS, UCLA — The thermodynamic quantities of pressurized superfluid ^{4}He near the λ-transition are calculated using a vortex-loop renormalization method. The superfluid density, specific heat, vortex core size, and vortex core energy are determined as functions of pressure and temperature, and compared with experiments. The theory predicts exponents describing the critical behavior of the superfluid density and specific heat that are in agreement with recent high-precision theoretical simulations. The vortex core size is found to increase with pressure, while the core energy decreases, the behavior found experimentally for both parameters. The specific heat, though strongly dependent on both of these parameters, is found to scale with pressure in agreement with experimental measurements.

[1]Work supported by the NSF, DMR 09-06467

4:42PM X33.00012 Topological and geometrical interactions between quantum vortices near zero temperature , RAN CHENG, XIAO LI, QIAN NIU, University of Texas at Austin — With new velocity-dependent term discovered, various types of interactions between quantum vortices in 2-d superfluid Helium and BEC near zero temperature are unified via Berry Phase theory. Originated from the finite compressibility of the fluid, the topological statistical gauge field of an vortex breaks down to geometrical gauge field mediating local interactions. This new interaction modifies the cyclotron motion of a pair of identical vortices, and changes the pattern of orbits of a pair of vortex-antivortex. Damping effect due to finite temperature is treated phenomenologically, which does not invalidate our essential conclusions.

4:54PM X33.00013 Semiclassical dynamics of vortices in superfluid helium thin films , XIAO LI, RAN CHENG, QIAN NIU, The University of Texas at Austin — Based on the Berry phase theory, we consider the case of two vortices in Bosonic superfluids and try to extract the interaction between them. Under the adiabatic approximation, we use semiclassical Lagrangian formalism to describe the system and found that in addition to the universal background "magnetic field" which results in the Magnus force, there exists a new interaction mediated by the density profile of the background fluid due to its finite compressibility. Finally, numerical solutions from the nonlinear Schrodinger equation were employed to gain better insight into this problem.

5:06PM X33.00014 Theory of the Bose-glass states in Br-doped Nickel-Tetrakis Thiourea (DTN) , RONG YU, Rice University, STEPHAN HAAS, University of Southern California, TOMMASO ROSCILDE, Ecole Normale Superieure de Lyon - France — We present extensive Quantum Monte Carlo calculations on bond-disordered coupled spin chains with strong single-ion anisotropy, modeling the behavior of Br-doped Nickel-Tetrakis Thiourea (DTN). Our model quantitatively describes the phase diagram of the experimental compound - in particular the low-temperature magnetization curve and the critical temperature for magnetic Bose-Einstein condensation as a function of the field. Hence it provides fundamental insight into the nature of the Bose-glass phases appearing at low temperature close to the two critical fields for condensation. Br-doped bonds act as nucleation centers of magnetic quasiparticles in the low-field Bose glass, while at high fields the Br-doped bonds represent the localization centers of magnetic quasiholes. The quantitative understanding of Br-doped DTN opens the way to a detailed investigation of Bose-glass physics in quantum magnets.

Thursday, March 24, 2011 2:30PM - 5:30PM –

Session X34 DCMP: Nanostructures: Assembly, Growth, and Characterization C141

2:30PM X34.00001 Vapor-Liquid-Solid Glancing Angle Deposition (VLS-GLAD): A New Approach to Fabricate Crystalline Semiconductor Nanowires , ARIF SINAN ALAGOZ, TANSEL KARABACAK, Department of Applied Science, University of Arkansas at Little Rock — Vapor-liquid-solid (VLS) method has become one of the few and most powerful bottom-up single crystal nanowire growth techniques. On the other hand, control of growth direction and crystal orientation of semiconductor nanowires stand as major issues in VLS technique. In order to overcome these challenges, we developed a new vapor-liquid-solid glancing angle deposition (VLS-GLAD) fabrication approach for the growth of semiconductor nanowire arrays with a controlled geometry and crystal orientations. VLS-GLAD is a physical vapor deposition nanowire fabrication approach based on selective deposition of nanowire source atoms onto metal catalyst nanoislands placed on a crystal wafer. In this technique, collimated obliquely incident flux of source atoms selectively deposit on catalyst islands by using "shadowing effect". Geometrical showing effect combined with conventional VLS growth mechanism leads to the growth of tilted crystalline semiconductor nanowire arrays. In this presentation, we show the morphological and structural properties of tilted single crystal Si and Ge nanowire arrays fabricated by utilizing a conventional thermal evaporation system for VLS-GLAD.

2:42PM X34.00002 LEEM and STM observations of Growth of Nanowires of Ag on Ge(110) and Surface Structural Phases of Ir on Ge(111)[1] , CORY MULLET, MARSHALL VAN ZIJLL, EMILIE HUFFMAN, SHIRLEY CHIANG, University of California, Davis — We have used both low energy electron microscopy (LEEM) and scanning tunneling microscopy (STM) to characterize the growth of silver on Ge(110) and iridium on Ge(111) as a function of coverage, deposition temperature, and annealing temperature. We observed 1D island growth along [-110] as Ag is deposited onto Ge(110) above 430 C. Island dimensions varied with deposition temperature. At 480 C, Ag islands are $\sim$100nm wide and 1-20 μm long for 9 ML coverage. Between 380 C and 430 C, we observed two novel low coverage phases, with the higher coverage phase completing at 0.12 ML. Ir deposited onto the Ge(111) c(2x8) above 400 C forms a $(\sqrt{3}x\sqrt{3})R30^o$ phase, with island size dependent upon substrate temperature during deposition. Deposition at 400-425 C produces Ir islands, which are 1-20 nm in diameter at 0.5 ML coverage. Island heights range from one to several atomic layers, and exhibit a unique growth mode with islands connected by "streamers" of Ir. We observed Stranski-Krastanov growth in LEEM at 670 C. Ir desorbs from Ge(111) at 870 C, beginning from areas of high step density.

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

2:54PM X34.00003 ABSTRACT WITHDRAWN –

3:06PM X34.00004 Alignment of Gold Nanorods in Thermoresponsive Hydrogels[1] , HEUNG-SHIK PARK, OLEG LAVRENTOVICH, Kent State University — The unique optoelectronic properties of the anisotropic metallic nanorods (NRs) are of great interest because of their potential applications in biomedical science, transformative optics and materials science. In order to utilize metallic NRs for the practical devices, the control of orientation and immobilization of NRs in bulk materials are essential. We report an experimental study of gold NR embedded in thermoresponsive gels which can align NRs by volume-contraction transition. When temperature increases, an NR hydrogel stripe experiences an abrupt shrinkage in two lateral (x,y) directions; in the third z-direction, the size remains fixed as the stripe is clamped. The shrunk stripes show high birefringence and anisotropic absorption associated with alignment of the NRs. The alignment of NRs in anisotropically shrunk hydrogels can be achieved also when one uses aggregates of side-by-side preassembled NRs rather than individual NRs. These aggregates can be transferred into a polymer hydrogel preserving their structural and optical features. The hydrogel stripes with preassembled NRs show optical anisotropy opposite to that one of stripes with isolated NRs.

[1]AFOSR FA9550-10-1-0527 and MURI FA9550-06-1-0337

3:18PM X34.00005 Programmable Nanofabrication of Nanoparticle Assemblies of arbitrarily Shapes on DNA Templates , MAURICIO PILO-PAIS, SARAH GOLDBERG, Duke University, ENRIQUE SAMANO, CNyN-UNAM, Ensenada, B.C., México, HENOK MEBRAHTU, THOMAS LABEAN, GLEB FINKELSTEIN, Duke University, GLEB FINKELSTEIN TEAM, THOMAS LABEAN TEAM — We present a method for producing metallic structures with nanoscale dimensions and programmable design. Rectangular "DNA origami" structures ($\sim$90x70nm) were modified to have uniquely coded binding sites and adsorbed onto silicon dioxide substrates. Gold nanoparticles functionalized with a complimentary DNA sequence were attached to these binding sites in a highly controllable fashion. The seed nanoparticles were then enlarged (and even fused, if desired) by a silver reduction chemistry. Using this method we constructed a variety of metallic structures, including parallel wires, H-shapes, and rings. Due to the flexibility of the design and the multiply parallel nature of the method, these structures may offer great promise for plasmonic applications.

3:30PM X34.00006 Controlling Nanostructure Self-assembly for Design of Three-dimensional Semiconductor Heterostructures[1] , SANTINO D. CARNEVALE, J. YANG, P.J. PHILLIPS, M.J. MILLS, R.C. MYERS, Dept. of Materials Science and Engineering, Ohio State University — We examine the control of vertical and coaxial growth in self-assembled GaN/AlN nanowires grown on Si (111) by plasma assisted molecular beam epitaxy. To grow nanowires vertically and not radially a two-step growth method is used. Nanowires are nucleated at low temperatures and grown vertically at high temperatures, allowing for independent control of density and height and constant radius. A second method is used to promote radial growth. GaN nanowire cores are formed, then growth temperature is reduced and growth continues. Vertically and coaxially oriented AlN/GaN heterostructures grown using these methods are presented. We discuss the structural and optical properties of these GaN/AlN quantum disk and core-shell heterostructures using scanning electron microscopy, scanning transmission electron microscopy, and temperature dependent photoluminescence measurements.

[1]Work supported by the Office of Naval Research.

3:42PM X34.00007 Preparation of monodisperse silicon nanocrystals through density-gradient unltracentrifugation in organic solvents[1] , JOSEPH B. MILLER, AUSTIN VAN SICKLE, SWATHI IYER, NDSU, REBECCA A. ANTHONY, UWE R. KORTSHAGEN, University of Minnesota, ERIK K. HOBBIE, NDSU — Monodisperse colloidal suspensions of ligand-coated silicon nanocrystals, synthesized through a nonthermal low-pressure plasma reaction, have been prepared through density-gradient ultracentrifugation in mixed organic solvents. Density-gradient profiles of mixed chloroform and m-xylene are used to tune and control the settling speed of the nanoparticles and hence optimize their transient separation by size along the depth of polyoxymethylene ultracentrifuge tubes. The mean size and polydispersity of the extracted fractions are characterized through photoluminescence spectroscopy and transmission electron microscopy, and the self-assembly of fractions into close-packed crystal lattices is achieved using an immiscible two-fluid evaporation scheme. The photophysical properties of the nanocrystal lattices are compared with those of the starting materials and suspensions, and the influence of atmospheric oxygen on the stability of the nanocrystal photoluminescence is measured.

[1]Supported by the DOE through DE-FG36-08GO88160

3:54PM X34.00008 Self-assembled Au Nanoparticle Arrays with Engineered Hot Spots for SERS , A. CHEN, U. WELP, V. VLASKO-VLASOV, Material Science Division, Argonne National Laboratory, A.E. DEPRINCE III, A. DEMORTIERE, A. JOSHI-IMRE, E.V. SHEVCHENKO, S.K. GRAY, Center for Nanoscale Materials, Argonne National Laboratory — We demonstrate a cost-effective bottom-up self-assembly of 80 nm Au nanoparticles (NPs) with controllable regular arrays of hot spots for high-fidelity and high-sensitivity sensor applications. The self-assembly of gold NPs is implemented using solvent evaporation techniques. By careful control of surface stabilizers on NPs and optimization of assembly conditions, we fabricated hcp arrays of NPs extended over more than 200 μm. Electromagnetic hot spots localized in the nanometer gaps between Au NPs are well defined and reproducible over large areas of the arrays. UV-Vis-NIR extinction spectra of our 2D plasmonic crystals exhibit unique resonances due to strong particle-particle interactions, in a good agreement with results of our finite-difference-time-domain (FDTD) simulations. We experimentally demonstrate large enhancements of both photoluminescence and surface enhanced Raman scatterings of 5nm CdSe quantum dots coated on 80nm Au NP arrays. High-resolution SEM imaging of quantum dots gave a precise estimate of their density and positions and allowed direct evaluation of the enhancement factors.

4:06PM X34.00009 Fine tuning nanoparticle spacing in freestanding membranes through ion and electron beams , PONGSAKORN KANJANABOOS, The University of Chicago, ALEXANDRA JOSHI-IMRE, XIAO-MIN LIN, Argonne National Laboratory, HEINRICH JAEGER, The University of Chicago — Freestanding membranes of ligated nanoparticles can be assembled in a one-step drying-mediated process. These 2D sheets have remarkable mechanical properties, in particular extreme bending flexibility coupled with effective Young's moduli in the range of 1-20GPa, depending on the nanoparticle and ligand types and sizes. We report on experiments in which used a focused Ga ion beam to strategically place cuts into freestanding monolayer membranes. Exposed to electron beams, the cuts expand and the membranes act as if additional strains were deposited. Given that the exposed membranes behave like strained elastic sheets, we can easily design various strain patterns. With calibration, the electron beam dose serves as a knob to fine-tune interparticle distances in these patterns.
K. E. Mueggenburg, X. Lin, R. H. Goldsmith, and H. M. Jaeger, Nature Materials 6, 656 (2007). J. He, P. Kanjanaboos, N. L. Frazer, X. Lin, and H. M. Jaeger, Small 6, 1449 (2010) W. Cheng et al. Nature Materials 8, 519 (2009)

4:18PM X34.00010 Mechanics of colloidal nanoparticle arrays , JIE YIN, MARKUS RETSCH, EDWIN L. THOMAS, MARY C. BOYCE, Massachusetts Institute of Technology, BOYCE TEAM, THOMAS TEAM — Hollow colloidal nanoparticles have become a focal point of studies for applications in drug delivery and nanostructured materials. The mechanical properties of individual nanoparticle and the collective behavior of colloidal nanoparticle arrays are of great importance. In this paper, the mechanics of colloidal arrays of hollow amorphous silica spherical nanoparticles during microindentation are explored. The study reveals that the consecutive contact process of nanoparticles during indentation results in highly nonlinear indentation load-displacement curves. The contacted nanoparticles successively become flattened and locally bend and buckle to form a localized dimple as the indentor encounters each particle. By using the contact mechanics model of single hollow particle, the indentation load-displacement formula is obtained for indentation on hollow spherical nanoparticle arrays and the Young's modulus of an individual particle is extracted from the measured load-displacement behavior of an array. The reduced Young's modulus is consistent with the measurement of single hollow amorphous silica nanoparticle by using AFM.

4:30PM X34.00011 Au/Fe nanoparticles prepared by multilayers annealing[1] , AIDA SERRANO, Institute for Ceramic and Glass- CSIC, OSCAR RODRIGUEZ DE LA FUENTE, Dpt. Material Physics - University Complutense at Madrid, MIGUEL ANGEL GARCIA, Institute for Ceramic and Glass- CSIC — Metallic nanoparticles supported onto a substrate can be obtained by thin film deposition and subsequent annealing. The stress relief after the thermal annealing due to the difference of thermal expansion coefficient between the metal and the substrate promotes hillock formation and subsequent hole nucleation, growth and percolation leading to the formation of nanoparticles layers. The nanoparticle size and inter-particle distance can be tuned by controlling the initial film thickness and the annealing time, temperature and atmosphere, providing a simple and low cost method to prepare NPs layers over large areas. The method has been successfully applied to obtain nanoparticles from a single metallic layer in the past. We report here the formation of complex nanoparticles ensembles by deposition and annealing of Au-Fe multilayers. The optical properties of gold nanoparticles (surface plasmon resonance absorption) and the magnetic properties of Fe/Fe oxide ones as well as cross-over effects are studied as a function of multilayers structure and annealing conditions.

[1]This work was supported by the Spanish Ministry of Science and Education through the project FIS-2008-06249

4:42PM X34.00012 Effects of ligand binding strength and facet coverage on the morphology of nanocrystal superlattices[1] , CLIVE BEALING, RICHARD HENNIG, Cornell University — Nanocrystals (NCs) of lead-salt have been proposed for a number of photovoltaic applications. These NCs consist of an inorganic core, in the rock salt structure, whose surface is usually passivated by oleate ligands. The self-assembly of NCs from colloidal solutions into mesoscale superlattices provides a path to materials with tunable electronic, physical and chemical properties that are promising for applications. The self-assembly is controlled by the NC shape and by ligand-mediated interactions between NCs; to understand this, it is necessary to know the effect of the ligands on the surface energies, as well as the relative coverage of the different facets. Our density functional calculations of the binding energies of carboxylic acid-based ligands on PbSe and PbS show that the ligands exhibit a strong energetic preference to particular facets. The results suggest that the transformation of the NC superlattice structure from *fcc* to *bcc* in aged NC assemblies is caused by the preferential detachment of ligands from particular facets, leading to anisotropic ligand coverage. Combined with the experimental results, our calculations present a potential route to greater control over the morphology of the NC superlattice assembly.

[1]This work was supported by Award No. KUS-C1-018-02, made by King Abdullah University of Science and Technology (KAUST).

4:54PM X34.00013 Scanning Tunneling Microscopy and Spectroscopy of Rare Earth-Monopnictide Nanostructures Embedded in a Semiconducting Matrix , JASON KAWASAKI, University of California Santa Barbara, RAINER TIMM, Lund University, TREVOR BUEHL, University of California Santa Barbara, EDVIN LUNDGREN, ANDERS MIKKELSEN, Lund University, ARTHUR GOSSARD, CHRIS PALMSTRØM, University of California Santa Barbara — The atomic and electronic structure of molecular beam epitaxy (MBE)-grown rare earth-monopnictide nanostructures embedded within a III-V semiconductor matrix are examined via scanning tunneling microscopy (STM) and spectroscopy (STS). We examine several systems, including ErSb nanoparticles embedded in GaSb, ScAs nanoparticles embedded in GaAs, and ErAs nanoparticles and nanorods embedded in GaAs. Tunneling current I(V) and differential conductance dI/dV spectra show that for both ErAs nanoparticles and nanorods the local density of states (LDOS) exhibits a sharp but finite minimum at the Fermi level, demonstrating that both the particles and rods are semimetallic and not semiconducting. This observation lies in contrast to previous models of quantum confinement in ErAs. We also use STS to measure the LDOS across the ErAs/GaAs interface and discuss the formation of interface states and band bending at the interface. Finally, we discuss possible changes in the LDOS with varying nanoparticle size and varying levels of doping in the semiconductor matrix.

5:06PM X34.00014 *Ab Initio* Studies of Si_mGe_n(m+n $\leq$ 5) Nanoclusters[1] , SARAH DUESMAN, ASOK RAY, University of Texas at Arlington — Electronic and geometric structure properties of Si_mGe_n(m+n $\leq$ 5) nanoclusters have been investigated using hybrid density functional B3LYP, 6-311G (3df, 3pd) basis set, and the GAUSSIAN 03 software. For the Si atom, the computed values of the ionization potential and electron affinity are 8.11 and 1.10eV, and for the Ge atom, the values are 7.90 and 1.14eV. The experimental values are 8.15, 1.39, 7.90, and 1.23eV, respectively. Various possible geometries have been spin-optimized to determine the global minimum for each nanocluster. We will present the electronic and geometric structures of the isomers of each nanocluster, including bond length, symmetry group, electronic state, binding energy, HOMO-LUMO gap, ionization potential, and electron affinity. In addition, the harmonic frequencies, fragmentation energies, average coordination number and Mulliken atomic charges will also be discussed for the ground states of the nanoclusters.

[1]This work is partially supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525).

5:18PM X34.00015 Competition of Nonlinear Optical Properties in ZnO Nanoparticles , JIE LIN, ANTONIO LLOPIS, BENNY URBAN, University of North Texas, YASUHISA FUJITA, Shimane University, ARUP NEOGI, University of North Texas — ZnO nanoparticles have attracted increased attention due to its large exciton binding energy. Moreover it has enhanced nonlinear optical properties due to its noncentrosymmetric crystal structure which results in a second order nonlinearity. The presence of oxygen vacancy and modified surface states also yields third order nonlinearity such as two photon absorption which yield significant two-photon emission. However, the presence of high second order nonlinearity in a system can result in the retardation of the third order nonlinearity. We thereby present the relative efficiencies of the second and the third-order nonlinear processes in ZnO nanoparticle system. Using tunable femtosecond laser irradiation the recombination lifetime due to single and two-photon induced electron-hole recombination process has been studied. Our results show that the second harmonic generation (SHG) process compete with the two photon emission(TPE) process in the region 700nm—900nm. The TPE process is more efficient in 700 nm-740nm whereas the SHG process is more efficient from 745-900nm) region. We also observed the increase of the two photon emission with excited energy is caused by the increased life of its virtual state.

Thursday, March 24, 2011 2:30PM - 5:42PM –
Session X35 DCMP: Topological Insulators: Theory III C140

2:30PM X35.00001 Search for New Topological Insulators , HSIN LIN, Northeastern U., L.A. WRAY, S.-Y. XU, M.Z. HASAN, Princeton U., T. DAS, Y.J. WANG, R.S. MARKIEWICZ, ARUN BANSIL, Northeastern U. — Topological insulators (TIs) host a novel quantum phase of electrons which is characterized by topologically protected surface states originating from the effects of spin-orbit and time-reversal symmetries. While several families of TIs have already been found, the intense world-wide search for new classes of TIs continues unabated. This interest is driven by the need for materials with greater structural flexibility and tunability to enable viable applications in spintronics and quantum computing. We have used first-principles band theory computations in combination with angle-resolved photoemission experiments to successfully predict many new classes of topologically interesting materials, including Bi2Se3 series, the ternary half-Heusler compounds, thallium-based chalcogenides, and the Li2AgSb and $Ge_nBi_{2m}Te_{3m+n}$ families. [1-5] Work supported by the Office of Basic Energy Sciences, US DOE.

[1] H. Lin, R. S. Markiewicz, L. A. Wray, L. Fu, M. Z. Hasan, and A. Bansil, Physical Review Letters **105**, 036404 (2010).
[2] H. Lin, L. A. Wray, Y. Xia. S. Y. Xu, S. Jia, R. J. Cava, A. Bansil, and M. Z. Hasan, Nature Materials **9**, 546 (2010).
[3] W. Al-Sawai *et al.*, Physical Review B **82**, 125208 (2010).
[4] L. A. Wray *et al.*, Nature Physics (2010, in press).
[5] S.-Y. Xu *et al.*, arXiv:1007.5111 (2010).

2:42PM X35.00002 Spin-texture of three-dimensional topological insulators: Bi_2Te_3, Bi_2Se_3 and Sb_2Te_3 , SUSMITA BASAK, HSIN LIN, Northeastern University, L.A. WRAY, S.-Y. XU, M.Z. HASAN, Princeton University, A. BANSIL, Northeastern University — We have investigated the nature of surface states in the Bi_2Te_3, Bi_2Se_3 and Sb_2Te_3 family of 3D topological insulators using first-principles calculation as well as $k \cdot p$ scheme [1]. Recent spin-resolved photoemission experiments suggest that electrons on the surface of a topological insulator behave as massless relativistic particles with an intrinsic angular momentum (spin) which is locked to their translational momentum [2,3]. We have computed the in-plane spin-textures of all three aforementioned compounds to demonstrate the 'spin-helical' nature of the 2D fermions. In addition, the spin must acquire a finite out-of-the-plane component to preserve the bulk topological invariant [1]. We study this quantity in particular since there are possibilities of observing new quantum effects. Work supported by the US DOE.

[1] L. Fu, Phys. Rev. Lett. **103**, 266801, (2009).
[2] D. Hsieh *et al.*, Science **323**, 919 (2009).
[3] D. Hsieh *et al.*, Nature **460**, 1101 (2009).

2:54PM X35.00003 First principles analysis of quantum transport in Bi2Se3 3D topological insulators , YONGHONG ZHAO, YIBIN HU, LEI LIU, YU ZHU, HONG GUO — By carrying out density functional theory (DFT) within the Keldysh nonequilibrium Green's function formalism (NEGF), we have investigated quantum transport properties of the Bi2Se3 topological insulator from atomistic first principles without any phenomenological parameters. Using the scattering states, our results vividly reveal the surface Dirac fermions and helical edge spin states in the momentum space. We have also determined the real-space distribution of the helical edge spin states which provide the penetration depth of the surface topological conducting channels into the bulk Bi2Se3 crystal. Our first principles calculations take into account the full non-collinear spin structure and spin-orbit interaction, the details of these technical advances within the NEGF-DFT quantum transport formalism will also be briefly discussed.

3:06PM X35.00004 Electrically controllable surface magnetism on the surface of topological insulator[1]

, JIA-JI ZHU, SKLSM, Institute of Semiconductors, Chinese Academy of Sciences, DAO-XIN YAO, School of Physics and Engineering, Sun Yat-sen University, SHOU-CHENG ZHANG, Department of Physics, Stanford University, KAI CHANG[2], SKLSM, Institute of Semiconductors, Chinese Academy of Sciences — We study theoretically the RKKY interaction between magnetic impurities on the surface of a three dimensional topological insulator, mediated by the massless and massive helical Dirac electrons. Exact analytical expression of RKKY interaction shows that the spin- spin interaction consists of the Heisenberg-like, Ising-like and Dzyaloshinskii-Moriya (DM)-like terms caused by the helicity of the topological surface states. It provides us a new way to realize various spin models, e.g., DM model, XXZ model and XZ model, and control surface magnetism by tuning the Fermi energy, and/or the distance between the two local spins. The gap opened by doped magnetic ions can lead to a short-range Bloembergen- Rowland interaction via the virtual interband interaction when the Fermi energy is located in the gap. The competition among the Heisenberg, Ising and DM terms leads to rich spin configurations and anomalous Hall effect on different lattices.

[1]This work was supported by the NSFC Grant Nos. 60525405 and 10874175, and the Knowledge Innovation Project of CAS. SCZ is supported by the NSF under grant numbers DMR-0904264.
[2]Speaker

3:18PM X35.00005 Ordering of magnetic impurities and tunable electronic properties of topological insulators[1]

, DMYTRO PESIN, The University of Texas at Austin, Austin, TX, DMITRY ABANIN, Princeton University, Princeton, NJ — We study collective behavior of magnetic adatoms randomly distributed on the surface of a topological insulator. As a consequence of the spin-momentum locking on the surface, the RKKY- type interactions of two adatom spins depend on the direction of the vector connecting them, thus interactions of an ensemble of adatoms are frustrated. We show that at low temperatures the frustrated RKKY interactions give rise to two phases: an ordered ferromagnetic phase with spins pointing perpendicular to the surface, and a disordered spin-glass-like phase. The two phases are separated by a quantum phase transition driven by the magnetic exchange anisotropy. Ferromagnetic ordering occurs via a finite-temperature phase transition. The ordered phase breaks time-reversal symmetry spontaneously, driving the surface states into a gapped state, which exhibits an anomalous quantum Hall effect and provides a realization of the parity anomaly. We find that the magnetic ordering is suppressed by potential scattering. Our work indicates that controlled deposition of magnetic impurities provides a way to modify the electronic properties of topological insulators.

[1]Supported by Welch Foundation grant F1473, and by the ARO MURI on bioassembled nanoparticle arrays

3:30PM X35.00006 Possible Strong Topological Insulator Phase in Li_2IrO_3

, HEUNG SIK KIM, CHOONG HYUN KIM, Department of Physics and Astronomy and Center for Strongly Correlated Materials Research, Seoul National University, Seoul 151-747, Korea, HOSUB JIN, Department of Physics and Astronomy, Northwestern University, Evanston, Illinois 60208, USA, JAEJUN YU, Department of Physics and Astronomy and Center for Strongly Correlated Materials Research, Seoul National University, Seoul 151-747, Korea — Recently Na_2IrO_3, a layered $5d$ transition metal oxide compound, was suggested to be a possible topological insulator (TI) based on the $j_{eff} = 1/2$ states induced by the strong spin-orbit coupling of Ir $5d$ states, but its realization has not been clarified yet. In search of the TI phase in transition metal oxides, we propose Li_2IrO_3 to be a candidate for the three-dimensional strong TI. By carrying out Wannier function analysis based on first-principles calculations, we constructed a low energy effective Hamiltonian, which leads to a three-dimensional extension of the Kane-Mele model with third-nearest-neighbor hopping within the Ir honeycomb layer and a significant inter-layer coupling. The nature of spin-orbit coupled states near the Fermi level depends on the change of the trigonal crystal field driven by the lattice deformations. A competition between the third next-nearest-neighbor hopping parameter and the trigonal crystal field is found to play a key role in determining the topological character of Li_2IrO_3.

3:42PM X35.00007 Half-Heusler Topological Insulators: A First-Principle Study with the Tran-Blaha Modified Becke-Johnson Density Functional[1]

, WANXIANG FENG, Institute of Physics, Chinese Academy of Sciences, DI XIAO, Oak Ridge National Lab, YING ZHANG, Beijing Normal University, China & University of Texas, YUGUI YAO, Institute of Physics, Chinese Academy of Sciences & University of Texas — We systematically investigate the topological band structures of half-Heusler compounds using first-principles calculations. The modified Becke-Johnson exchange potential together with local density approximation for the correlation potential (MBJLDA) has been used here to obtain accurate band inversion strength and band order. Our results show that a large number of half-Heusler compounds are candidates for three-dimensional topological insulators. The difference between band structures obtained using the local density approximation (LDA) and MBJLDA potential is also discussed.

[1]Research sponsored by the Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, and Institute of Physics, Chinese Academic Science

3:54PM X35.00008 Toplogical electronic structure in half-Heusler topological insulators[1]

, WAEL AL-SAWAI, HSIN LIN, ROBERT MARKIEWICZ, Northeastern University, L. WRAY, Y. XIA, S. XU, M. HASAN, Princeton University, A. BANSIL, Northeastern University — We investigate the details of electronic band structure of a series of 28 ternary half-Heusler compounds MM′X of MgAgAs-type where M = (Lu, La, Sc, Y) and M′X=(PtBi, AuPb, PdBi, PtSb, AuSn, NiBi, PdSb). Our results show that the Z_2 topological order is due to a single band inversion at the Γ-point. Half-Heusler compounds can be either topologically nontrivial semimetals, nontrivial metals, or trivial insulators. Our analysis reveals a straightforward relationship between the band inversion strength (extent of deviation from the critical point), the atomic charge of constituents, and the lattice parameter. Our findings suggest a general method for identifying Z_2 topological insulators in nonmagnetic ternary compounds.

[1]Work supported by the US DOE.

4:06PM X35.00009 Topological insulating behavior in conducting property of crystalline Ge-Sb-Te

, JEONGWOO KIM, JINWOONG KIM, SEUNG-HOON JHI, Physics, POSTECH — Phase-change random access memory (PRAM) is one of the most promising materials for data storage application. Especially, Ge-Sb-Te(GST) is considered as the best candidates for next generation nonvolatile memories because of the rapid and reversible cycles between the crystalline and amorphous structures. GeTe and $Sb_2Te_3$are the main components of GSTs, and have finite band gaps in the bulk phase. Sb_2Te_3 is topological insulator that has gapless edge states while maintaining bulk energy gap. These surface states are robust to external perturbations because they are protected by time-reversal symmetry. We report a discovery, through first-principles calculations, that crystalline GST phase-change materials exhibit the topological insulating property. Our calculations show that the materials become topological insulator or develop conducting surface-like interface states depending on the layer stacking sequence. It is shown that the conducting interface states originate from topological insulating Sb_2Te_3 layers in GSTs and can be crucial to the electronic property of the compounds. These interface states are found to be quite resilient to atomic disorders but sensitive to the uniaxial strains. We presented the mechanisms that destroy the topological insulating order in GSTs and investigated the role of Ge migration that is believed to be responsible for the amorphorization of GSTs.

4:18PM X35.00010 Ab initio study of topological order induced by symmetry breaking in PbTe , JINWOONG KIM, Department of Physics, POSTECH, SEUNG-HOON JHI, Department of Physics and Advanced Materials Science Division, POSTECH — Topological insulator (TI) is a new class of materials that have an energy gap in bulk phase but contain linear and chiral band dispersions on their surface. The topological insulating order can be initiated by parity inversion in time-reversal symmetric momenta. We studied the topological insulating properties of PbTe under uniaxial strain using first-principles methods. PbTe is a narrow-gap semiconductor with trivial topological insulating order. While it is known to have band inversion under pressure at a time-reversal symmetric k-point, the degeneracy at the k-point prevents the overall parity inversion which is needed to induce the TI order. In this presentation, we show that uniaxial strain can break the symmetry and thus induce topologically nontrivial order in PbTe.

4:30PM X35.00011 Electronic structure of the side surface of Bi_2Se_3[1] , CHANG-YOUN MOON, JINHEE HAN, HYUNGJUN LEE, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University, Korea — We investigate the electronic band structure of a side surface geometry, other than the conventional [111] surface, of the topological insulator Bi_2Se_3 using the first-principles pseudopotential calculations. As Bi_2Se_3 is known to be a strong topological insulator, it is expected that an arbitrary surface would have the topological surface state characterized by Dirac-cone-like band dispersion and spin-momentum coupling. Here we indeed obtain surface states with linear band dispersion around the Gamma point, but with a strong anisotropy with different group velocities along different k-directions. Low energy effective hamiltonian is proposed, and physical implications of the anisotropic Dirac fermions are also discussed.

[1]This work was supported by NRF of Korea (Grant No. 2009-0081204) and KISTI Supercomputing Center (Project No. KSC-2008-S02-0004).

4:42PM X35.00012 Spatial characters of metallic surface states of topological insulators , JINHEE HAN, HYUNGJUN LEE, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University — We study the electronic structure of metallic surface states in Bi_2Se_3, Bi_2Te_3, and Sb_2Te_3 using an ab-initio pseudopotential density-functional method. We implemented the spin-orbit interaction into the SIESTA in a form of additional fully non-local projectors. For surface states on (001) surface, we used a supercell containing 10 quintuple layers. We obtained bulk and surface electronic structures of topological insulators Bi_2Se_3, Bi_2Te_3, and Sb_2Te_3, which are close to previous theoretical results and consistent with Dirac-cone band dispersions measured by angle-resolved photoemission spectroscopy. Then, we analyzed the wavefunctions of the metallic surface states near the Fermi level to find out spatial distributions of the surface-state wavefunctions, which turn out to be localized in the surface region with a typical spread of about 2 quintuple layers, and the shapes of the wavefunctions around Bi (or Sb) atoms close to the surface. This work was supported by the NRF of Korea (Grant No. 2009-0081204) and KISTI Supercomputing Center (Project No. KSC-2008-S02-0004).

4:54PM X35.00013 Chern-Simons orbital magnetoelectric coupling in generic insulators , SINISA COH, DAVID VANDERBILT, Rutgers University, ANDREI MALASHEVICH, UC Berkeley, IVO SOUZA, Centro de Fisica de Materiales, San Sebastian — The isotropic Chern-Simons coupling θ is a component of the orbital contribution to the magnetoelectric coupling.[1] In a generic insulator it can have any value, while it must be exactly π in a strong Z_2 topological insulator. The results of our first-principles density-functional calculations for the ordinary magnetoelectrics Cr_2O_3, $BiFeO_3$ and $GdAlO_3$ confirm that the Chern-Simons contribution is quite small in these materials.[2] We discuss various strategies for finding insulators for which θ is large but not equal to π. For example, we show that if the spatial inversion and time-reversal symmetries of the Z_2 topological insulator Bi_2Se_3 are broken by hand, large induced changes appear in the Chern-Simons magnetoelectric coupling. We also perform an analysis based on space-group representation theory to determine the simplest possible magnetic structures which allow for a non-zero and possibly large value of θ.

[1]A. Malashevich *et al.*, New J. Phys. **12**, 053032 (2010); A. M. Essin *et al.*, Phys. Rev. B **81**, 205104 (2010).
[2]S. Coh *et al.*, arXiv:1010.6071.

5:06PM X35.00014 Theoretical prediction of new topological insulators in filled skutterudites , BINGHAI YAN, Department of Physics, McCullough Building, Stanford University, Stanford, CA 94305-4045, LUKAS MUECHLER, Institut fuer Anorganische Chemie und Analytische Chemie, Johannes Gutenberg - Universtitaet, 55099 Mainz, Germany, XIAO-LIANG QI, Department of Physics, McCullough Building, Stanford University, Stanford, CA 94305-4045, CLAUDIA FELSER, Institut fuer Anorganische Chemie und Analytische Chemie, Johannes Gutenberg - Universtitaet, 55099 Mainz, Germany, SHOU-CHENG ZHANG, Department of Physics, McCullough Building, Stanford University, Stanford, CA 94305-4045 — We have reported a unique class of topological insulators, filled skutterudite (FS) compounds, using ab initio calculations. We find that several FSs are not only two-dimensional topological insulators as quantum wells like HgTe, but also three-dimensional topological Kondo insulators. Different from previously reported topological insulators, they have unique band inversion feature in band structures. Their advantages are discussed to realize superconductivity proximity and other topological phenomena.

5:18PM X35.00015 Three-Dimensional Topological Insulators in I-III-VI_2 and II-IV-V_2 Chalcopyrite Semiconductors[1] , DI XIAO, Oak Ridge National Lab, WANXIANG FENG, JUN DING, YUGUI YAO, Institute of Physics, Chinese Academy of Sciences — Using first-principles calculations, we investigate the band topology of the ternary chalcopyrite family. Our method is based on the adiabatic continuity of the Hamiltonian combined with direct calculation of the Z2 topological invariants in inversion-symmetry breaking systems. We show that a large number of these compounds are candidates for three-dimensional topological insulators. Moreover, The topological order can be tuned and controlled by lattice strain. The excellent physical properties of these compounds make them an appealing platform for novel quantum phenomena.

[1]Research sponsored by the DOE, Office of BES, Materials Sciences and Engineering Division, and by the NSF and MOST of China

5:30PM X35.00016 Edge states and the bulk-boundary correspondence in Dirac Hamiltonians , VASUDHA SHIVAMOGGI, ROGER MONG, University of California, Berkeley — We present an analytic prescription for computing the edge dispersion $E(k)$ of a tight-binding Dirac Hamiltonian terminated at an abrupt crystalline edge. Specifically, we consider translationally invariant Dirac Hamiltonians with nearest-layer interaction. The result is a geometric formula that relates the existence of surface states as well as their energy dispersion to properties of the bulk Hamiltonian. We give examples of how the formula can be used to find the edge state dispersion in various topologically ordered systems. We further prove the bulk-boundary correspondence between the Chern number and the chiral edge modes for quantum Hall systems within the class of Hamiltonians studied here. Our results can be extended to the case of continuum theories which are quadratic in momentum, as well as other symmetry classes.

Thursday, March 24, 2011 2:30PM - 5:30PM –
Session X36 DCMP: Graphene: Quantum Hall Effect C142

2:30PM X36.00001 Graphene in a periodically alternating magnetic field: an unusual quantization of the anomalous Hall effect , PATRICK BRUNO, ESRF, Grenoble, France, MATHIEU TAILLEFUMIER, University of Oslo, Norway, VITALII K. DUGAEV, Rzeszow University of Technology, Poland, BENJAMIN CANALS, CLAUDINE LACROIX, Institut Néel, CNRS, Grenoble, France — We study the energy spectrum and electronic properties of graphene in a periodic magnetic field of zero average with a symmetry of triangular lattice. The periodic field leads to formation of a set of minibands separated by the gaps, which can be manipulated by external field. The Berry phase, related to the motion of electrons in k space, and the corresponding Chern numbers characterizing topology of the energy bands are calculated analytically and numerically. In this connection, we discuss the anomalous Hall effect in the insulator state, when the Fermi level is located in the minigap. The results of calculations show that in the model of gapless Dirac spectrum of graphene the anomalous Hall effect can be treated as a sum of fractional quantum numbers, related to the nonequivalent Dirac points.

2:42PM X36.00002 Quantum Hall Edge States in Bilayer Graphene Ribbons[1] , HERBERT FERTIG, Indiana University, VICTORIA MAZO, EFRAT SHIMSHONI, Bar-Ilan University — We study the low energy edge states of bilayer graphene ribbons subject to a strong perpendicular magnetic field B, and show that they can be described within a continuum model (the Dirac equation). We are mainly interested in investigating the energy- band structure of ribbons with a zigzag termination. At the zero Landau Level there are eight degenerate bands, whose degeneracy can be broken and controlled by an external inter- layer voltage bias V. This leads to the opening of a gap in the bulk. On the edges, due to a mixture of hole- and particle- like bands (from the same valley), an avoided crossing occurs which can be understood within a perturbative expansion in the inter-layer hopping. On the other hand, edge states from different valleys are protected from mixing by a long-range disorder potential. Hence, hole- and particle-like states can cross without mixing, and the system has properties of a topological insulator. In the presence of interactions, the rich behavior of crossing single-electron edge states may lead to a variety of collective edge-modes, whose properties dominate the transport behavior of this system.

[1]US-Israel Binational Science Foundation

2:54PM X36.00003 Hofstadter's Fractal Energy Spectrum in Twisted Bilayer Graphene[1] , ZHENGFEI WANG, School of Physics, Georgia Institute of Technology. Department of Materials Science and Engineering, University of Utah, FENG LIU, Department of Materials Science and Engineering, University of Utah, M.Y. CHOU, School of Physics, Georgia Institute of Technology — Hofstadter butterfly, the fractal spectrum of 2D lattice electrons in a magnetic field, has been studied theoretically for a few prototypical systems. However, due to the small unit cell in traditional materials, it is difficult to directly observe such a structure in the experiment. In this work we demonstrate that the Hofstadter butterfly structure can be detected in twisted bilayer graphene with a reasonable strength of the magnetic field. Based on the recursive tight-binding method, we have systematically studied the landau level dependence on the magnetic field as a function of the twist angle, with the underlying electronic structure ranging from the parabolic dispersion of Bernal bilayer graphene to the linear dispersion of decoupled graphene layers. The signature of transition is characterized by some low-lying landau levels in slightly twisted bilayer graphene, which are related to the flat bands induced in the layer decoupling process.

[1]This work was supported by DOE.

3:06PM X36.00004 Multi-Domain Model of Bilayer Graphene with Broken Time Reversal Symmetry[1] , GILAD BEN-SHACH, AMIR YACOBY, BERTRAND I. HALPERIN, Harvard University — Recent experiments suggest strange new states for bilayer graphene at zero electric and magnetic fields [1]. We consider recent models for the ground state of bilayer graphene with interactions [2,3]. These models predict domains with non-zero local Hall conductance but an expected overall average Hall conductance of $\sigma_{xy} = 0$, and should exhibit broken time reversal symmetry. We examine theoretical models for random four-probe measurements for various domain geometries in bilayer graphene at zero electric and magnetic fields. We find non-zero Hall conductance of magnitude dependent on domain geometry and network structure.

[1] Weitz, R.T., Allen, M.T., Feldman, B.E., Martin, J. Yacoby, A. Science. **330**, 6005 (2010).
[2] Nandkishore, R., Levitov, LPhys. Rev. Lett. **104**, 156803 (2010)
[3] Zhang F., Jung J., Fiete, G.A., Niu, Q., MacDonald, A.H. arXiv:1010.4003v1 (2010)

[1]Supported by NSERC and FQRNT.

3:18PM X36.00005 Fractional quantum Hall effect in graphene: multicomponent states and tunable interactions[1] , ZLATKO PAPIC, Department of Electrical Engineering, Princeton University, DMITRY ABANIN, Princeton Center for Theoretical Science, Princeton University, NICOLAS REGNAULT, Laboratoire Pierre Aigrain, Ecole Normale Superieure, CNRS, MARK GOERBIG, Laboratoire de Physique des Solides, CNRS, Universite Paris-Sud, Orsay — We study the fractional quantum Hall (FQH) states in graphene using exact diagonalization and taking into account the multicomponent degrees of freedom and the possibility of tuning the interaction potential. The recently observed graphene FQH state at a filling factor $\nu_G = 1/3$ is found to be adiabatically connected to the $1/3$ Laughlin state in the upper spin branch, with SU(2) valley-isospin ferromagnetic ordering and a completely filled lower spin branch. At the experimentally relevant values of the Zeeman field, however, the state possesses characteristic low-energy spin-flip excitations (different from the magneto-roton expected at large Zeeman fields) that may be unveiled in inelastic light-scattering experiments. We also discuss the possibility of realizing other Abelian and non-Abelian FQH states in graphene by modifying the effective interaction potential using a combination of insulating substrates.

[1]This work was supported in part by DOE grant DE-SC 000 2140.

3:30PM X36.00006 Decomposition into half-integer quantum Hall numbers from Dirac cones in a graphene-related lattice model , HARUKI WATANABE, Department of Physics, University of Tokyo, HATSUGAI YASUHIRO, Institute of Physics, University of Tsukuba, HIDEO AOKI, Department of Physics, University of Tokyo — In field theory it is well-known that the Hall conductivity of a massive Dirac particle is equal to $1/2\ \mathrm{sgn}\,(m)$ (in units of $-e^2/h$) when the Fermi energy lies in the mass gap. By contrast, any lattice model must have an integer quantum Hall number when we consider noninteracting electrons, as dictated by the TKNN formula arising from the periodicity in the Brillouin zone. Usually, this is understood to be consistent with the fact that in lattice models such as graphene honeycomb lattice Dirac dispersions tend to appear in pairs (as dictated by the Nielsen-Ninomiya theorem for chiral cases), but this does obscure a half-integer contribution from each Dirac cone. To resolve this, here we show that it is possible to identify half-integer contributions by constructing a lattice model with systematically shifted Dirac points [1]. Edge-state spectrum also confirms this.

[1] H. Watanabe, Y. Hatsugai and H. Aoki, arXiv:1008.0130, to appear in Phys. Rev. B (R).

3:42PM X36.00007 Lattice Theory of Pseudospin Ferromagnetism in Bilayer Graphene: Competing Orders and Interaction Induced Quantum Hall States , JEIL JUNG, FAN ZHANG, ALLAN MACDONALD, Department of Physics, University of Texas at Austin — In mean-field-theory bilayer graphene's massive Dirac fermion model has a family of broken inversion symmetry ground states with charge gaps and spin-valley flavor dependent spontaneous charge transfers between layers. We use a lattice Hartree-Fock model to explore some of the physics which controls whether or not this type of broken symmetry state, which can be viewed as a pseudospin ferromagnet, occurs in nature. We find that inversion symmetry is still broken in the lattice model and estimate that transferred areal densities are $\sim 10^{-5}$ per carbon atom, that the associated energy gaps are $\sim 10^{-2}$eV, the ordering condensation energies are $\sim 10^{-7}eV$ per carbon atom and the energy differences between competing orders at the neutrality point to be of the order of $\sim 10^{-9}eV$ per carbon atom. We explore the quantum phase transitions between different states induced by external magnetic fields and by externally controlled electric potential differences between the layers. We find, in particular, that in an external magnetic field coupling to spontaneous orbital moments favors broken time-reversal-symmetry states that have spontaneous quantized anomalous Hall effects. Our theory predicts a non monotonic behavior of the band gap as a function of electric field in qualitative agreement with recent experiments.

3:54PM X36.00008 $\nu = 0$ quantum Hall ferromagnet in a monolayer graphene: bulk ground states and charged edge excitations[1] , MAXIM KHARITONOV, Department of Physics and Astronomy, Rutgers University — The $\nu = 0$ quantum Hall state in a defect-free graphene sample is studied within the framework of the quantum Hall ferromagnetism. Starting from the low-energy electron Hamiltonian, in which all allowed by symmetry sublattice- and valley-anisotropic terms due to the Coulomb and leading electron-phonon interactions are taken into account, the energy functional for the quantum Hall ferromagnet is derived. Paying special attention to the signs of anisotropies, we find that the anisotropy due to the repulsive Coulomb interactions always favors the spin-polarized pseudospin-singlet state. On the other hand, the anisotropy due to the phonon-mediated attractive interactions favors the XY pseudospin-polarized spin-singlet state. It is then demonstrated that, in the case of the XY pseudospin bulk order and armchair boundary, the Skyrmion-type charged excitations are gapped at the edge, which makes the whole sample insulating. These findings suggest that the experimentally observed insulating $\nu = 0$ state is an XY pseudospin ferromagnet favored by electron-phonon interactions.

[1]This work was supported by the Center for Materials Theory at Rutgers University and US DOE under the Contract No. DE-AC02-06CH11357 while at Argonne National Laboratory.

4:06PM X36.00009 Disorder-induced magnetooscillations in bilayer graphene at high bias , MIKHAIL RAIKH, VAGHARSH MKHITARYAN, Department of Physics and Astronomy, University of Utah, Salt Lake City, UT 84112, USA — Energy spectrum of biased bilayer graphene near the bottom has a "Mexican-hat"-like shape. For the Fermi level within the Mexican hat we demonstrate that, apart from conventional magnetooscillations which vanish with temperature, there are additional magnetooscillations of capacitance and conductance which are weakly sensitive to temperature. These oscillations are also insensitive to a long-range disorder. Their period in magnetic field scales with bias, V, as V^2. The origin of these oscillations is the disorder-induced scattering between electron-like and hole-like Fermi-surfaces, specific for Mexican hat. At low temperatures, oscillations transform into quantum Hall plateaus in σ_{xy}. We predict that evolution of σ_{xy} with magnetic field is highly non-trivial. This is because the contributions to σ_{xy} from electron-like and hole-like Landau levels have opposite signs.

4:18PM X36.00010 Dynamical scaling analysis of the optical Hall conductivity in the quantum Hall regime , TAKAHIRO MORIMOTO, University of Tokyo, YSHAI AVISHAI, Ben Gurion University, HIDEO AOKI, University of Tokyo — We study the optical Hall conductivity $\sigma_{xy}(\varepsilon_F, \omega)$ in two-dimensional electron gas (2DEG) and in graphene in the quantum Hall regime, which is measurable by the Faraday rotation. It was previously demonstrated that both conductivities retain their plateau structure at finite frequency, up to the optical frequency regime. Physically, the robustness of the plateau structure in the ac optical regime can be attributed to the localization of electrons in the QHE. To quantify this picture, a dynamical scaling analysis of $\sigma_{xy}(\varepsilon_F, \omega)$ is performed for the $n = 0$ Landau level in graphene as well as for the conventional quantum Hall system. This analysis examines whether the system size dependence of $\sigma_{xy}(\varepsilon_F, \omega)$ can be captured with a universal scaling function that involves the localization exponent ν and the dynamic critical exponents z. Based on exact diagonalization of these systems with potential disorder, employing the Kubo formula, it is shown that $\sigma_{xy}(\varepsilon_F, \omega)$ obeys a well-defined dynamical scaling behavior. For both systems, the static exponents ν are similar and the dynamical exponents z are found to be ≈ 2. Our quantitative analysis indicates that the plateau structure in the ac Hall conductivity should be robust and experimentally testable in the THz regime.

4:30PM X36.00011 Disorder Effect of Quantum Anomalous Hall effect in Graphene , ZHENHUA QIAO, SHENGYUAN A. YANG, WANG-KONG TSE, The University of Texas at Austin, YUGUI YAO, Institue of Physics, Chinese Academy of Sciences, China, JIAN WANG, The University of Hong Kong, QIAN NIU, The University of Texas at Austin — We investigate the possibility of realizing quantum anomalous Hall effect in graphene. We show that a bulk energy gap can be opened in the presence of both Rashba spin-orbit coupling and an exchange field. We calculate the Berry curvature distribution and find a nonzero Chern number for the valence bands and demonstrate the existence of gapless edge states. Inspired by this finding, we also study, by first-principles method, a concrete example of graphene with Fe atoms adsorbed on top, obtaining the same result. We further study the disorder effect of this quantum anomalous Hall effect and show how this state is localized in the presence of strong disorders.

4:42PM X36.00012 Multiferroïc-like behavior in the quantum Hall ferromagnetic states of a graphene bilayer , RENE COTE, JULES LAMBERT, Universite de Sherbrooke — In a quantizing magnetic field, a graphene bilayer has an octet of degenerate states in the Landau level $N = 0$. An electron in this level must be described by three quantum numbers: its spin, its valley index K or K' and an orbital quantum number $n = 0, 1$. In the Hartree-Fock approximation, the ground states of the graphene bilayer at integer filling factors $\nu \in [-3, 4]$ can be described as different kinds of quantum Hall ferromagnets (QHF's) with finite interlayer, inter- orbital, or inter-spin coherence. In this talk, we present the phase diagram of the two-dimensional electron gas (2DEG) in $N = 0$ when the filling factor or a finite interlayer voltage, Δ_B is varied. A finite density of $electric$ dipoles is either spontaneously present in the QHF phases with inter-orbital coherence or can be generated by applying an external electric field in the plane of the layers. We show that by changing the strength of this electric field, and so the coupling with the electric dipoles, it is possible to control the degree of $magnetic$ polarisation of the 2DEG.

4:54PM X36.00013 Longitudinal Conductivity of Bilayer Graphene in the Integer Quantum Hall Regime , ROHIT HEGDE, ALLAN MACDONALD, University of Texas at Austin — We investigate the frequency dependent conductivity of disordered bilayer graphene near neutral filling, in a strong magnetic field. Absent Zeeman coupling, and with two independent valleys, a graphene bilayer's lowest Landau level is eightfold-degenerate, comprising two Landau orbitals of equal energy. Its spectral properties are altered by an inter-layer bias potential, which can open a gap between the constituent orbitals. We establish the dependence of the one and two-particle disorder-averaged Greens' functions on inter-layer bias, and show that the longitudinal conductivity exhibits the signature of disorder-induced Landau orbital mixing.

5:06PM X36.00014 Transverse Thermoelectric Conductivity of Bi-layer graphene in quantum Hall Regime[1] , WEI-LI LEE, CHANG-RAN WANG, WEN-SEN LU, Institute of Physics, Academia Sinica, INSTITUTE OF PHYSICS, ACADEMIA SINICA TEAM — We performed electric and thermoelectric transport measurements of bilayer graphene in a magnetic field up to 15 Tesla. The transverse thermoelectric conductivity α_{xy}, determined from four transport coefficients, attains a peak value of $\alpha_{xy,peak}$ whenever chemical potential lies in the center of a Landau level. The temperature dependence of $\alpha_{xy,peak}$ is dictated by the disorder width W_L. For $k_BT/W_L \leq 0.2$, $\alpha_{xy,peak}$ is nominally linear in temperature, which gives $\alpha_{xy,peak}/T = 0.19 \pm 0.03 nA/K^2$ independent of the magnetic field, temperature and Landau Level index. At $k_BT/W_L \geq 0.5$, $\alpha_{xy,peak}$ saturates to a value close to the predicted universal value of $4 \times (\ln 2) k_B e/h$ according to the theory of Girvin and Jonson. We remark that an anomaly is found in α_{xy} near the charge neutral point, similar to that in single-layer graphene.

[1]Phys. Rev. B 82, 121406(R) (2010).

5:18PM X36.00015 Interface Landau levels in graphene monolayer-bilayer junction , MIKITO KOSHINO, Department of Physics, Tohoku University, TAKESHI NAKANISHI, Nanotube Research Center, AIST, TSUNEYA ANDO, Department of Physics, Tokyo Institute of Technology — Electronic structure of graphene monolayer-bilayer junction in a magnetic field is studied within an effective-mass approximation. The energy spectrum is characterized by interface Landau levels, i.e., the locally flat bands appearing near the boundary region, resulting in a series of characteristic peaks in the local density of states. Their energies are independent of boundary types such as zigzag or armchair. In the atomic scale, the local density of states shows a Kekulé pattern due to the valley mixing in the armchair boundary, while does not in the zigzag boundary.

Thursday, March 24, 2011 2:30PM - 5:30PM –

Session X37 DMP: Focus Session: Graphene Structure, Dopants, and Defects: Magnetism and Nanoribbons C146

2:30PM X37.00001 Oxygen- and Sulfur- driven Ferromagnetism in Graphitic Fragments: Ab-Initio Study , IVAN NAUMOV, Hewlett-Packard Laboratories, YAKOV KOPELEVICH, Instituto de Física "Gleb Wataghin," Universidade Estadual de Campinas, UNICAMP 13083-970, Campinas, São Paulo, Brasil, ALEXANDER BRATKOVSKY, Hewlett-Packard Laboratories, HEWLETT-PACKARD LABORATORIES COLLABORATION — We study the origins of high-temperature ferromagnetic behavior in graphite by means of unbiased ab-initio calculations and compare them with our data. The experimental results show that oxygen/sulfur-induced edges of graphitic fragments (via unzipping effect) play an essential role in this phenomenon, and that the finite magnetic moment appears if edges in a graphitic ribbon are occupied asymmetrically by either oxygen or sulphur. In particular, our ab-initio calculations performed within the LDA and GGA approximations showed that in the case of pure graphene ribbon, its zig-zag edge carbon atoms carry large magnetic moment ($\sim 1\ \mu_B$/C). In an oxidized or sulfurized graphene, however, the magnetic moment at the edge with absorbed atoms gets considerably reduced, leading to effective ferromagnetic (more precisely, ferri-magnetic) behavior of the sample.

2:42PM X37.00002 Defect Induced Resonances and Magnetic Patterns in Graphene , YI CHEN CHANG, Department of Physics and Astronomy, University of southern California — We investergate the effects of point and line defects in monolayer graphene was investigated within the framework of the Hubbard model, using a self-consistent mean field theory. These defects are found to induce characteristic patterns into the electronic density of states and cause non-uniform distributions of magnetic moments in the vicinity of the impurity sites. Specifically, defect induced resonance bound states in the local density of states are observed at energies close to the Dirac points. The magnitudes of the frequencies of these resonance states are shown to decrease with the strength of the scattering potential, whereas their amplitudes decay algebraically with increasing distance from the defect. Furthermore, non-trivial impurity induced magnetic patterns are observed in the presence of line defects: zigzag line defects are found to introduce stronger-amplitude magnetic patterns than single line defect and armchair line defects. When the scattering strength of these topological defects is increased, the induced patterns of magnetic moments become more strongly localized.

2:54PM X37.00003 Theory of Magnetic Edge States in Chiral Graphene Nanoribbons , RODRIGO CAPAZ, Instituto de Fisica, Universidade Federal do Rio de Janeiro, OLEG YAZYEV, STEVEN LOUIE, Department of Physics, U. C. Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — Using a model Hamiltonian approach including electron Coulomb interactions, we systematically investigate the electronic structure and magnetic properties of chiral graphene nanoribbons. We show that the presence of magnetic edge states is an intrinsic feature of any smooth graphene nanoribbons with chiral edges, and discover a number of structure-property relations. Specifically, we describe how the edge-state energy gap, zone-boundary edge-state energy splitting, and magnetic moment per edge length depend on the nanoribbon width and chiral angle. The role of environmental screening effects is also studied. Our results address a recent experimental observation of signatures of magnetic ordering at smooth edges of chiral graphene nanoribbons and provide an avenue towards tuning their properties via the structural and environmental degrees of freedom. This work was supported by National Science Foundation Grant No. DMR10-1006184, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231 and the ONR MURI program. RBC acknowledges financial support from Brazilian agencies CNPq, FAPERJ and INCT-Nanomateriais de Carbono.

3:06PM X37.00004 Spin-orbit interactions in graphene nanoribbons : Effects of the edge profile , JUN-WON RHIM, KYUNGSUN MOON, Yonsei University, CONDENSED MATTER THEORY TEAM — In graphene, it has been shown by Kane and Mele that the spin orbit coupling (SOC) connects the Dirac particles to the low- lying p_x and p_y orbitals so that the quantum spin Hall effect(QSHE) arises at the edges of the graphene. Their theory has drawn considerable attention as a realization of Haldane's idea of quantum Hall effect without magnetic field and as a trigger for the surging field of topological insulator. In the work, we study the band structure of the zigzag nanoribbons with the spin-orbit interaction and argue that the role of graphene edge should be considered more carefully since the realization of the QSHE is found to be largely dependent on the edge profile such as the kinds of molecules passivated. When the edge p_x, p_y and s orbitals are dangling without any passivation, the Dirac states at the edges seem to be no longer chiral for each spin species and the QSHE is not guaranteed to occur. We notice that upon the hydrogen passivation at the edges, the spin filtered chiral edge states become available. We will explain that these are due to the interaction between π-edges states and σ-edge states. The similar calculations are also performed for the armchair nanoribbons and compared with those of zigzag nanoribbons.

3:18PM X37.00005 Quantum Monte Carlo Study of Edge Magnetism in Nanoribbons of Graphene , Z.Y. MENG, Institut für Theoretische Physik III, Universität Stuttgart, H. FELDNER, IPCMS Université de Strasbourg France, Institut für Theoretische Physik, Georg-August-Universität Göttingen, T.C. LANG, Institut für Theoretische Physik und Astrophysik, Universität Würzburg, S. WESSEL, Institut für Theoretische Physik III, Universität Stuttgart, A. HONECKER, Institut für Theoretische Physik, Georg-August-Universität Göttingen, F. ASSAAD, Institut für Theoretische Physik und Astrophysik, Universität Würzburg — We study the electronic and magnetic properties of graphene nanoribbons, employing projective quantum Monte Carlo simulations within the Hubbard model description of electrons in graphene. We also compare our numerical results to a self-consistent mean field approximation in the weak coupling regime. Motivated by recent STM experiments about electronic resonance around atomic vacancies on multilayer graphene and graphene nanoisland, we in particular examine the local density of states throughout the sample. From this, we verify that interacting zig-zag ribbons develop an insulating ground state with a finite single particle gap from the localized edge modes observed in the non-interacting limit. In addition, we observe a drastic increase of the spin-spin correlation length along the zig-zag edge with the ribbon width. Effectively, on our finite samples ferromagnetic edges appear already for moderately wide zig-zag ribbons. This ferromagnetism is accompanied by an essentially gapless edge magnon mode, that we identify in the spin excitation spectrum.

3:30PM X37.00006 First principles study of edge effects in electronic structures of graphene nanoflakes and nanoribbons , CHENGBO HAN, WENCHANG LU, JERRY BERNHOLC, North Carolina State University, Raleigh, NC, CENTER FOR HIGH PERFORMANCE SIMULATION (CHIPS) TEAM — Graphene is a promising material for future nanoelectronics. Understanding of the edge effects on the electronic structure of graphene nanoflakes and nanoribbons is important for its nanoscale applications. Using the real space multigrid method within density functional theory, we systematically simulate STM images of nanoflakes and nanoribbons with both zigzag and armchair edges. Our results explain several STM patterns seen in experiments [1], such as triangular and hexagonal lattices for different shapes of flakes. We also find that localization of edge states in zigzag flakes depends on the interior angle between two edges. Furthermore, we show that the influence of Si(001)-2x1-H substrate on the local density of states of graphene nanoflakes is not significant when the graphene layer is 0.3 nm above the substrate.

[1] K. A. Ritter and J. W. Lyding, Nature Materials 8, 235 (2009).

3:42PM X37.00007 Spin states in graphene quantum dots , KLAUS ENSSLIN, ETH Zurich — Graphene quantum dots [1,2], douple dots [3], rings [4] and nanoribbons [5] have been fabricated by electron beam lithography and dry etching. The orbital [1] properties of graphene quantum dots have been investigated in perpendicular magnetic fields and the details of the electron-hole crossover in graphene leads to a situation where electron (hole) states move down (up) in magnetic field opposite to what has been observed in standard semiconductor based quantum dots. Graphene quantum dots are thought to be good candidates for spin-based quantum information processing since spin-orbit interactions and hyperfine coupling are both expected to be weak. We investigated graphene quantum dots in the single-level transport regime in in-plane magnetic fields where orbital effects are expected to have a minor effect [6]. The g-factor is found to be $g \approx 2$ and the spin filling sequence of orbital levels can be understood in view of the strength of the exchange interaction which is independent of carrier density in graphene.

[1] J. Guttinger, C. Stampfer, F. Libisch, T. Frey, J. Burgdoerfer, T. Ihn, K. Ensslin, Phys. Rev. Lett. 103, 046810 (2009)
[2] T. Ihn, J. Guttinger, F. Molitor, S. Schnez, E. Schurtenberger, A. Jacobsen, S. Hellmuller, T. Frey, S. Droscher, C. Stampfer, and K. Ensslin, Materials Today 13, 44 (2010)
[3] F. Molitor, H. Knowles, S. Droscher, U. Gasser, T. Choi, P. Roulleau, J. Guttinger, A. Jacobsen, C. Stampfer, K. Ensslin and T. Ihn, Europhys. Lett. 89, 67005 (2010)
[4] M. Huefner, F. Molitor, A. Jacobsen, A. Pioda, C.Stampfer, K. Ensslin and T. Ihn, N. J. of Phys. 12, 043054 (2010)
[5] C. Stampfer, J. Guttinger, S. Hellmuller, F. Molitor, K. Ensslin, and T. Ihn, Phys. Rev. Lett. 102, 056403 (2009)
[6] J. Guttinger, T. Frey, C. Stampfer, T. Ihn, and K. Ensslin, Phys. Rev. Lett. 105, 116801 (2010)

4:18PM X37.00008 Complex edge effects in graphene nanoribbons due to hydrogenation[1] , BIPLAB SANYAL, Associate Professor, Uppsala University, Sweden, SUMANTA BHANDARY, Ph.D. student, Uppsala University, Sweden, MIKHAIL KATSNELSON, Professor, Radboud University Nijmegen, The Netherlands, OLLE ERIKSSON, Professor, Uppsala University, Sweden — We have performed density-functional calculations as well as employed a tight-binding theory, to study the effect of hydrogenation of zigzag graphene nanoribbons (ZGNR). We show that each edge C atom bonded with 2 H atoms open up a gap and magnetism collapses for small widths of the nanoribbon. However, a re-entrant magnetism accompanied by a metallic electronic structure is observed from eight rows and thicker nanoribbons. The electronic structure and magnetic state are quite complex for this type of termination, with sp^3 bonded edge atoms being nonmagnetic whereas the nearest neighboring atoms are metallic and magnetic. We have also evaluated the phase stability of several thicknesses of ZGNR and demonstrate that sp^3 bonded edge atoms with 2 H atoms at the edge can be stabilized over 1 H atom terminated edge at high temperatures and pressures.

[1]We gratefully acknowledge financial support from the Swedish Research Council, Carl Tryggers Foundation, STINT, the EU-India FP-7 collaboration under MONAMI, and a KOF grant from Uppsala University.

4:30PM X37.00009 Magnetism in bulk and finite size graphene multilayers and its effect on the band gaps[1] , BHAGAWAN SAHU, HONGKI MIN, SANJAY BANERJEE, ALLAN MACDONALD, University of Texas at Austin — In this talk, we will address the edge state magnetism and the resulting modulation of band gaps induced by quantum confinements in multilayer graphene ribbons and flakes. The magnetism arising from random point defects such as vacancies in bulk graphene layers will also be presented. The robustness of magnetism with respect to the edge disorder and the saturating agents in finite size graphene layers and with respect to the defect concentrations in bulk graphene layers will be discussed. A numerical approach based on density functional theory which uses plane-wave basis set and pseudopotentials for ion-electron interactions will be used for elucidating the complex interplay of magnetism, external electric field applied perpendicular to the layers and the resulting band gaps.

[1]Financial support from SRC-NRI SWAN center is acknowledged.

4:42PM X37.00010 Exploring the Structure of Graphene Nanoribbons Using Scanning Tunneling Microscopy , YEN-CHIA CHEN, JUANJUAN FENG, CHENGGANG TAO, LIYING JIAO, XIAOWEI ZHANG, OLEG YAZYEV, RODRIGO CAPAZ, ALEX ZETTL, STEVEN LOUIE, HONGJIE DAI, MICHAEL CROMMIE — The confined dimension and edges of graphene nanoribbons (GNRs) are predicted to result in novel magnetic edge states and tunable energy gaps. Such properties should be strongly dependent on GNR nanoscale structure. Here we report a scanning tunneling microscopy (STM) study of the structure of GNRs derived from unzipped carbon nanotubes that are deposited onto different substrates. These GNRs are found to have different chiralities and widths, and show some unexpected geometrical structure near the edges. We will also present new results obtained from GNRs with disordered edges.

4:54PM X37.00011 STM and STS studies of CVD grown graphene nanoribbons , XIAOTING JIA, MIT, MINGHU PAN, CNMS, ORNL, SREEKAR BHAVIRIPUDI, MIT, VINCENT MEUNIER, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, JING KONG, MILDRED DRESSELHAUS, MIT — Graphene nanoribbons (GNRs) are quasi one dimensional structures which have unique transport properties, and have a potential to open a bandgap at small ribbon widths. They have been extensively studied in recent years due to their high potential for future electronics applications. We have experimentally found some GNRs in our CVD grown graphene layers. In this work, we investigated the morphology and electronic properties of the GNRs on top of a graphene layer transferred to a SiO_2 substrate by using scanning tunneling microscopy. Our results suggest that these GNRs have a surprisingly high crystallinity with one side folded. Atomic resolution images were obtained on the folded layer and the bottom layer of the GNR, which enables clear identification of the chirality for both layers. By combining with theoretical modeling we conclude that a (5,7) line defect exists at the zone of maximum curvatures to help reducing the strain energy of the folding. Low temperature spectroscopic measurements suggest that different electronic states may exist at GNR edges, when compared to the ribbon interior regions.

5:06PM X37.00012 ABSTRACT WITHDRAWN –

5:18PM X37.00013 Large intrinsic energy band gaps in annealed nanotube-derived graphene nanoribbons[1] , J. HARUYAMA, T. SHIMIZU, Aoyama Gakuin University, D.C. MARCANO, D.V. KOSINKIN, J.M. TOUR, Rice University, K. HIROSE, K. SUENAGA, AIST, Japan — The usefulness of graphene for electronics is diminished by an absent energy bandgap. While graphene nanoribbons have non-zero bandgaps, lithographic fabrication methods introduce defects which decouple the bandgap from electronic properties and compromise performance [1]. Here, we present direct measurements of a large intrinsic energy bandgap of approximately 50 meV in 100 nm-width level nanoribbons fabricated by high-temperature annealing of unzipped carbon nanotubes [2]. The activation energy is seven times greater than those in [1], and is close to the width of the transport gap in the differential conductance. This similarity suggests that the activation energy is in fact the intrinsic bandgap. High-resolution TEM and Raman spectroscopy, along with an absence of hopping conductance and stochastic charging effects, suggest a low defect density. [1] M.Y. Han, P. Kim et al., PRL 104, 056801 (2010) [2] J.Haruyama, J.M.Tour, et al., Nature Nanotech. (December 2010)

[1]We thank a Grant-in-aid for Scientific Research in MEXT, the AFOSR (FA9550-09-1-0581), the Alliance for Nanohealth, the AFRL through University Technology Corporation, 09-S568-064-01-C1, and the Office of Naval Research MURI program.

Thursday, March 24, 2011 2:30PM - 5:18PM –

Session X38 DCP DBP: Focus Session: Non-Equilibrium Insights into Single Molecules and Cell Function I A130/131

2:30PM X38.00001 The Statistical Mechanics of Trajectories and Weights: Applications to Gene Expression , ROB PHILLIPS, California Institute of Technology — Many fascinating questions concerning the behavior of systems ranging from chemical reaction patterns to the patterns of gene expression in living systems do not concern their terminal states, but rather the various microscopic trajectories connecting those states. Some of the most intriguing examples of these kinds of phenomena center on the time evolution of the many molecular machines that populate living cells. Motivated by studies of the time evolution of gene expression, this talk will review both classic approaches to time evolution using rate equations (but couched in the language of trajectories and weights) and more controversial ideas based upon the principle of maximum entropy.

3:06PM X38.00002 Challenges in Characterizing and Controlling Complex Cellular Systems[1] , JOHN WIKSWO, Vanderbilt University — Multicellular dynamic biological processes such as developmental differentiation, wound repair, disease, aging, and even homeostasis can be represented by trajectories through a phase space whose extent reflects the genetic, post-translational, and metabolic complexity of the process - easily extending to tens of thousands of dimensions. Intra- and inter-cellular sensing and regulatory systems and their nested, redundant, and non-linear feed-forward and feed-back controls create high-dimensioned attractors in this phase space. Metabolism provides free energy to drive non-equilibrium processes and dynamically reconfigure attractors. Studies of single molecules and cells provide only minimalist projections onto a small number of axes. It may be difficult to infer larger-scale emergent behavior from linearized experiments that perform only small amplitude perturbations on a limited number of the dimensions. Complete characterization may succeed for bounded component problems, such as an individual cell cycle or signaling cascade, but larger systems problems will require a coarse-grained approach. Hence a new experimental and analytical framework is needed. Possibly one could utilize high-amplitude, multi-variable driving of the system to infer coarse-grained, effective models, which in turn can be tested by their ability to control systems behavior. Navigation at will between attractors in a high-dimensioned dynamical system will provide not only detailed knowledge of the shape of attractor basins, but also measures of underlying stochastic events such as noise in gene expression or receptor binding and how both affect system stability and robustness. Needed for this are wide-bandwidth methods to sense and actuate large numbers of intracellular and extracellular variables and automatically and rapidly infer dynamic control models. The success of this approach may be determined by how broadly the sensors and actuators can span the full dimensionality of the phase space.

[1]Supported by the Defense Threat Reduction Agency HDTRA-09-1-0013, NIH National Institute on Drug Abuse RC2DA028981, the National Academies Keck Futures Initiative, and the Vanderbilt Institute for Integrative Biosystems Research and Education

3:42PM X38.00003 Maximizing efficiency of molecular machines , GAVIN CROOKS, Lawrence Berkeley Natl. Lab. — I will discuss how to locate protocols that minimize dissipation in non-equilibrium, molecular scale processes, adapting ideas from finite-time thermodynamics.

4:18PM X38.00004 Autonomous Boolean models for logic, timing, and stability in regulatory networks[1] , JOSHUA E.S. SOCOLAR, Physics Department and Center for Systems Biology, Duke University — The dynamics of gene expression in a cell is controlled by a dizzying array of biochemical processes. Natural selection, however, has created regulatory systems with a level of logical organization that can be modeled without detailed knowledge of the biochemistry. In cases where graded responses are not relevant, autonomous Boolean network (ABN) models can effectively represent the logic of gene regulation. These are models in which Boolean logic governs the output value of each node and the timing of updates is determined according to delay parameters associated with each link. An advantage of ABNs over synchronous or random asynchronous Boolean networks is that noise associated with molecular concentrations or transport times can be represented through fluctuations in the timing of updates. We have used ABN models to investigate the stability of oscillations in a model of transcriptional oscillations in yeast and the parameter constraints in a model of segment polarity maintenance in the fly embryo, and also to characterize chaotic dynamics observed in a free–running digital electronic circuit. The yeast study highlights architectural and dynamical features of oscillators that rely on pulse transmission rather than a frustrated feedback loop; the fly study reveals timing constraints that are hidden in ODE models; and the electronics study shows that Boolean chaos can occur if and only if time delays are history dependent.

[1]Joint work with V. Sevim, X. Gong, X. Cheng, M. Sun, D. Gauthier, H. Cavalcante, and R. Zhang. Supported by NSF Grant PHY-0417372 and NIH Grant P50-GM081883.

4:54PM X38.00005 Maximum Caliber Analysis of Ion-Channel Gating , ROY CAMPBELL, Walla Walla University — The principle of maximum caliber, MaxCal, is a generalization to nonequilibrium statistical mechanics of the principle of maximum entropy, MaxEnt. E. T. Jaynes introduced the MaxEnt approach to equilibrium statistical mechanics in 1957 and its MaxCal generalization in 1980. MaxCal has recently been used to derive dynamical laws of transport, analyze single particle two-state dynamics, and study few state models of non-equilibrium processes. We use MaxCal to analyze ion-channel gating data and make logical inferences concerning the underlying dynamics. The inferred trajectory probabilities are used to calculate the fluctuations responsible for channel noise.

5:06PM X38.00006 Driving denaturation: Nanoscale thermal transport as a probe of DNA melting , YONATAN DUBI, School of Physics and Astronomy, Tel-Aviv University, Tel-Aviv, Israel, KIRILL VELIZHANIN, CHIH-CHUN CHIEN, MICHAEL ZWOLAK, Los Alamos National Laboratory — The microscopic dynamics of DNA denaturation have long been a subject of intense study but many aspects of this phenomenon remain poorly understood. Experiments typically measure the degree of denaturation versus temperature which, unfortunately, introduces only a relatively weak constraint: Although many existing models reproduce this denaturation transition well, they give, e.g., incorrect time scales for fluctuations in base pair unbinding. Here, we propose a critical test of DNA models based on driving DNA out of thermal equilibrium via two heat reservoirs. Contrary to what might be expected, we find that the preeminent model of denaturation predicts the thermal conductance to increase substantially as DNA melts. Furthermore, we show that different models can possess qualitatively different thermal transport properties. Measuring the thermal conductance of DNA will thus shed new light on the nonlinear physics of this important molecule and may lead to novel thermal technologies, such as a DNA thermal switch.

Thursday, March 24, 2011 2:30PM - 5:30PM –

Session X39 DBP DCOMP: Biomechanics: From Subcellular to Multicellular Scales A124/127

2:30PM X39.00001 Simple, Voltage Dependent Statistics Governing Cell-Substrate Contact Times , BRET N. FLANDERS, Department of Physics, Kansas State University — The distribution of contact times between a nanofilament-based contact sensor and individual pseudopods of *D. discoideum* have been measured as a function of voltage applied to the filament. The distributions are well described by exponential distributions. The average duration of the pseudopod-filament contact was found to increase across the +20 mV to -50 mV range of filament-voltages. These results are consistent with the predictions of a simple model based on rather general considerations of energy usage by the cell. This analysis indicates that the exponential functionality (of the contact time distributions) results from competition between a large number of cellular processes for the available energy. The evolution of these distributions across the +20 mV to -50 mV voltage range suggests that the negatively biased filament enhances adhesion to the filament by activating additional adhesion molecules to bind to its surface. These results will be discussed in the context of recent findings on the coupling of voltage gated ion channels and cellular adhesion.

3:06PM X39.00002 Multiscale modeling of the dynamics of multicellular systems[1] , IOAN KOSZTIN, University of Missouri - Columbia — Describing the biomechanical properties of cellular systems, regarded as complex highly viscoelastic materials, is a difficult problem of great conceptual and practical value. Here we present a novel approach, referred to as the Cellular Particle Dynamics (CPD) method, for: (i) quantitatively relating biomechanical properties at the cell level to those at the multicellular and tissue level, and (ii) describing and predicting the time evolution of multicellular systems that undergo biomechanical relaxations. In CPD cells are modeled as an ensemble of cellular particles (CPs) that interact via short range contact interactions, characterized by an attractive (adhesive interaction) and a repulsive (excluded volume interaction) component. The time evolution of the spatial conformation of the multicellular system is determined by following the trajectories of all CPs through integration of their equations of motion. Cell and multicellular level biomechanical properties (e.g., viscosity, surface tension and shear modulus) are determined through the combined use of experiments and theory of continuum viscoelastic media. The same biomechanical properties are also "measured" computationally by employing the CPD method, the results being expressed in terms of CPD parameters. Once these parameters have been calibrated experimentally, the formalism provides a systematic framework to predict the time evolution of complex multicellular systems during shape-changing biomechanical transformations. By design, the CPD method is rather flexible and most suitable for multiscale modeling of multicellular system. The spatial level of detail of the system can be easily tuned by changing the number of CPs in a cell. Thus, CPD can be used equally well to describe both cell level processes (e.g., the adhesion of two cells) and tissue level processes (e.g., the formation of 3D constructs of millions of cells through bioprinting).

[1]Work supported by NSF [FIBR-0526854 and PHY-0957914]. Computer time provided by the University of Missouri Bioinformatics Consortium.

3:42PM X39.00003 Theoretical estimation of the breakage intensity of microtubules at resonance using ultrasound waves , ABDORREZA SAMARBAKHSH[1], JACK TUSZYNSKI[2], Department of Oncology, University of Alberta — Microtubules (MTs) are protein filaments forming a major part of the cytoskeleton of all eukaryotic cells which directly contribute to the process of cell division by forming mitotic spindles and providing force for the segregation of chromosomes. In this work first we show the resonance condition for MTs subject to ultrasound wave by solving the beam equation for MT analytically. Then we estimate the required minimum intensity of the ultrasound at the location of the MT in order to break it. We have shown that this intensity is of the order of 100KW per unit of area which corresponds to 170 dB.

[1]Also at Department of Physics
[2]also at Department of Physics

3:54PM X39.00004 Flexural Rigidity of MCF-7 Microtubules Measured from Thermal Fluctuations in Shape , MITRA SHOJANIA FEIZABADI, Physics Department, Seton Hall University, KIRYAKO MUTAFOPULOS, Biology Department, Seton Hall University, ADAM BEHR, Physics Department, Seton Hall University — Microtubules play a key role in the mechanical and elastic properties of eukaryotic cells. For this reason, measuring the flexural rigidity of bovine brain microtubules have been extensively investigated through different methods of measurement. Beta tubulin isotypes, a noticeable trait to consider as we transfer from mammalian neural microtubules to mammalian non-neural microtubules, are assembled differently in distributions among various types of microtubules. Different studies have shown that microtubules made from different beta-tubulin isotypes express unique polymerization and dynamic behavior. This study focuses on measuring mechanical properties of one of non-neural microtubules, MCF-7. We will discuss the structure differences between brain bovine microtubules and MCF-7, along with the rigidity of single microtubules polymerized from MCF-7 tubulin through monitoring the curvature of microtubule due to thermal fluctuations.

4:06PM X39.00005 ABSTRACT WITHDRAWN –

4:18PM X39.00006 Persistence Length of Stable Microtubules[1] , TAVIARE HAWKINS, University of Massachusetts Amherst, MATTHEW MIRIGIAN, National Institutes of Health, M. SELCUK YASAR, JENNIFER ROSS, University of Massachusetts Amherst — Microtubules are a vital component of the cytoskeleton. As the most rigid of the cytoskeleton filaments, they give shape and support to the cell. They are also essential for intracellular traffic by providing the roadways onto which organelles are transported, and they are required to reorganize during cellular division. To perform its function in the cell, the microtubule must be rigid yet dynamic. We are interested in how the mechanical properties of stable microtubules change over time. Some "stable" microtubules of the cell are recycled after days, such as in the axons of neurons or the cilia and flagella. We measured the persistence length of freely fluctuating taxol-stabilized microtubules over the span of a week and analyzed them via Fourier decomposition. As measured on a daily basis, the persistence length is independent of the contour length. Although measured over the span of the week, the accuracy of the measurement and the persistence length varies. We also studied how fluorescently-labeling the microtubule affects the persistence length and observed that a higher labeling ratio corresponded to greater flexibility.

[1]National Science Foundation Grant No: 0928540 to JLR

4:30PM X39.00007 Modeling actin waves in dictyostelium cells , VAIBHAV WASNIK, RANJAN MUKHOPADHYAY, Clark University — Actin networks in living cells demonstrate a high capacity for self-organization and are responsible for the formation of a variety of structures such as lamellopodia, phagocytic cups, and cleavage furrows. Recent experiments have studied actin waves formed on the surface of dictyostelium cells that have been treated with a depolymerizing agent. These waves are believed to be physiologically important, for example, for the formation of phagocytic cups. We propose and study a minimal model, based on the dendritic nucleation of actin polymers, to explain the formation of these waves. This model can be extended to study the dynamics of the coupled actin-membrane system.

4:42PM X39.00008 ABSTRACT WITHDRAWN –

4:54PM X39.00009 Force Generated by Actin Array , KONSTANTINOS TSEKOURAS, Institut Curie, DAVID LACOSTE, Ecole Superieure de Physique et Chimie Industrielles, KIRONE MALLICK, CEA Saclay, JEAN-FRANCOIS JOANNY, Institut Curie — We study a theoretical model for a group of parallel filaments growing against a barrier held by a constant force. An array of N filaments nucleate on a fixed surface and grow towards a rigid barrier which is held in place by a constant force. Filaments are coupled only by mechanical contact against the barrier. We obtain the filament density distribution in terms of the distance from the barrier, and force-velocity curves. We apply our model to the case of an array of actin filaments. All results are validated by extensive Monte-Carlo simulations. For a small value of N we find the stall force to be N times the stall force of a single filament ($f_{stall} \approx N f^1_{stall}$). For large N we find that the velocity *appears* to be considerably smaller, an effect due to its exponential decrease as the theoretical stall force is approached.

5:06PM X39.00010 BSDB: the Biomolecule Stretching Database[1] , MAREK CIEPLAK, MATEUSZ SIKORA, Institute of Physics, Polish Academy of Sciences, JOANNA I. SULKOWSKA, UCSD, BARTLOMIEJ WITKOWSKI, Institute of Physics, Polish Academy of Sciences — Despite more than a decade of experiments on single biomolecule manipulation, mechanical properties of only several scores of proteins have been measured. A characteristic scale of the force of resistance to stretching, F_{max}, has been found to range between ∼10 and 480 pN. The Biomolecule Stretching Data Base (BSDB) described here provides information about expected values of F_{max} for, currently, 17 134 proteins. The values and other characteristics of the unfolding proces, including the nature of identified mechanical clamps, are available at www://info.ifpan.edu.pl/BSDB/. They have been obtained through simulations within a structure-based model which correlates satisfactorily with the available experimental data on stretching. BSDB also lists experimental data and results of the existing all-atom simulations. The database offers a Protein-Data-Bank-wide guide to mechano-stability of proteins. Its description is provided by a forthcoming Nucleic Acids Research paper.

[1]Supported by EC FUNMOL project FP7-NMP-2007-SMALL-1, and European Regional Development Fund: Innovative Economy (POIG.01.01.02-00-008/08)

5:18PM X39.00011 The nonequilibrium thermodynamics and kinetics of focal adhesion dynamics , KRISHNA GARIKIPATI, JOSEPH OLBERDING, MICHAEL THOULESS, ELLEN ARRUDA, University of Michigan — We consider a focal adhesion (FA) to be made up of molecular complexes consisting of ligands, integrins, and associated plaque proteins. Free energy changes drive the binding and unbinding of these complexes, thus controlling the FA's dynamic modes of growth, treadmilling and resorption via the following mechanisms: (i) work done during the addition of molecular complexes, (ii) the chemical free energy of addition of a molecular complex, (iii) the elastic free energy of deformation of FAs and the cell membrane, and (iv) the work done on a molecular conformational change. We have developed a treatment of FA dynamics as a nonlinear rate process driven by out-of-equilibrium thermodynamic driving forces, and modulated by kinetics. The mechanisms governed by the above four effects allow FAs to exhibit a rich variety of behavior, predicting growth, treadmilling and resorption. Treadmilling requires symmetry breaking between the ends of the focal adhesion, and is achieved by driving force (i) above. In contrast, the remaining mechanisms cause symmetric growth or resorption. These findings hold for a range of conditions: temporally-constant force or stress, and for spatially-uniform and non-uniform stress distribution over the FA. This treatment of FA dynamics can be coupled with models of cytoskeleton dynamics and contribute to the understanding of cell motility.

Thursday, March 24, 2011 2:30PM - 5:18PM –

Session X40 DBP: Biological Networks and Systems Biology A122/123

2:30PM X40.00001 Computer Simulations of Loss of Organization of Neurons as a Model for Age-related Cognitive Decline[1] , LUIS CRUZ, ELENE FENGOMETIDIS, FRANK JONES, SRINIVAS JAMPANI, Physics Dept., 3141 Chestnut St., Drexel University, Philadelphia PA 19104 — In normal aging, brains suffer from progressive cognitive decline not linked with loss of neurons common in neurodegenerative disorders such as Alzheimer's disease. However, in some brain areas neurons have lost positional organization specifically within microcolumns: arrays of interconnected neurons which may constitute fundamental computational units in the brain. This age-related loss of organization, likely a result of micron-sized random displacements in neuronal positions, is hypothesized to be a by-product of the loss of support from the surrounding medium, including dendrites. Using a dynamical model applied to virtual 3D representation of neuronal arrangements, that previously showed loss of organization in brains of cognitively tested rhesus monkeys, the relationship between these displacements and changes to the surrounding dendrite network are presented. The consequences of these displacements on the structure of the dendritic network, with possible disruptions in signal synchrony important to cognitive function, are discussed.

[1]NIH R01AG021133

2:42PM X40.00002 Coupled feedback loops govern bistability properties in gene networks , ABHINAV TIWARI, OLEG IGOSHIN, Rice University — Positive feedback is a necessary component for network bistability - the simplest design being a positive autoregulatory circuit. Then why some biological systems have multiple feedback loops? We hypothesize that the presence of multiple additively or multiplicatively coupled feedback loops affects the net cooperativity of the system, thereby influencing the possibility of bistability. We find that additively coupled feedback loops in the MprAB-SigE-RseA network in mycobacteria do not lead to bistability. Only the inclusion of post-translational regulation of SigE by RseA makes the system robustly bistable. In general we find that if two one-feedback networks are individually monostable, then only multiplicative coupling can generate bistability in the combined circuit. We analytically perform pair-wise controlled comparisons between the autoregulation circuit, additively and multiplicatively coupled two-gene circuits that reveal neither of the circuits has an advantage with regards to bistability range. We numerically validate our results by employing Monte Carlo parameter sampling for the comparisons.

2:54PM X40.00003 Better Bet-Hedging with coupled positive and negative feedback loops , JATIN NARULA, OLEG IGOSHIN, Dept. of Bioengineering, Rice University — Bacteria use the phenotypic heterogeneity associated with bistable switches to distribute the risk of activating stress response strategies like sporulation and persistence. However bistable switches offer little control over the timing of phenotype switching and first passage times (FPT) for individual cells are found to be exponentially distributed. We show that a genetic circuit consisting of interlinked positive and negative feedback loops allows cells to control the timing of phenotypic switching. Using a mathematical model we find that in this system a stable high expression state and stable low expression limit cycle coexist and the FPT distribution for stochastic transitions between them shows multiple peaks at regular intervals. A multimodal FPT distribution allows cells to detect the persistence of stress and control the rate of phenotype transition of the population. We further show that extracellular signals from cell-cell communication that change the strength of the feedback loops can modulate the FPT distribution and allow cells even greater control in a bet-hedging strategy.

3:06PM X40.00004 Attractor Distribution in Random Biological Networks Described by ODEs and Diminished Order-Chaos Transition , ZHIYUAN LI, UCSF, Dept of Biophysics, CHAO TANG, UCSF — Ordinary Differential Equations (ODEs) are widely used to model biological network in a continuous manner. The state of an ODE system after infinitely long time is called attractor, which indicates the ultimate fate of the corresponding biological system. Even though the attractor behaviors of many biological systems have been understood, yet the distribution of attractors for networks followings biological reaction rules is in general unknown. In our work, we study the final state for all 3 nodes networks that follow transcriptional regulation or enzymatic reaction rules, under random parameter sets. Surprisingly, mono-stable behavior appears most frequently, while bi-stable and tri-stable behavior is less frequently observed. Oscillations are rarely seen, and chaos is almost never observed. We extend the study to random networks with a large number of nodes, and the outcome does not change qualitatively. Furthermore, with increased connectivity, the transition from order to chaos predicted by discrete models is not observed. Our results provide a null-distribution for attractors in bio-networks, and have important implication for cell fate decision.

3:18PM X40.00005 Beyond Critical Exponents in Neuronal Avalanches , NIR FRIEDMAN, Department of Physics, University of Illinois at Urbana-Champaign, TOM BUTLER, Massachusetts Institute of Technology, ROBERT DEVILLE, Department of Mathematics, University of Illinois at Urbana-Champaign, JOHN BEGGS, University of Indiana, KARIN DAHMEN, Department of Physics, University of Illinois at Urbana-Champaign — Neurons form a complex network in the brain, where they interact with one another by firing electrical signals. Neurons firing can trigger other neurons to fire, potentially causing avalanches of activity in the network. In many cases these avalanches have been found to be scale independent, similar to critical phenomena in diverse systems such as magnets and earthquakes. We discuss models for neuronal activity that allow for the extraction of testable, statistical predictions. We compare these models to experimental results, and go beyond critical exponents.

3:30PM X40.00006 Stochastic Modeling of Regulation of Gene Expression by Multiple Competing Small RNAs , CHARLES BAKER, TAO JIA, RAHUL KULKARNI, Virginia Polytechnic Institute and State University — A wealth of new research has highlighted the critical roles of small RNAs (sRNAs) in diverse processes such as quorum sensing and cellular responses to stress. The pathways controlling these processes often have a central motif comprised of a key protein regulated by multiple sRNAs. However, the regulation of stochastic gene expression of a single target gene by multiple sRNAs is currently not well understood. To address this issue, we analyze a stochastic model of regulation of gene expression by multiple sRNAs. For this model, we derive exact analytic results for the regulated protein distribution including compact expressions for its mean and variance. The derived results provide novel insights into the roles of multiple sRNAs in fine-tuning the noise in gene expression. In particular, we show that, in contrast to regulation by a single sRNA, multiple sRNAs provide a mechanism for independently controlling the mean and variance of the regulated protein distribution.

3:42PM X40.00007 The up and down states of cortical networks , MARYAM GHORBANI, ALEX J. LEVINE, MAYANK MEHTA, ROBIJN BRUINSMA, UCLA — The cortical networks show a collective activity of alternating active and silent states known as up and down states during slow wave sleep or anesthesia. The mechanism of this spontaneous activity as well as the anesthesia or sleep are still not clear. Here, using a mean field approach, we present a simple model to study the spontaneous activity of a homogenous cortical network of excitatory and inhibitory neurons that are recurrently connected. A key new ingredient in this model is that the activity-dependant synaptic depression is considered only for the excitatory neurons. We find depending on the strength of the synaptic depression and synaptic efficacies, the phase space contains strange attractors or stable fixed points at active or quiescent regimes. At the strange attractor phase, we can have oscillations similar to up and down states with flat and noisy up states. Moreover, we show that by increasing the synaptic efficacy corresponding to the connections between the excitatory neurons, the characteristics of the up and down states change in agreement with the changes that we observe in the intracellular recordings of the membrane potential from the entorhinal cortex by varying the depth of anesthesia. Thus, we propose that by measuring the value of this synaptic efficacy, one can quantify the depth of anesthesia which is clinically very important. These findings provide a simple, analytical understanding of the spontaneous cortical dynamics.

3:54PM X40.00008 Adiabatic and Non-Adiabatic Non-Equilibrium Stochastic Dynamics of Single Regulating Genes , HAIDONG FENG, BO HAN, JIN WANG, Department of Chemistry, State University of New York at Stony Brook — We explore the stochastic dynamics of self regulative genes from fluctuations of molecular numbers and of on and off switching of gene states due to regulatory protein binding/unbinding to the genes. We found when the binding/unbinding is relatively fast (slow) compared with the synthesis/degradation of proteins in adiabatic (non-adiabatic) case, the self regulators can exhibit one or two peak (two peak) distributions in protein concentrations. This shows even with the same architecture (topology of wiring), networks can have quite different functions (phenotypes), consistent with recent single molecule single gene experiments. We derive the non-equilibrium phase diagrams of mono-stability and bi-stability in adiabatic and non-adiabatic regimes. We study the stability and robustness of the systems through mean first passage time (MFPT) from one peak (basin of attraction) to another. In addition, using the new method for quantifying the paths and the associated weights for complex systems in discrete state space (Markov chains), we identified the dominant paths among all possible paths from the "off" basin to the "on" basin for self-activators, and observe turnover kinetic behavior of transitions and MFPT from non-adiabatic to adiabatic regimes.

4:06PM X40.00009 Steady state growth of *E. Coli* in low ammonium environment , MINSU KIM, BARRET DERIS, ZHONGGE ZHANG, TERRY HWA, UCSD — Ammonium is the preferred nitrogen source for many microorganisms. In medium with low ammonium concentrations, enteric bacteria turn on the nitrogen responsive (ntr) genes to assimilate ammonium. Two proteins in *E. coli*, Glutamine synthetase (GS) and the Ammonium/methylammonium transporter AmtB play crucial roles in this regard. GS is the major ammonium assimilation enzyme below 1mM of NH_4^+. AmtB is an inner membrane protein that transports NH_4^+ across the cell membrane against a concentration gradient. In order to study ammonium uptake at low NH_4^+ concentration at neutral pH, we developed a microfluidic flow chamber that maintains a homogenous nutrient environment during the course of exponential cell growth, even at very low concentration of nutrients. Cell growth can be accurately monitored using time-lapse microscopy. We followed steady state growth down to micro-molar range of NH_4^+ for the wild type and ΔamtB strains. The wild type strain is able to maintain the growth rate from 10mM down to a few uM of NH_4^+, while the mutant exhibited reduced growth below $\sim$20 uM of NH_4^+. Simultaneous characterization of the expression levels of GS and AmtB using fluorescence reporters reveals that AmtB is turned on already at 1mM, but contributes to function only below $\sim$30 uM in the wild-type. Down to $\sim$20 uM of NH_4^+, *E. coli* can compensate the loss of AmtB by GS alone.

4:18PM X40.00010 Threshold response and bimodality in non-cooperative auto-activation circuits[1] , RUTGER HERMSEN, DAVID ERICKSON, TERENCE HWA, Center for Theoretical Biological Physics, UC San Diego — In prokaryotes as well as in eukaryotes, many transcription factors (TFs) activate their own gene. For that reason the benefits of auto-activation have been studied extensively. However, little attention is paid to the fact that many TFs are modified by a signal, usually through phosphorylation or binding of a ligand. Typically only one version of the TF—the modified or the unmodified one—can activate transcription. Consequently the TF's expression level responds to changes in the signal. Here, we use stochastic models to study the response properties of such circuits. In real examples the auto-activation is often mediated by a single binding site. Surprisingly, in that case we find that an arbitrarily sensitive threshold response can be obtained, while the bistability and hysteresis associated with multiple cooperative binding sites are avoided. Also, we find that the steady-state probability distributions of the TF expression level can be bimodal even though the system is not bistable. This is not caused by slow TF–DNA binding kinetics or bursty protein production, as in earlier studies, but by strongly reduced production and degradation rates at low expression levels.

[1]This work was supported by the CTBP sponsored by the NSF (Grant PHY-0822283).

4:30PM X40.00011 Inferring Complex Network Topology from Spatio-Temporal Spike Patterns , FRANK VAN BUSSEL, BIRGIT KRIENER, MARC TIMME, Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — The problem of reconstructing or reverse-engineering the connectivity of networks consisting of dynamically interacting units has become an active area of study in fields such as genetics, ecology, and neuroscience. The collective dynamics of such networks is often sensitive to the presence (or absence) of individual interactions, but there is commonly no direct way to probe for their existence. We present an explicit method for reconstructing neuronal networks from their spiking activity. The approach works well for networks in simple collective states, but is also applicable to networks exhibiting complex spatio-temporal spike patterns. In particular, stationarity of spiking time series is not required.

4:42PM X40.00012 ABSTRACT WITHDRAWN –

4:54PM X40.00013 Temporal competition between differentiation programs determines cell fate choice , ANNA KUCHINA, UT Southwestern Medical Center, LORENA ESPINAR, Universitat Politècnica de Catalunya, TOLGA CAGATAY, ALEJANDRO BALBIN, ALMA ALVARADO, UT Southwestern Medical Center, JORDI GARCIA-OJALVO, Universitat Politècnica de Catalunya, GUROL SUEL, UT Southwestern Medical Center — During pluripotent differentiation, cells adopt one of several distinct fates. The dynamics of this decision-making process are poorly understood, since cell fate choice may be governed by interactions between differentiation programs that are active at the same time. We studied the dynamics of decision-making in the model organism *Bacillus subtilis* by simultaneously measuring the activities of competing differentiation programs (sporulation and competence) in single cells. We discovered a precise switch-like point of cell fate choice previously hidden by cell-cell variability. Engineered artificial crosslinks between competence and sporulation circuits revealed that the precision of this choice is generated by temporal competition between the key players of two differentiation programs. Modeling suggests that variable progression towards a switch-like decision might represent a general strategy to maximize adaptability and robustness of cellular decision-making.

5:06PM X40.00014 Comparison of Control Approaches in Genetic Regulatory Networks by Using Stochastic Master Equation Models, Probabilistic Boolean Network Models and Differential Equation Models and Estimated Error Analyzes , MEHMET UMUT CAGLAR, RANADIP PAL, Texas Tech University — Central dogma of molecular biology states that "information cannot be transferred back from protein to either protein or nucleic acid" . However, this assumption is not exactly correct in most of the cases. There are a lot of feedback loops and interactions between different levels of systems. These types of interactions are hard to analyze due to the lack of cell level data and probabilistic - nonlinear nature of interactions. Several models widely used to analyze and simulate these types of nonlinear interactions. Stochastic Master Equation (SME) models give probabilistic nature of the interactions in a detailed manner, with a high calculation cost. On the other hand Probabilistic Boolean Network (PBN) models give a coarse scale picture of the stochastic processes, with a less calculation cost. Differential Equation (DE) models give the time evolution of mean values of processes in a highly cost effective way. The understanding of the relations between the predictions of these models is important to understand the reliability of the simulations of genetic regulatory networks. In this work the success of the mapping between SME, PBN and DE models is analyzed and the accuracy and affectivity of the control policies generated by using PBN and DE models is compared.

Thursday, March 24, 2011 2:30PM - 5:18PM –

Session X41 DCP: Focus Session: Electronic Structure and Applications to Energy Conversion II A115/117

2:30PM X41.00001 Fundamental understanding and computational design of thin-film photovoltaics materials , JEFFREY C. GROSSMAN, Massachusetts Institute of Technology — The search for abundant and clean energy sources has placed photovoltaics at the focus of research over a variety of disciplines spanning physics, chemistry and materials science. However, the quest for more cost-efficient photovoltaics is challenged by limitations in efficiency of charge excitation and collection in the materials and their interfaces. We will present our recent *ab initio* calculations aimed at understanding important microscopic mechanisms in solar photovoltaic materials. Our goal is to predict accurately key properties that govern the efficiency in these materials, including structural and electronic effects, interfacial charge separation, electron and hole traps, excited state phenomena, band level alignment, and binding energies. Examples of our work in the areas of organic and other thin-film photovoltaics will be presented. We use these examples to illustrate how accurate electronic structure approaches can improve our understanding and lead to more efficient materials.

3:06PM X41.00002 Effect of environment and long range behaviour of exchange functional on polaron formation in π-conjugated polymers , IFFAT NAYYAR, Theoretical Div, Los Alamos National Lab, NM and NanoScience Technology Center, Dept. of Physics, University of Central Florida, Orlando, FL, ENRIQUE BATISTA, SERGEI TRETIAK, AVADH SAXENA, DARRYL SMITH, RICHARD MARTIN, Theoretical Division, Los Alamos National Lab, NM — Organic conjugated polymers find a variety of applications in devices such as solar cells, light emitting diodes and lasers. An accurate understanding of the role of nonlinear excitations as polarons in charge carrier transport is critical to improve the efficiency of these devices. PPV and MEH-PPV are the candidates of choice for the extensive experimental data and relative simplicity compared to other polymers. This motivated us to perform a density functional theory study to describe the charge defects in these systems. We emphasize on the role of surrounding dielectric medium and the amount of long range orbital exchange in the density functional to predict the polaron localization in agreement with experiment. The particle-hole symmetry observed in trans-geometries is broken by introducing certain cis defects.

3:18PM X41.00003 Photo-induced modulation in the dipole moment of a donor-acceptor pair of organic molecules[1] , YOSHIYUKI MIYAMOTO, National Institute of Advanced Industrial Science and Technology, Japan, MINA YOON, ORNL, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft — We have investigated the photo-induced electron dynamics in donor-acceptor pairs of organic molecules. Specifically we will discuss TTF and TCNQ molecules and study their electron dynamics under illumination by means of time-dependent density functional theory within the local-density approximation. In their stable molecular structure, we find that these molecules align in parallel and show maximum optical oscillator strength with an optical polarization parallel to their molecular axis. Without illumination, a dipole moment from TTF to TCNQ directs perpendicular to the molecular axis. This dipole-moment is further increased upon illumination with an optical polarization parallel to the molecular axis at resonant excitation energies of 2.00 eV and 3.55 eV. The light-induced increase of the dipole moment, which reflects the separation of electron and hole pair, is caused by the internal electric field between these molecules. Therefore, these molecules may have a high potential as building blocks of future organic photovoltaic devices.

[1]Supported by the Next Generation Supercomputer Project (MEXT Japan), and by the US DOE, Office of Basic Energy Sciences, Materials Sciences and Engineering Division and the Max Planck Society

3:30PM X41.00004 Exciton transport and dissociation at organic interfaces , DAVID BELJONNE, University of Mons — This paper focuses on modeling studies of exciton transport and dissociation at organic interfaces and includes three parts: 1) Experiments have shown that the values of exciton diffusion length L_D in conjugated polymers (CPs) are rather low, in the range of 5-10 nm, apparently regardless of their chemical structure and solid-state packing. In contrast, larger L_D values have been reported in molecular materials that are chemically more well-defined than CPs. Here we demonstrate that energetic disorder alone reduces the exciton diffusion length more than one order of magnitude, from values typically encountered in molecules (>50nm) to values actually measured in CPs (<10nm). 2) A number of organic crystals show anisotropic excitonic couplings, with weak interlayer interactions between molecules that are more strongly coupled within the layers. The resulting energy carriers are intra-layer 2D excitons that diffuse along the interlayer direction. We model this analytically for infinite layers and using quantum-chemical calculations of the electronic couplings for anthracene clusters. We show that the exciton hopping rates and diffusion lengths depend in a subtle manner on the size and shape of the interacting aggregates, temperature and the presence of energetic disorder. 3) The electronic structure at organic/organic interfaces plays a key role, among others, in defining the quantum efficiency of organic-based photovoltaic cells. Here, we perform quantum-chemical and microelectrostatic calculations on molecular aggregates of various sizes and shapes to characterize the interfacial dipole moment at pentacene/C60 heterojunctions. The results show that the interfacial dipole mostly originates in polarization effects due to the asymmetry in the multipolar expansion of the electronic density distribution between the interacting molecules. We will discuss how the quadrupoles on the pentacene molecules produce direct electrostatic interactions with charge carriers and how these interactions in turn affect the energy landscape around the interface and therefore also the energy barrier for exciton dissociation into free carriers.

4:06PM X41.00005 Correlating First-Principles Electronic Structure with Device Performance of Organic Photovoltaic Cells , ERIC B. ISAACS, SAHAR SHARIFZADEH, BIWU MA, JEFFREY B. NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory — Organic photovoltaic cells (OPVs) are promising candidates for low-cost solar energy conversion. Here, we employ static and time-dependent density functional theory calculations to predict the excitation energy of the donor-acceptor charge transfer state (E_{CT}) at the interface between C_{60} and several boron(subphthalocyanine)- and azadipyrromethene-based donor moieties, comparing to measured open-circuit voltage (V_{oc}) in bilayer heterojunction OPVs [1]. When E_{CT} is approximated as the difference between the ionization potential and electron affinity of the isolated donor and acceptor molecules, respectively, we observe no apparent correlation between E_{CT} and V_{oc}. Both bulk polarization and excitonic effects at the interface are found to influence the energetics significantly, the latter being strongly morphology dependent. We demonstrate that a linear relationship between V_{oc} and E_{CT} may be obtained once the interface morphology is considered. We acknowledge support from DOE, NSF-NCN, and NERSC.

[1] C. E. Mauldin *et al.*, ACS Appl. Mater. Interfaces **2**, 2833 (2010).

4:18PM X41.00006 Photo-induced Charge Separation in Nanoscale Donor-Bridge-Acceptor Systems: Theory and Experiment , PETER DOAK, Molecular Foundry, LBNL; Department of Chemistry, UC-Berkeley, PIERRE DARANCET, Molecular Foundry, LBNL, KASPER MOTH-POULSEN, Department of Chemical and Biological Engineering, Chalmers U. of Technology, JESSE JENKINS, Department of Chemistry, UC-Berkeley, RACHEL SEGALMAN, Department of Chemical Engineering, UC-Berkeley, DON TILLEY, Department of Chemistry, UC-Berkeley, JEFF NEATON, Molecular Foundry, LBNL — Understanding and control of light-harvesting processes at the molecular-scale remains a fundamental challenge in solar energy conversion. Donor-bridge-acceptor molecules (DBAM), with atomically-defined interfaces made by a covalently bound bridge between donor and acceptor moieties, allow probing of excited states relevant to optical absorption and charge separation. In close collaboration with experiment, we use first-principles many-body perturbation theory, within the GW approximation and the Bethe-Salpeter equation approach, to compute excited states for six DBAMs. We compare with experiments, and quantitative agreement is obtained. Implications of our results for nanoscale light-harvesting are thoroughly discussed. Support: DOE via the Molecular Foundry and Helios SERC, and NSF via NCN. Computational support provided by NERSC.

4:30PM X41.00007 Exciton Scattering in Branched Conjugated Molecules: Towards Photoinduced Dynamics and Energy Transfer , VLADIMIR CHERNYAK, Wayne State University — The exciton scattering (ES) approach attributes excited electronic states in quasi-one-dimensional (branched) conjugated molecules with perfect geometry to standing waves on the linear segments of a molecule formed by scattering of quantum quasi-particles (excitons). We extract their dispersion and frequency-dependent scattering matrices at termini, including donor/acceptor substitutions, joints, and branching centers from time-dependent density functional theory (TD-DFT) calculations, with applications to for conjugated phenylacetylene-based molecules. This allows electronic spectra for any structure of arbitrary size within the considered molecular family to be obtained with insignificant numerical effort. To extend the capability of the ES approach to treating photoinduced dynamics, including absorption and fluorescence lineshapes and energy transfer, the methodology should be modified to account for non-ideal molecular geometry. Geometry distortions break down translational symmetry of the linear segments, and excitations are not represented by perfect standing waves anymore. To overcome this difficulty we associate electronic excitations with the eigenstate of a quantum particle on an irregular lattice (graph), referred to as a tight-binding model. The morphology of the underlying lattice, together with the tight-binding parameters, can be identified by studying the topological and analytical properties of excitons at molecular termini, joints, and branching centers. The dependence of the tight-binding parameters on geometry distortions that controls effects of disorder and coupling to vibrational modes can be extracted from quantum chemical calculations by studying exciton scattering on localized geometry distortions, the latter considered as scattering centers.

5:06PM X41.00008 NA-ESMD modeling of photoinduced dynamics in conjugated molecules , TAMMIE NELSON, Los Alamos National Laboratory, SEBASTIAN FERNANDEZ-ALBERTI, Universidad Nacional de Quilmes, VLADIMIR CHERNYAK, Wayne State University, ADRIAN ROITBERG, University of Florida, SERGEI TRETIAK, Los Alamos National Laboratory — The evolution of electronic excitations in optically active molecules can generally be defined by non-adiabatic (NA) dynamics. A number of fundamental and complex processes are associated with NA dynamics. To treat ultrafast excited state dynamics we have developed a non-adiabatic excited state molecular dynamics (NA-ESMD) framework incorporating quantum transitions. Our calculations combine the Collective Electronic Oscillator (CEO) package with the Tully's fewest switches algorithm for surface hopping, and the actual potential energy surfaces of the excited states are used. This method is applied to model the photoinduced dynamics of distyrylbenzene. Our analysis shows intricate details of vibronic relaxation and identifies specific slow and fast nuclear motions that are strongly coupled to the electronic degrees of freedom. Non-adiabatic relaxation of the highly excited mAg state is predicted to occur on a femtosecond timescale at room temperature and on a picosecond timescale at low temperature.

Thursday, March 24, 2011 2:30PM - 5:30PM –
Session X42 DPOLY: Polymeric Glasses A302/303

2:30PM X42.00001 Molecular Mobility on the Surface of Glassy Tris-naphthylbenzene (TNB) , ZAHRA FAKHRAAI, University of Wisconsin-Madison, CHAD DALEY, University of Waterloo, STEPHEN F. SWALLEN, DANIEL SCIFO, University of Wisconsin-Madison, JAMES A. FORREST, University of Waterloo, MARK D. EDIGER, University of Wisconsin-Madison — Mechanical relaxation measurements on the surface of polymeric glasses show that as the bulk material falls out of equilibrium at Tg a thin layer at the surface behaves like a liquid with relaxation times that are orders of magnitude faster and more weakly temperature dependent compared to those of the bulk glass. However the origin of this phenomenon remains elusive. Recently exceptionally stable glasses of small organic molecules have been produced by physical vapor deposition at temperatures below Tg, suggesting that these glasses also exhibit enhanced surface mobility. In this study gold nanoparticles were used to probe micron size meniscus formation on the surface of organic glass former TNB below Tg, a direct evidence of surface mobility in this material. Neutron scattering measurements of inter-diffusion between stacks of d-TNB and regular TNB layers during the deposition suggest that the temperature dependence of the diffusion on the surface is very similar to what is observed on polymeric films.

2:42PM X42.00002 Tuning the Dynamics of Penetrant Transport in Glassy Polymers through Network Structure Modification , ADAM EKENSEAIR, NICHOLAS PEPPAS, Department of Chemical Engineering, The University of Texas at Austin — The relative rates of the diffusional and relaxational processes during the absorption of penetrant molecules in glassy polymers determine the nature of the transport process and lead to Fickian, Case II, and anomalous absorption behavior. While previous models account for anomalous behavior, there is still a disconnect between theory and experiment, as data must be fit to the model with previously determined independent parameters. With trends leading to smaller device scales and increasingly complex polymer structures, there is a need for a quantitative understanding of the manner in which a polymer's network structure alters both the rate and the mode of penetrant transport. To this end, the effects of the basic network parameters of PMMA, including the degree of crosslinking, polymer mesh size, and the crosslink interchain bridge length, on the integral sorption of methanol were studied utilizing gravimetric integral sorption studies. The effects of sub-T_g annealing/aging, temperature, and the presence of un-reacted monomer were also investigated. Controlling the relative timescale of the relaxational process by altering the polymer network structure was shown to directly influence the Case II front propagation velocity and control the overall nature of the observed transport behavior.

2:54PM X42.00003 A Surrogate for Debye-Waller Factors from Stokes Shifts[1] , MARCUS CICERONE, QIN ZHONG, MADHUSUDAN TYAGI, NIST — We show that short-time relaxation behavior characteristic of the intermediate scattering function at q near the peak in the static structure factor can be obtained from time-resolved Stokes shifts (TRSS) in glassforming materials. We extract Debye- Waller factor ($\langle u^2 \rangle$) analogs from the TRSS data from four glassforming liquids and apply these to a proposed relationship between α relaxation and the Debye-Waller factor; $\tau_\alpha = \tau_\infty \, Exp\left[\frac{a^2}{2\langle u^2\rangle} + \frac{\sigma_{a^2}^2}{8\langle u^2\rangle^2}\right]$. This putative relationship has previously been evaluated using experimental Debye-Waller factors obtained in the time range (40 to 2000) ps. We show that the relation yields physically meaningful fit values only when relaxation on a 1 ps timescale is considered. We also observe an unexpected dependence of short-time Debye-Waller factors on fragility.

[1]We acknowledge funding from NIH/NIBIB under grant R01 EB006398-01A1

3:06PM X42.00004 Comparison of the KWW and BSW Model Descriptions of the Dynamic Responses of Polymeric and Colloidal Glass Formers , BEN XU, GREGORY B. MCKENNA, Department of Chemical Engineering, Texas Tech University — In this work, we present the results of the KWW and BSW[1] descriptions of the dynamic data for a colloid and a polymer (PVAc) in their respective glass transition regions. It was found that the KWW function is not able to describe the dynamic data for the colloidal system, while BSW function, provides an acceptable description to the dynamic response of the polymer. The fitting parameters n_e and n_g in the BSW function, which indicate the slopes of the relaxation spectrum, remain constant at different temperatures consistent with the validity of the time-temperature superposition principle. We also used the G_g obtained from the KWW and BSW functions, where appropriate, to evaluate the Dyre shoving model.[2] Here, as is the case for small molecule glass formers, we found the temperature dependences of the G_g highly sensitive to the model chosen to describe the experimental data. This suggests that evaluation of the shoving model requires very broad frequency and temperature experiments beyond those normally performed in dynamic rheometry.

[1]M. Baumgärtel, A. Schausberger, H.H. Winter, Rheol. Acta. 29:400–408 (1990).
[2]J. C. Dyre, N. B. Olsen, T. Christensen, Physical Review B.53, 5 (1996).

3:18PM X42.00005 Aging and structural recovery behaviors in epoxy films subjected to carbon dioxide plasticization jumps: Evidence for a new glassy state , GREGORY MCKENNA, SHANKAR SUBRAMANIAN, JING ZHAO, MATAZ ALCOUTLABI, LAMECK BANDA, Texas Tech University — Structural recovery and physical aging of glassy polymers after temperature jumps have been very well studied in the literature. On the contrary, there is only limited work available on the aging and recovery behaviors of glassy polymers subjected to plasticizer jumps. We have shown in our previous works, using strong and weakly polar plasticizers that qualitatively they mimic the behaviors of temperature jumps but quantitatively they are different [1, 2]. In this work, we further investigate this anomalous behavior by studying the structural recovery and physical aging of an epoxy film subjected to carbon dioxide pressure jumps and compare the results with temperature jump experiments such that the final conditions are identical. The results are surprising and we observe evidence for existence of a new glassy state.

[1] Zheng. Y., and McKenna, G.B., *Macromolecules,* **36**, 2387-2396, 2003
[2] Alcoutlabi, M., Briatico-Vengosa, F., and McKenna, G.B., JPSB., **40**, 2050-2064, 2002

3:30PM X42.00006 Effect of Quench Conditions on the Subsequent Physical Aging Rate of Polymer Glasses , LAURA GOLICK, PAUL YOON, ANDY PAHNER, CONNIE ROTH, Dept. of Physics, Emory University — We investigate the stability of polymer glasses when thermally quenched under different conditions. Ellipsometry is used to measure the physical aging rate of polystyrene (PS) films supported or transferred onto silicon wafers. The aging rate quantifies the time-dependent decrease in film thickness that results from the increase in average film density during aging. Although all films are subsequently aged in a supported state, we observe significant differences between films quenched in a free-standing compared to supported state. Films quenched in a free-standing state exhibit a strong thickness dependence to their physical aging rate at micron length scales, an order of magnitude or two larger than thicknesses where nanoconfinement effects on the glass transition and modulus are typically observed. In contrast, supported films do not display any film thickness dependence to their aging rate at this large length scale. This indicates that the physical aging of the material is strongly dependent on conditions during the formation of the glassy state. In an effort to determine the key factors underlying the aging dynamics, we have measured the physical aging rate of supported PS films quenched at various controlled rates. In addition, we have explored the effects of quenching free-standing films held on different frames such that either biaxial or uniaxial stress is applied.

3:42PM X42.00007 Low Temperature Flow of PVC Chains , WEI CHEN, GI XUE[1] — PVC is usually processed at temperature above 180 °C, however, it starts to degrade at 130 °C. If PVC can flow at temperatures below glass transition temperature (Tg), the manufacturing procedure will be energy-conserving and environment-friendly. We find that PVC powders with controlled inter-segment van der Waals attraction can be compressed into a transparent pellet with high modulus at low temperatures. The molecular mechanism underlying this phenomenon involves shear-induced unjamming transition. PVC chains are unjammed by cold-pressing freeze-dried powder with decreased packing density. Because the Tg of freeze-dried PVC is dramatically reduced to the test temperatures under compression, PVC chains are able to flow by applying pressure solely. These results help us better understanding glass transition and can possible to develop a theory for cold processes.

[1]corresponding author

3:54PM X42.00008 Evolution of Entanglements During Crazing of Glassy Polymers[1] , TING GE, MARK O. ROBBINS, Johns Hopkins University, ROBERT HOY, Yale University, STEFANOS ANOGIANNAKIS, CHRISTOS TZOUMANEKAS, DOROS THEODOROU, National Technical University of Athens — Craze formation increases the fracture energy of glassy polymers by orders of magnitude. The polymer volume expands by an extension ratio which is assumed to be determined by the entanglement network. We test this assumption with molecular simulations that use the Contour Reduction Topological Analysis (CReTA) algorithm to follow topological constraints (TCs) associated with the entanglement network. The TCs are identified with contacts between chains after applying CReTA. Within systematic errors, crazing does not change the number of TCs or the distribution of chemical distances between them. Moreover, about 75% of the contacts remain between the same chains at nearly the same location. The 25% of contacts that change do not reflect a comparable loss of entanglements. Instead, small displacements within the tube change which chains contact after CReTA. This interpretation is tested by adding fixed crosslinks to a sparse entanglement network and crazing preoriented samples.

[1]This material is based upon work supported by NSF Grant DMR 108474.

4:06PM X42.00009 Surface Softening in Polymers and Their Nanocomposites Determined by Surface Mechanical Properties through Spontaneous Particle Embedment , TASKIN KARIM, GREGORY MCKENNA, Texas Tech University — In the present work, we have used the particle embedment technique with sub-micron particles to estimate the surface modulus of epoxy/POSS composites at a temperature far below the glass transition temperature. The embedment of the particle is determined from atomic force microscope measurements and the modulus was determined using the elastic analysis of Johnson, Kendall and Roberts (JKR) with surface energy estimates of the work of adhesion as the driving force for embedment. The surface modulus values were found much smaller than the macroscopic modulus values. The maximum embedment depth obtained for all surfaces was low enough so that it did not cause plastic deformation on the surface. The maximum stress values on all surfaces induced by the particle embedment were estimated to verify the expected response in close to the linear regime.

[1] K. L. Johnson, K. Kendall and A. D. Roberts, *P. Royal Society of Lonodon A,* **324**, 301-313 (1971).
[2] J. H. Teichroeb and J. A. Forrest, *Physical Review Letter,* **91**, 016104 (2003).

4:18PM X42.00010 Effect of molecular weight on gold nanoparticle embedding into polystyrene films near and below the bulk glass transition temperature , CHAD DALEY, DONGPING QI, JAMES FORREST, University of Waterloo — We use gold nanoparticle embedding to probe the surface properties of glassy polystyrene films at temperatures ranging from a few degrees above to 10's of degrees below the bulk glass transition temperature (T_g). These studies employed monodisperse polymer samples with molecular weights (M_w) ranging from 3000-80000 kg/mol. A qualitative change in the surface response is observed between the high M_w and low M_w regimes. At low M_w a buildup of polymer material forms around the base of the nanoparticles similar to the observed behavior in molecular glasses. For the higher molecular weights this buildup is not observed and the system instead relaxes through nanoparticle embedding. We also observe changes in the complete embedding process observed only near the bulk T_g. These changes suggest that nanoparticle embedding can be used as a probe of polymer entanglements.

4:30PM X42.00011 Glass Transition and Free Volume Behavior in Epoxy-amine Network Glasses: Effect of Diiamine Isomers , SERGEI NAZARENKO, MUKUL KAUSHIK, MATTHEW JACKSON, JEFFREY WIGGINS, School of Polymers and High Performance Materials The University of Southern Mississippi, Hattiesburg, MS 39406 — A systematic investigation of the effect of meta and para isomers of diamino diphenyl sulfone (DDS) crosslinker on glass transition temperature (T_g) and free volume properties of DGEBF based epoxy-amine network was carried out. The pressure volume temperature (PVT) properties were measured experimentally from 0 to 120 MPa and 30 °C to 240 °C in a high pressure dilatometer-type PVT apparatus. It was observed that the glass transition temperature of epoxy system with para isomer is higher than the one consisting of meta isomer by 30 °C. PVT data were also fitted using Simha-Somcynsky, equation of state to calculate occupied and free volume. Positron annihilation lifetime spectroscopy (PALS) was used to calculate average hole free volume below and above glass transition temperature. The average free volume size in para isomer cured systems is larger than in meta isomer cured systems below their glass transition temperature, while in the melt state they are the same.

4:42PM X42.00012 Difference in the heat capacity and the coefficient of thermal expansion responses during thermal cycling , GRIGORI MEDVEDEV, EUN-WOONG LEE, JAMES CARUTHERS, Purdue University — An observation that different experimental methods give different values of Tg is part of the lore of the field of the glassy polymers. We report on a careful study of a series of polymeric systems both thermoplastic and thermoset, including PMMA, PC, PS, and 3,3' DDS Epon 825, conducted using DSC and TMA techniques. We found that for the same thermal history the heat capacity and the coefficient of thermal expansion (both measured upon heating) as functions of temperature transition from the glassy asymptote to the equilibrium asymptote at significantly different temperatures; this difference was in the range from 8 to 17 degrees, depending on the system. We argue that such a large difference in the enthalpy and volume responses during the same thermal history is inconsistent with the commonly used material clock models, but is consistent with the view of the glassy materials as containing dynamically heterogeneous regions.

4:54PM X42.00013 Formation of Glassy Polymer Films by Matrix Assisted Pulsed Laser Evaporation , RODNEY PRIESTLEY, YUNLONG GUO, Department of Chemical and Biological Engineering, Princeton University, CRAIG ARNOLD, Department of Mechanical and Aerospace Engineering, Princeton University — The properties of glasses strongly depend on the path to glass formation. The most common method of making polymer glasses is by cooling from the liquid state. Recently, it has been shown that alternative routes to the vitreous state can lead to dramatically improved glassy-state stability. In this talk, we present our initial work on the thermal and kinetic stability of glassy polymer films prepared by Matrix Assisted Pulsed Laser Evaporation (MAPLE). In comparison to glassy films prepared by spin coating, MAPLE-deposited glassy films can exhibit higher glass transition temperatures and greater kinetic stability.

5:06PM X42.00014 Characterization of pre-mature nanocomposite crazes , GREGORY N. TOEPPERWEIN, JUAN J. DE PABLO, University of Wisconsin Madison — Crazing is a unique mode of failure by which polymer strands are stretched into a periodic array of columns. It has been shown that these crazes follow cavitation under deformation. Inclusion of nanoparticles drastically alters the glass transition temperature and the globally measurable mechanical properties of these polymer glasses. However, limited literature exists to explain the behavior on the lengths scales of the heterogeneous domains within the glass in the context of nanocomposites. In this work, we investigate the nucleation and growth of voids that precede craze formation to elucidate the role these inclusions play in failure and further characterize the pre-mature craze itself. Extensive Molecular Dynamics and Monte Carlo simulations of highly entangled polymer nanocomposites allow for calculation of local densities, local elastic moduli, and local orientation of additives. We find that the site of void formation is inexorably linked to the local mechanical properties of polymer. This relationship is more evident upon the inclusion of reinforcing additives which induce a broader distribution of local moduli leading to the nucleation of more, smaller voids. Within the developing craze, larger additives resist incorporation, but those that do are subject to ordering.

5:18PM X42.00015 Structural Characterization of a Polymer of Intrinsic Microporosity: X-ray Scattering With Insight From Molecular Dynamics Simulations[1] , AMANDA G. MCDERMOTT, GREGORY S. LARSEN, Penn State University, PETER M. BUDD, University of Manchester, CORAY M. COLINA, JAMES RUNT, Penn State University — Polymers of intrinsic microporosity (PIMs) are high-T_g, amorphous materials exhibiting high gas permeability and a large concentration of pores smaller than 2 nm, arising from a combination of rigid segments and sites of contortion. Structures generated by molecular dynamics simulations accurately reproduce characteristic scattering features from PIM-1 at high q, allowing us to investigate their origin by examining partial structure factors. Unlike scattering patterns typical of nonporous amorphous polymers, broad q range PIM scattering patterns include a shoulder at the size scale corresponding to pore sizes measured by other techniques. We discuss the development of a model for extracting pore sizes from scattering patterns.

[1]Supported by NSF/Materials World Network/EPSRC and the NSF Graduate Research Fellowship Program.

Thursday, March 24, 2011 2:30PM - 5:30PM –

Session X43 DPOLY: Focus Session: Assembly, Structure, & Instabilities in Polymer Films, Network Films, & Interfaces II A306/307

2:30PM X43.00001 Hydrogels with Spatially and Temporally Controlled Properties to Control Cellular Interactions , JASON BURDICK, University of Pennsylvania — Stem cells (e.g., mesenchymal stem cells, MSCs) respond to many cues from their microenvironment, which may include chemical signals, mechanics, and topography. Importantly, these cues may be incorporated into scaffolding to control stem cell differentiation and optimize their ability to produce tissues in regenerative medicine. Despite the significant amount of work in this area, the materials have been primarily static and uniform. To this end, we have developed a sequential crosslinking process that relies on our ability to crosslinked functional biopolymers (e.g., methacrylated hyaluronic acid, HA) in two steps, namely a Michael-type addition reaction to partially consume reactive groups and then a light-initiated free-radical polymerization to further crosslink the material. With light exposure during the second step comes control over the material in space (via masks and lasers) and time (via intermittent light exposure). We are applying this technique for numerous applications. For example, when the HA hydrogels are crosslinked with MMP degradable peptides with thiol termini during the first step, a material that can be degraded by cells is obtained. However, cell-mediated degradation is obstructed with the introduction of kinetic chains during the second step, leading to spatially controlled cell degradability. Due to the influence of cellular spreading on MSC differentiation, we have controlled cell fates by controlling their spread ability, for instance towards osteoblasts in spread areas and adipocytes when cell remained rounded. We are also using the process of stiffening with time to investigate mechanically induced differentiation, particularly in materials with evolving mechanics. Overall, these advanced HA hydrogels provide us the opportunity to investigate diverse and controlled material properties on MSC interactions.

3:06PM X43.00002 Hydrogel Stamping of Polyelectrolyte Multilayers for Directed Cell Growth , NICOLE ZACHARIA, Texas A&M University, CHUNGYEON CHO, Texas A&M University, Materials Science and Engineering — The authors have recently introduced the use of hydrogel stamp materials to pattern polyelectrolyte multilayer (PEM) films. It has been demonstrated that using a stamp equilibrated in either low or high pH can cause local swelling in these films, leading to patterns. It has also been shown that stamps soaked in high ionic strength salt solutions are able to locally etch PEM films. This hydrogel stamping technique gives both lateral control of surface properties and depth control over the film's properties. This technique is a promising way to pattern chemical reactions within PEM, phase transformation, and physical properties such as film thickness, Young's modulus, and swelling. By using hydrogels for the stamp material, stamping becomes a process of continuously delivering aqueous reagent of interest to a film, instead of merely a single layer of material, as is the case when using hydrophobic stamp materials such as PDMS. While chemical modification of only the surface may be desirable in some cases, the hydrogel stamping technique is more versatile. By creating local variations in swelling, we are able to pattern mechanical stiffness, and in turn cell adhesion. We demonstrate the creation of gradients in mechanical stiffness which we are able to use to direct cell growth and adhesion on these films.

3:18PM X43.00003 Patterned Poly-N-isopropylacrylamide Surfaces for Culture and Harvest of Muscle Fibers , SAMUEL DUPONT, KRANTHI KUMAR ELINENI, NATHAN GALLANT, RYAN TOOMEY, University of South Florida — Swelling of surface confined poly-N-isopropylacrylamide (pNIPAAm) structures leads to non-uniform patterns that can be switched by a thermal cue. Based on the geometry of the surface confined patterns, various forms of structural instabilities arise such as bulk buckling, differential lateral swelling and edge buckling. Instabilities that arise from the swelling of patterned pNIPAAm surfaces present a unique platform for tissue engineering applications. Recent work has demonstrated the attachment, survivability, and alignment of fibroblasts grown atop rectangular pNIPAAm surface extrusions. Detachment of contiguous and aligned fibroblasts grown on these surfaces was observed when the geometry of the structure was such that a bulk buckling instability formed upon thermally induced gel swelling. Current work is aimed at utilizing this switchable platform to culture aligned myoblasts, which upon differentiation, form multicellular myotubes, an important structure in skeletal muscle. Myotubes for tissue engineering can then be harvested by non-enzymatic detachment facilitated by thermally induced non-uniform gel swelling.

3:30PM X43.00004 Controlled Release from Model Blended Polyelectrolyte Multilayer Films , BULENT AKGUN, NIST Center for Neutron Research, NIST, Gaithersburg, MD 20899, YEONGSEON JANG, School of Chemical and Biological Engineering, Seoul National University, Seoul, Korea , SUSHIL SATIJA, NIST Center for Neutron Research, NIST, Gaithersburg, MD 20899, KOOKHEON CHAR, School of Chemical and Biological Engineering, Seoul National University, Seoul, Korea — We propose a new concept of controlled release platforms based on the model blended multilayer films composed of positively charged weak polyelectrolyte (linear poly(ethylenimine),LPEI) layer and blended layer with negatively charged strong (poly(sodium-4-styrene sulfonic acid),PSS) and weak (poly(methacrylic acid),PMAA) polyelectrolytes. The blended multilayer films $((\text{LPEI/PSS:PMAA})_n)$ with well-defined internal structure are prepared by spin-assisted LbL deposition method, and their release behavior is systematically characterized with combined techniques of neutron reflectivity, ellipsometry, AFM, QCM and FT-IR. Since PSS provides the robust skeleton within the multilayer films independently on pH variation, the burst erosion of multilayer films is dramatically suppressed, and the release kinetics of PMAA can be precisely controlled by simply changing PSS contents within the multilayer films.

3:42PM X43.00005 Surface wrinkling driven by swelling and its applications , HYUN SUK KIM, ALFRED CROSBY, University of Massachusetts Amherst — The nature of reversible surface wrinkling offers great promise for designing responsive or adaptive materials. We experimentally explore the reversibility and geometry of surface wrinkles driven by swelling an elstically-supported stiff plate by solvent vapor and liquid. We use crosslinked polydimethylsiloxane (PDMS) substrates with surfaces modified by ultraviolet-ozone (UVO) processing, creating materials with rigid, surface films that swell differentially in comparison to the underlying substrates. We observe the dependence of the wrinkle wavelength on the UVO time and thickness of elastomers. Furthermore, we identify a critical length scale for the swelling region below which wrinkle formation is suppressed. Taking advantage of the reversibility and geometric relations, we demonstrate advanced applications such as smart windows with swichable optical transparency and responsive channels in microfluidics.

3:54PM X43.00006 Nanoporous Conductive Films Derived from Polymeric Bicontinuous Microemulsions , BRAD JONES, KAI-YUAN CHENG, RUSSELL HOLMES, Department of Chemical Engineering and Materials Science, University of Minnesota, TIMOTHY LODGE, Department of Chemistry and Department of Chemical Engineering and Materials Science, University of Minnesota — Ternary blends of two homopolymers and a diblock copolymer can self-assemble into interpenetrating, 3D-continuous networks with a characteristic length scale of 100 nm. These polymeric bicontinuous microemulsions (BμE) can be designed to serve as templates for the synthesis of nanoporous materials with 3D-continuous pore networks. We have investigated the behavior of BμE-forming blends of polyolefins as precursors to nanoporous polyethylene (PE) films. The effect of interfaces in these films can drastically disrupt the BμE structure, leading to a macro-phase separated morphology. Proper consideration of several factors, including substrate surface energy, film thickness, and annealing time, is necessary to retain a BμE structure in such films. Finally, we use the BμE-like, nanoporous PE films as templates in the synthesis of nanoporous films of the conducting polymer poly(3,4-ethylenedioxythiophene), having potential application in organic electronic devices.

4:06PM X43.00007 Particle Behavior at Anisotropically Curved Liquid Interfaces , KATHLEEN MCENNIS, CHUAN ZENG, BENNY DAVIDOVITCH, ANTHONY DINSMORE, THOMAS RUSSELL, University of Massachusetts Amherst — A particle bound to an anisotropically curved liquid interface, such as a cylinder or catenoid, cannot maintain a constant contact angle without deforming the interface. Theory suggests that the particles will experience a force that depends on the interfacial shape and migrate to minimize the total interfacial energy. To test these predictions, particles were deposited on top of liquid semi-cylinders of ionic liquid or melted polystyrene confined on chemically patterned surfaces. Particles were also deposited on liquid catenoid structures created by placing a melted polymer film under an electric field. The location of the particles on these structures was observed by optical, confocal, and scanning electron microscopy. The implications for the directed assembly of particles and stability of Pickering emulsions are also discussed.

4:18PM X43.00008 Hierarchically Ordered Block Copolymer Micelles Formed by Controlled Evaporative Self-Assembly , WEI HAN, MYUNGHWAN BYUN, ZHIQUN LIN, Iowa State University — Highly ordered gradient stripes of PS-b-P4VP block copolymer were obtained by combining the microscopic controlled evaporative self-assembly (CESA) of confined microfluid of PS-b-P4VP toluene solution in a "cylinder-on-Si" geometry with spontaneous self-assembly of micellar hexagonal arrays of PS-b-P4VP at the nanometer scale. The order of packed micelles within microstripes could be significantly improved by subsequent THF vapor annealing. The surface reconstruction of micelles led to the formation of nanoporous arrays when immersed in a selective solvent of the pore component. Gold nanoparticles were then selectively deposited into the core of micelles, and eventually forming the hexagonal arrays of gold nanoparticles after removal of polymer templates by oxygen plasma. The formation of gold particle arrays was verified by XPS measurement.

4:30PM X43.00009 Viscoelastic properties of ultrathin polymer films using the liquid dewetting technique , JINHUA WANG, GREGORY MCKENNA, Department of Chemical Engineering, Texas Tech University, Lubbock, Texas, 79409 — There is considerable interest in studying the behavior of polymers at the nanoscale. Here we describe experiments using the Bidiguel and Fretigny's liquid dewetting technique in which no great glass transition temperature (Tg) reduction or rubbery plateau compliance change for polystyrene (PS) films was observed [1]. These results are contrary to observations by others of Tg reductions on free standing polystyrene films and of large rubbery stiffening observed in our lab using a bubble inflation method [2,3]. Preliminary results of PS film dewetting are consistent with the Bidiguel and Fretigny's results. Also, annealing time and confinement effects on the creep behavior of polystyrene thin film were examined. Then, the range of investigated materials is being expanded to polycarbonate (PC) and poly(methyl methacrylate) PMMA with the ultimate goal to determine the reasons for the differences between the bubble inflation method and liquid dewetting technique of polymer film charicterization. References: [1] H. Bodiguel and C. Fretigny, "Viscoelastic dewetting of a polymer film on a liquid substrate," *Eur.Phys. J. E.*, 19, 185-193 (2006). [2] K. Dalnoki-Veress, J. A. Forrest, P. G. de Gennes and J. R. Dutcher, *J. Phys. IV.*, 10, 221-226 (2000). [3] O' Connell P. A. and McKenna G. B., "Rheological Measurements of the Thermoviscoelastic Response of Ultrathin Polymer Films", *Science*, 307, 1760-1763 (2005).

4:42PM X43.00010 Elastic Moduli of Nanoparticle-Polymer Composite Thin Films via Buckling on Elastomeric Substrates , HONGYI YUAN, ALAMGIR KARIM, Department of Polymer Engineering, The University of Akron, Akron, OH, USA, UNIVERSITY OF AKRON TEAM — Polymeric thin films find applications in diverse areas such as coatings, barriers and packaging. The dispersion of nanoparticles into the films was proven to be an effective method to generate tunable properties, particularly mechanical strength. However, there are very few methods for mechanical characterization of the composite thin films with high accuracy. In this study, nanometric polystyrene and polyvinyl alcohol films with uniformly dispersed cobalt and Cloisite nanoparticles at varying concentrations were synthesized via flow-coating and then transferred to crosslinked polydimethylsiloxane (PDMS) flexible substrates. The technique of Strain-Induced Elastic Buckling Instability for Mechanical Measurements (SIEBIMM) was employed to determine the elastic moduli of the films, which were calculated from the buckling patterns generated by applying compressive stresses. Results on moduli of films as a function of the concentrations of nanoparticles and the thicknesses of the composite films will be presented. *Corresponding author: alamgir@uakron.edu

4:54PM X43.00011 Effect of Chain Architecture on the Physical Aging of Thin Polymer Filims , BRADLEY FRIEBERG, EMMANOUIL GLYNOS, PETER GREEN, University of Michigan — Physical aging, glassy structural relaxations, is an important phenomenon that has an important influence on a range of physical properties, such as optical, mechanical and electrical, of polymeric materials properties. When a polymeric material is cooled below its glass transition temperature (Tg) it resides in a non-equilibrium state, and over time it attempts to return to equilibrium via a structural relaxation process. We have previously demonstrated that chain architecture can influence the Tg in supported thin films. Specifically, star-shaped molecules possessing sufficiently high functionality (f) and low molecular weight of the arm (Mw), exhibit significant differences in vitrification trends from their linear analogs. In this presentation we show that when f is sufficiently high, or Mw is sufficiently low, the physical aging rate is suppressed compared to linear chains. Moreover, the aging rates of thin, supported films of star shaped molecules are strongly thickness dependent.

5:06PM X43.00012 Perturbing the Tg of Polymers by 50-100 K in Nanoconfined Freely Standing Films and by the Presence of Neighboring Layers of Other Polymers , JOHN TORKELSON, SOYOUNG KIM, Northwestern University — We demonstrate via the temperature dependence of fluorescence intensity intrinsic to the polymer of interest or from dye labels that the glass transition temperature (Tg) of a polymer can be altered by 50-100 K by nanoconfinement in freely standing films and in multilayer systems in which the neighboring layers are different polymers. In the former case, Tg always decreases from bulk Tg; in the latter case, Tg decreases or increases depending on the Tg of the neighboring polymer layer and factors that may be related to fragility. We employ fluorescence to characterize the gradient in Tg from the perturbing interfaces. These studies reveal that the theory by de Gennes for the Tg reduction in freely standing films cannot be correct and that the perturbation to Tg by a neighboring layer of another polymer can extend as much as 100 nm into the layer of interest.

5:18PM X43.00013 ABSTRACT WITHDRAWN –

Thursday, March 24, 2011 2:30PM - 5:42PM –

Session X44 DPOLY DFD: Focus Session: Polymer Colloids-Structure, Function, and Dynamics II A309

2:30PM X44.00001 Nanoparticle Organic Hybrid Suspensions: Structure and Rheology , SAMANVAYA SRIVASTAVA, LYNDEN ARCHER, Cornell University — Nanoparticle Organic Hybrid Materials (NOHMs) are a new class of tethered nanoparticle systems with high grafting densities and behave as model systems for studying spherical polymer brushes. Here we report rheology and scattering measurements of NOHMs with a silica core and PEG corona suspended in PEG oligomers at varying volume fractions. Our rheology results reveal a liquid-glassy transition at strikingly low core volume fractions in these suspensions and prominent stress overshoots in flow startups indicative of yielding in the high volume fraction suspensions. Further, we elucidate the form of particle interactions in the glassy suspensions and compare them with established models. Also, a negative first normal stress difference in the moderate volume fraction suspensions is reported, which is in agreement with recent theoretical and experimental findings. We also report small angle scattering measurements of these suspensions to reveal their equilibrium structure, which are in qualitative agreement with a recent theoretical study (Langmuir, 2010, 26, 16801).

2:42PM X44.00002 Measuring and Modeling the Interactions Between DNA-Functionalized Colloids , WILLIAM ROGERS, JOHN CROCKER, Department of Chemical and Biomolecular Engineering, University of Pennsylvania — DNA hybridization is an ideal tool to direct "bottom-up" assembly of complex materials and has been used to form crystalline assemblies of quantum dots, polymer microspheres and other materials made exclusively of DNA. In order to fully realize the potential of DNA-directed self-assembly, one must be able to quantitatively predict the binding energies and interaction potentials between the relevant "building blocks." In this work, we use a scanning-line optical tweezers instrument to measure DNA-induced interactions between colloidal microspheres. We then use well-known concepts in statistical mechanics to model the pair-potentials, whose functional form and energetics of binding are intimately related to the equilibrium configurations of grafted polymers and polymer bridges. By measuring and modeling the pair interaction energies as a function of the essential system parameters (solution hybridization free energies, DNA concentrations, temperature, interparticle separation, etc.), we are able to develop simple, numerical tools that can be used to guide both experiment and simulation.

2:54PM X44.00003 Rheological and scattering properties of cross-linker-free microgels , ZHIYONG MENG, CHINEDUM OSUJI, Yale University — Microgel suspensions are intriguing tunable systems in part due to their pH/temperature responsivity at the single particle level. Particle collapse during volume transitions is heavily mediated by the presence of cross-links in the system. Here we examine the rheology and light scattering of microgel suspensions based on poly(N-isopropylacrylamide-*co*-acrylic acid) (pNIPAm-AAc) in the limit of vanishing cross-linking density. One issue of concern is centered on the nature of these fluids – are they simple polymer solutions or real particulate suspensions? A combination of concentration-dependent viscometry and static light scattering demonstrates conclusively that these are particulate suspensions. The absence of cross-linkers provides a sharper volume collapse at the LCST in comparison with heavily cross-linked particles. Furthermore, at fixed mass content, cross-linker-free microgel suspersions display a much higher shear modulus than cross-linked counterparts due to their larger particle size, which implicates the use of these particles in rheological modification. We survey the frequency dependence and yielding response of these suspensions as a function of temperature and composition.

3:06PM X44.00004 Normal Modes and Density of States of Disordered Colloidal Solids , MOHAMMAD ISLAM, Department of Materials Science & Engineering, Carnegie Mellon University, Pittsburgh, PA 15213 — The normal modes and the density of states (DOS) of any material provide a basis for understanding its thermal and mechanical transport properties. In perfect crystals, normal modes take the form of planewaves, but they can be complex in disordered systems. I will show our recent experimental measurements of the normal modes, the DOS and dynamical structure factor (DSF) in disordered colloidal solids: disordered colloidal crystals composed of thermally sensitive micron-sized hydrogel particles at several different particle volume fractions, ϕ. Particle positions are tracked over long times using optical microscopy and particle tracking algorithms in a single two dimensional (2D) [111] plane of a 3D face-centered-cubic single crystal. The dynamical fluctuations are spatially heterogeneous while the lattice itself is highly ordered. At all ϕ, the DOS exhibits an excess of low frequency modes, a so-called boson peak (BP), and the DSF exhibits a crossover from propagating to non-propagating behavior, a so-called Ioffe-Regel (IR) crossover, at a common frequency somewhat below the BP for both longitudinal and transverse modes. As we tune ϕ from 0.64 to 0.56, the Lindemann parameter grows from $\sim$3% to $\sim$8%, however, the shape of the DOS and DSF remain largely unchanged when rescaled by the Debye level. This invariance indicates that the effective degree of disorder and the structure of the underlying normal modes remain essentially unchanged even in the vicinity of melting. This work was supported by NSF through grants DMR-0645596 & DMR-0619424, the Sloan Foundation and American Chemical Society Petroleum Research Fund.

3:42PM X44.00005 Signatures of Aging: Comparison between Colloidal and Molecular Glasses , XIAOJUN DI, Dept of ChE, Texas Tech Univ., K.Z. WIN, GREGORY MCKENNA, T. NARITA, F. LEQUEUX, S. PULLELA, Z. CHENG, DEPT OF CHE, TEXAS TECH UNIV TEAM, PPMD, UPMC-ESPCI-CNRS, FRANCE TEAM, DEPT OF CHE, TEXAS A&M UNIV TEAM — Colloids near to the glass concentration are often taken as models for molecular glass formers. Yet, one of the most important aspects of the dynamics of molecular glasses, structural recovery, remains to be examined in colloids. We use DWS to investigate structural recovery in a thermosensitive PNIPAM colloidal suspension in the glass concentration range. The three classical aging signatures observed in molecular glasses: intrinsic isotherms, asymmetry of approach and memory effect, are investigated with this colloid and the results are compared with those typical of molecular glasses. We find: 1 for the intrinsic isotherms, the colloid shows dramatic changes in relaxation time at equilibrium while the times required to reach the equilibrium state are nearly independent of the concentration; 2 for the asymmetry of approach, the observed nonlinearity is similar to that in molecular glasses; 3 for the memory experiment, while the memory effect is seen in the colloid, the response is qualitatively different than in the molecular glass.

3:54PM X44.00006 Packings of soft disks[1] , PRIMOZ ZIHERL, University of Ljubljana and Jozef Stefan Institute, MARIJA VIDMAR, University of Ljubljana — We explore the stability of 2D ordered structures formed by soft disks treated as isotropic solid bodies. Using a variational model, we compute the equilibrium shapes and the elastic energy of disks in regular columnar, honeycomb, square, and hexagonal lattice. The results reproduce the Hertzian interaction in the regime of small deformations. The phase diagram of elastic disks is characterized by broad regions of phase coexistence; its main feature is that the coordination number of the stable phases decreases with density. These results may provide an insight into structure of the non-close-packed lattices observed in certain nanocolloidal systems.

[1]This work was supported by Slovenian Research Agency (grant No. P1-0055) and by EU through ITN COMPLOIDS (grant FP7-People-ITN-2008 No. 234810).

4:06PM X44.00007 Theory of effective interactions and dispersion of soft nanoparticles in polymer melts , JIAN YANG, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — Integral equation theory is employed to investigate the consequences of nanoparticle softness (surface fluctuations) and corrugation (discrete roughness) on the equilibrium behavior of polymer-particle mixtures in the dilute filler limit. Monomer-particle pair correlations exhibit qualitatively different features relative to hard spheres which depend on both roughness and softness. Under athermal nonadsorbing polymer conditions, depletion effects on the interparticle potential-of-mean-force (PMF) are qualitatively modified by surface corrugation and/or fluctuations. As particle softness increases, monomer-scale PMF oscillations are destroyed, and the strongest attraction occurs at a particle separation and attraction depth that depends sensitively on surface fluctuation amplitude, as does the dependence on monomer-nanoparticle size asymmetry ratio (R). For corrugated particles, the most attractive nanoparticle separation does not occur at contact, and is far weaker and less sensitive to R than for hard spheres. Second virial coefficient calculations are performed to estimate how particle softness/roughness modifies miscibility in chemically matched blends. How surface corrugation and softness modifies bridging and sterically stabilized states has also been studied..

4:18PM X44.00008 Density functional theory for the structure and dynamics of solvent-free nanoparticle–organic hybrid materials , HSIU-YU YU, DONALD KOCH, Cornell University — Nanoparticle–organic hybrid materials consist of inorganic nanocores functionalized with oligomeric organic molecules. They exhibit fluid behavior in the absence of solvent with the fluidity provided by the attached oligomers. We present a density-functional theory for the equilibrium structure and transport properties of these materials based on an assumption that the intercore forces are mediated by entropic effects associated with the conformations of the hairs subject to the constraint that the oligomer fluid is incompressible. Because each core particle carries its share of the fluid phase, the structure factor at zero wave number is equal to zero. When the radius of gyration of the oligomers is large compared with the core radius, each core experiences weak interactions with many other cores residing in its neighborhood. Exploiting this limit, the transport properties can be determined in a quasi-analytical manner based on a solution of the non-equilibrium probability density for pairs of particles experiencing a non-pairwise-additive intercore potential.

4:30PM X44.00009 Yielding mechanisms and particle rearrangements in colloidal glasses and gels under shear , GEORGE PETEKIDIS, IESL-FORTH — Steady and oscillatory rheology was utilized to study the mechanical response of colloidal glasses and gels with particular emphasis in the way these are shear melted (yield) [1,2]. We used suspensions of hard sphere colloids with short-range depletion attractions induced by the addition of non-adsorbing linear polymer. The linear viscoelasticity and the yielding mechanisms at different regimes of colloid volume fraction and particle attractions are discussed. While hard sphere glasses exhibit a single step yielding due to cage breaking, attractive glasses show a two-step yielding reflecting bond and cage breaking respectively [1]. Here we present experimental data both along a line of equal attraction, varying the particle volume fraction, from an attractive glass to a low volume fraction gel as well as at intermediate and high volume fractions with increasing the attraction strength. In attractive gels yielding remains a two step process until very low ϕ's. The first yield strain is related with in-cage or inter-cluster bond braking while the second yield point is attributed to braking of cages or clusters into smaller constituents [3]. The latter increases as volume fraction is decreased due to enhancement of structural inhomogeneities. When the range of attraction was increased, both yield strains increase, scaling with the range of attraction and accompanied structural changes. Brownian Dynamics simulations and Dynamic Light scattering under shear (LS-echo) provide information on the microscopic particle rearrangements and structural changes during yielding and flow such as the size and structure of clusters that change under steady shear as a function of shear rate. Work in collaboration with: N. Koumakis, (FORTH), M. Laurati, S.U. Egelhaaf (U. Duesseldorf) and J. F. Brady (Caltech).

[1] K. Pham et al. J. Rheology 52, 649 (2008)
[2] M. Laurati, J. Chem. Phys. 130, 134907 (2009)
[3] Koumakis and Petekidis, submitted (2010); Laurati et al, submitted (2010)

5:06PM X44.00010 Ridge formation of charged end group ligands grafted on faceted nanoparticle , PEIJUN GUO, RASTKO SKNEPNEK, MONICA OLVERA DE LA CRUZ, Northwestern University — We have investigated the conformations of charged end group ligands grafted on icosahedral nanoparticles, using a coarse-grained molecular dynamics approach. Due to a competition between the electrostatic repulsion and the hydrophobic ligand-ligand attraction, the ligand coatings form a variety of different conformations. These conformations have been compared with the case of non-charged grafted ligands. We have found that the electrostatic interaction between the charged ends drives the formation of a ridge-like structure of the ligands, which makes the nanoparticle surface highly anisotropic. We argue that the ridge-like ligand structure induces controllable directional interaction between the nanoparticles, and can drive the self-assembly of the nanoparticles into crystalline structures.

5:18PM X44.00011 Dynamics of Polymers in Colloidal Flows , HSIEH CHEN, ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology — This research is motivated by recent studies on the von Willebrand factor (vWF), a large multimeric protein that plays an essential role in the initial stages of blood clotting in blood vessels. Recent experiments substantiated the hypothesis that the vWF is activated by shear stress in blood flow that causes its shape to transform from a compact globule to an extended state [1], and biological function is obtained only in the extended state. Simple simulations (which only consider a single polymer in bulk shear flow) have successfully reproduced the observed dynamics of the vWF [2]. However, a more refined model is still demanding for the better understanding of the behaviors of this biomolecule in the physiological environments. Here we refine the existing model by adding the drifting colloids into the flows to mimic the presence of the blood cells in the bloodstream. Preliminary result shows that colloids greatly influence the dynamics of the polymers. It is observed that the average extensions of polymers along and perpendicular to the shear flow direction are both increased with the presence of the colloids.

[1] S.W. Schneider, et. al. PNAS (2007) 104 19 7899-7903
[2] A. Alexander-Katz, et. al. Phys. Rev. Lett. (2006) 97 13 138101

5:30PM X44.00012 Spontaneous asymmetry in coated spherical nanoparticles in solution and at liquid-vapor interfaces , J. MATTHEW D. LANE, GARY S. GREST, Sandia National Laboratories — Nanoparticles in solution are often stabilized with functional coatings to prevent aggregation. We'll present recent simulations results showing that small spherical nanoparticles produce highly asymmetric coating arrangements, when coated with simple polymer chains. These coatings are not symmetric even when extremely uniform grafting arrangements and full coverages are employed. I will also discuss the geometric properties which dictate the coating shape. When particles are placed in an anisotropic environment, such as the liquid/vapor interface, the asymmetric coatings are amplified and oriented by the surface. Particle shape and its responsive behavior is seen to strongly influence interactions. Implications and examples of controlled self-assembly will be presented.

Thursday, March 24, 2011 2:30PM - 5:18PM –

Session X45 DPOLY: Focus Session: Nanocomposite Physics I-Dispersions and Physical Properties A310

2:30PM X45.00001 Dynamical Aspects of Percolation Networks of Carbon Nanotubes in Polymer Composites , GYEMIN KWON, BONG JUNE SUNG, Department of Chemistry, Sogang University, Korea — Carbon nanotubes (CNTs) form a percolating network easily in polymer nanocomposites due to their high aspect ratios, thus improving both electrical and mechanical properties of composites. However, poor dispersion of CNTs has been a stumbling block to their application in industry. Therefore, extensive studies on the structure and thermodynamics of CNTs have been carried out to enhance the dispersion of CNTs in composites and find optimal conditions for better electrical and mechanical properties. But little attention has been paid to the dynamic aspects of percolation networks of CNTs, which should be also a critical factor to determine physical properties of composites. In this study, we investigate the 1st order survival rate, the assortative coefficients, and the bond connectivity time correlation function of percolation networks by using molecular dynamics simulations. We find that the CNT network dynamics becomes significantly slow and the CNT networks become dynamically stable as the concentration of CNTs increases beyond the percolation threshold concentration. We also investigate the effect of intermolecular interaction between CNTs and polymers on the dynamic behaviors of CNT networks.

2:42PM X45.00002 Langevin Approach to Optimizing Thermal Conductivity in Composite Materials , ABDELLAH AIT MOUSSA, K.G.S.H. GUNAWARDANA, KIERAN MULLEN, Homer L. Dodge Dept. of Physics and Astronomy, University of Oklahoma — The quest for high thermal conductivity materials has lead to nano-composites incorporating materials with excellent thermal conductivity in a matrix of poorer thermal conductivity. To minimize the interface thermal resistance the stiff, incorporated materials can be chemically functionalized with various side chains. We report here an efficient theoretical method to evaluate different choices for functionalization. We use this method to examine how effective different alkane chains improve the heat flux through a graphene nano-sheet.

2:54PM X45.00003 Use of embedded metal nanoparticles as photothermal heaters in polymer nanocomposites , SOMSUBHRA MAITY, JASON BOCHINSKI, LAURA CLARKE, NC State University — Embedded metallic nanoparticles within polymer nanofibers can internally heat and thus thermally-modify (soften, melt, or bond) polymer composites when irradiated with visible light via excitation and non-radiative relaxation of the nanoparticle surface plasmon resonance. Because the heating originates at the nanoparticle surface and propagates outward, a strong spatial temperature gradient exists. We discuss a non-contact, temperature-sensitive fluorescence technique to determine local temperature within the composite, which utilizes changes in the emission spectrum of perylene.....,[1] in addition to determining temperature from changes in polymer morphology. The efficacy of plasmonic heating in different morphologies (nanofibers/films) as well as its effect on material mechanical properties when heated between T_g and T_m is discussed. The spatial specificity of the photothermal heating as determined by the nanoparticle location represents a unique nanoprocessing tool.

[1]Bur, A. J.; Vangel, M. G.; Roth, S. *Applied Spectroscopy* **2002,** 56, (2), 174-181.

3:06PM X45.00004 Resistive switching in bulk polymer nanocomposites containing silver nanowires , KAREN WINEY, University of Pennsylvania, SADIE WHITE, PATRICK VORA, JAY KIKKAWA, ROSE MUTISO, University of Pennsylvania — Traditionally, bulk nanocomposites of electrically conducting particles and insulating polymers have been categorized as either insulating or conducting when the nanoparticle concentration is below or above the percolation threshold, respectively. We present the first examples of reversible resistive switching in bulk, glassy polymer nanocomposites. At compositions close to the electrical percolation threshold, silver nanowire-polystyrene nanocomposites demonstrate reversible resistive switching upon increase voltage at room temperature. Nanocomposites with compositions outside of this range exhibit either irreversible switching, or no switching at all. We propose that resistive switching in these materials is the result of the field-induced formation of silver filaments that bridge adjacent nanowire clusters, extending the percolation network and decreasing the sample's bulk resistivity. We also describe the temperature-dependent characterization of resistive switching in these nanocomposites between 10 and 300K. These findings break from the usual dichotomy of insulating or conducting properties in polymer nanocomposites and could inspire new devices that capitalize on this responsive behavior in these versatile materials.

3:18PM X45.00005 The Development of Structure in Nanoscale Colloidal Silica – Polymer Nanocomposites , JEFF METH, J. DAVID LONDONO, CHANGZAI CHI, BARBARA WOOD, PATRICIA COTTS, Nanocomposite Technologies, Central R&D, DuPont Co., SANGAH GAM, KAREN WINEY, RUSSELL COMPOSTO, Dept. of Materials Science & Engineering, Univ. of Pennsylvania — Controlling the state of dispersion or agglomeration in polymeric nanocomposites has a profound impact on their properties. Many nanocomposites are manufactured by a solution process. In such processes, colloidal silica dispersed in a formulation possesses a certain interparticle structure, and this structure changes as the coating formulation dries. In this work, we have measured the structure of colloidal silica – PMMA formulations as a function of solvent content using small angle X-ray scattering (SAXS). We found that the formulations dried in two stages: concentration and neutralization. In the concentrating stage, the charged colloid structure prevails, and the formulation simply concentrated down. In the neutralization stage, the colloid gradually lost its charge. Controlling the matrix viscosity enables one to control the final state of dispersion. These findings explain how and why it is possible to create good nanodispersions in some material systems. These general findings are applicable to a wide range of material systems.

3:30PM X45.00006 Dispersion Behavior of Au Nanorods in Polymer Thin Films Mediated by Brush-Matrix Interactions , MICHAEL J.A. HORE, RUSSELL J. COMPOSTO, Department of Materials Science and Engineering, University of Pennsylvania — Moderate volume fractions (∼5 v%) of poly(ethylene glycol) or polystyrene-functionalized Au nanorods are incorporated into poly(ethylene oxide), poly(methyl methacrylate), or polystyrene thin films (thickness ∼30 nm). Their dispersion is characterized via TEM, AFM, and x-ray reflectivity. When the chemical species of the brush is identical to that of the matrix, nanorod dispersion is dominated primarily by entropy and controlled by the ratio of the chain lengths of the brush and matrix. When there is a favorable enthalpic interaction between the brush and matrix, the dispersion is independent of the molecular weights of the brush and matrix. These experimental data are compared to Monte Carlo simulations.

3:42PM X45.00007 Particle networks through aggregation in polymer nanocomposites , MEISHA SHOFNER, Georgia Institute of Technology, JASMEET KAUR, JI HOON LEE — Structure-property research in polymer nanocomposites has often focused on producing systems that are homogeneously dispersed in order to capitalize on the large amount of specific surface area available from nanoparticles. However, inhomogeneous dispersion is often obtained and in some cases has been deliberately sought to enhance functional properties through the formation of particle networks. In this research, we are seeking to understand how particle aggregation impacts network formation in polymer nanocomposites as a function of native particle shape. Specifically, we are characterizing nanocomposites comprised of calcium phosphate particles with different shapes and a polyhydroxybutyrate matrix. Experimental results concerning the effect of particle aggregation and shape on polymer crystalline structure, thermal transitions and mechanical properties are presented to correlate particle aggregation to network formation and understand structure-property relationships in these materials.

3:54PM X45.00008 A silica nanoparticle based ionic material[1] , NIKHIL FERNANDES, ZUBAIR AZAD, EMMANUEL GIANNELIS, Cornell University — We report an ionic fluid consisting of silica nanoparticles as the anion, and amine-terminated polyethylene glycol as the cation. Unlike previous work that has required chemical functionalization of the silica surface, the charge on the nanoparticle anion is carried by the intrinsic surface hydroxyls, simplifying the synthesis, and thus making this a simple test system to probe the physics of these nanoscale ionic materials. Charge and steric factors result in excellent dispersion of the nanoparticles in the polymer matrix. The resulting material is a soft glass that has thermal and rheological properties that depend on the silica:polymer ratio. In particular, at a critical silica:polymer ratio, the ionic material shows a significant depression of the normalized heat of melting and the melting temperature compared to samples with higher or lower silica content (showing eutectic-like behaviour), and to controls without the ionic interaction between the polymer and the particle.

[1]Funded by KAUST-CU

4:06PM X45.00009 Structure-Properties Relationship in Segmented Polyurethane/Silica Nanoparticle Composites , MATTHEW HOOD, Drexel University, JAMES SANDS, JOHN LA SCALA, FREDERICK BEYER, Army Research Laboratory, CHRISTOPHER LI, Drexel University — Segmented polyurethanes (SPUs) phase separate into hard and soft domains due to differences in segment composition, resulting in extraordinary mechanical properties. We have synthesized a set of SPU/nanoparticle composites possessing 25, 35 or 45wt.% hard segment content and loaded with less than 5wt.% silica nanoparticles (SiNPs). SiNPs were added either during SPU synthesis or blended after. Drastic effects on morphology and mechanical properties were observed. Blended composites, due to their destabilizing of the hard domain, showed decreased mechanical robustness. When particles are added, at very low SiNP concentrations, during SPU synthesis the SiNPs are covalently attached to the SPU matrix and hard domains are intact which enhanced elongation to break and tensile strength considerably. With increasing SiNP concentration this effect was reversed and hard domain crystallization was hindered. Thermal, mechanical and diffraction experiments were used to correlate the relationship between interfacial chemistry of the SiNP and SPU matrix and the mechanical properties of the composites.

4:18PM X45.00010 Polyurethane Nanocomposites Reinforced with Core-shell Magnetic Particles for Microwave Absorption Applications , ZHANHU GUO, Lamar University, JIAHUA ZHU, RAHUL PATIL, NEEL HALDOLAARACHCHIGE, DAVID YOUNG, SUYING WEI — Iron-silica core-shell particles with controlled shell thickness are fabricated using a sol-gel method. Polyurethane nanocomposites are fabricated with a surface initialized polymerization (SIP) method. The thermal stability of iron-silica NPs and its corresponding PNCs is significantly enhanced due to the barrier effect of silica shell. The anti-corrosive property of the core-shell particle is dramatically improved which is able to keep stable in 1M acid solutions. Salt fog exposure tests on PNCs reveal a better anti-corrosive performance with the incorporation of core-shell particles. By embedding different NPs, unique physical properties such as enlarged coercivity and dielectric constant (real permittivity) are observed. After coating a silica layer on iron NPs, the PNCs show lower real permittivity as compared to the PNCs filled with pure NPs. However, it is interesting to observe that only slight difference in real permeability is observed in both samples at the same loading. The permittivity and permeability of the PNCs are investigated with frequency ranging from 2-18 GHz. Results indicate that the PNCs reinforced with core-shell NPs exhibit a reflection loss in a wider frequency ranges. The maximum reflection loss is around -20 dB.

4:30PM X45.00011 Studies of Microwave Absorption Properties of Carbon Nanotubes-Epoxy Composites , Z. YE, Z. LI, Southern University and A&M College, J.A. ROBERTS, University of North Texas, G.L. ZHAO, Southern University and A&M College — Less weight, excellent mechanical properties, and high efficiency in absorbing electromagnetic (EM) wave make carbon nanotubes (CNTs) composites attractive for microwave technology applications. Six groups of multi-walled carbon nanotube (MWCNT)-epoxy composite samples with various outside diameter (OD) distributions were fabricated. The weight percentages of MWCNTs in the polymer composites were controlled in the range from 1 to 10%. A microwave resonant cavity technique was utilized to measure the microwave absorption properties of all the sixty samples near a central frequency of 9.968 GHz. The results show that the maxima of EM wave absorptions for the six groups of samples were all around 7% MWCNTs weight percentage. In general, the MWCNTs with smaller diameters have higher microwave absorption at 9.968 GHz. However, the sample group M5 (OD<8nm) shows unusual results, a lower microwave absorption than other samples. SEM was used to study the morphologies of the MWCNT samples. Based on the SEM analysis and microwave absorption measurements, it was found that the efficiency of the microwave absorption of MWCNT-Epoxy composites is also affected by the morphologies/structures of MWCNTs in individual bundles. *The work is funded in part by AFOSR, NSF, and Louisiana Board of Regents.

4:42PM X45.00012 Ecobionanocomposites: a new class of green materials , JOHN DORGAN, Colorado School of Mines — This abstract not available.

Friday, March 25, 2011 8:00AM - 11:00AM –

Session Y1 DCMP: New Insights Into the Mott Transition Ballroom A1

8:00AM Y1.00001 Renewed Understanding on Doped Mott Insulators[1] , MASATOSHI IMADA, Dept. Applied Physics, Univ. Tokyo and JST CREST — Mott transitions and nearby underdoped metals in two dimensions remain a major challenge in condensed matter physics, because of large spatial and quantum fluctuations, with its relevance to cuprate superconductors. Recent theoretical and computational developments have renewed its understanding with a unified picture for the unconventional metals. We overview historical backgrounds followed by a recent coherent picture obtained by path-integral renormalization group, many-variable variational Monte Carlo methods, and cluster-type dynamical mean-field theory [1]. Coexisting zeros and poles of the single-particle Green's function hold a key for Mott physics. Non-Fermi-liquid caused by topological transitions of Fermi surface including Lifshitz transitions naturally emerges. The energy-momentum dependent spectra reproduce the arc/pocket and pseudogap formation. We propose that the pseudogap in the cuprates is d-wave-like only below the Fermi level while it retains s-wave-like full gap above the Fermi energy even in the nodal point. In addition, the spectral asymmetry, back-bending and waterfall dispersions as well as the low-energy kink emerge within the same framework in agreement with the underdoped cuprates, excluding the scenarios by preformed pairs and d-density-waves, but supporting the proximity to the Mott insulator. We also propose that an extension of the exciton concept to doped Mott insulators by using cofermions accounts for the above unconventionality and superconductivity [2].

[1] S. Sakai et al., Phys. Rev. Lett. 102, 056404 (2009); Phys. Rev. B 82, 134505 (2010)
[2] Y. Yamaji and M. Imada, arXiv:1009.1197.

[1]This work is supported from MEXT Japan (grant # 17071003 and 22104010).

8:36AM Y1.00002 Quantum criticality in the Hubbard model[1] , MARK JARRELL, Louisiana State University — In large scale dynamical cluster quantum Monte Carlo simulations of the two-dimensional (2D) Hubbard model with only nearest neighbor hopping, we find a quantum critical point (QCP) at finite doping separating a Fermi liquid region at low filling from a non-Fermi liquid pseudogap region near half-filling. Marginal Fermi liquid behavior is seen in the thermodynamics and single-particle properties for a wide range of doping and temperatures above the QCP. The QCP is due to the second-order terminus of a line of first order phase separation transitions that is driven to zero temperature as the next near-neighbor hopping t' vanishes. The superconducting dome surrounds the QCP. The proximity the QCP and the dome is due to an algebraic divergence, replacing the BCS log divergence, of the bare pairing polarization. This behavior is captured with a simple variation of the quantum critical BCS formalism.

[1]Supported by NSF DMR-0706379 and EPS-1003897 and DOE SciDAC DE-FC02-06ER25792

9:12AM Y1.00003 Cluster Dynamical Mean Field Methods and the Momentum-selective Mott transition[1] , EMANUEL GULL, Columbia University — Innovations in methodology and computational power have enabled cluster dynamical mean field calculations of the Hubbard model with interaction strengths and band structures representative of high temperature copper oxide superconductors, for clusters large enough that the thermodyamic limit behavior may be determined. We present the methods and show how extrapolations to the thermodynamic limit work in practice. We show that the Hubbard model with next-nearest neighbor hopping at intermediate interaction strength captures much of the exotic behavior characteristic of the high temperature superconductors. An important feature of the results is a pseudogap for hole doping but not for electron doping. The pseudogap regime is characterized by a gap for momenta near Brillouin zone face and gapless behavior near the zone diagonal. for dopings outside of the pseudogap regime we find scattering rates which vary around the fermi surface in a way consistent with recent transport measurements. Using the maximum entropy method we calculate spectra, self-energies, and response functions for Raman spectroscopy and optical conductivities, finding results also in good agreement with experiment.

[1]Olivier Parcollet, Philipp Werner, Nan Lin, Michel Ferrero, Antoine Georges, Andrew J. Millis; NSF-DMR-0705847

9:48AM Y1.00004 Finite doping signatures of the Mott transition in the two-dimensional Hubbard model , GIOVANNI SORDI, Departement de physique and RQMP, Universite de Sherbrooke, Sherbrooke, Quebec, Canada J1K 2R1 — The evolution from the conventional metal at high doping to the Mott insulator at zero doping remains a central problem in physics of copper-oxide superconductors. Here we solve the cellular dynamical mean-field equations [1,2] for the two-dimensional Hubbard model on a plaquette with continuous-time quantum Monte Carlo [3,4]. The normal-state phase diagram as a function of temperature T, interaction strength U, and filling n reveals that, upon increasing n towards the Mott insulator, there is a surface of first-order transition between two metals at nonzero doping. That surface ends at a finite temperature critical line originating at the half-filled Mott critical point [5,6]. There is a maximum in scattering rate associated with this transition. These findings suggest a new scenario for the normal-state phase diagram of the high temperature superconductors. The criticality surmised in these systems can originate not from a T=0 quantum critical point, nor from the proximity of a long-range ordered phase, but from a very low temperature transition between two types of normal state metals at finite doping. The influence of Mott physics extends well beyond half-filling.

[1] G. Kotliar et al., Rev. Mod. Phys. 78, 865 (2006).
[2] T. Maier et al., Rev. Mod. Phys. 77, 1027 (2005).
[3] P. Werner and A.J. Millis, Phys. Rev. B 74, 155107 (2006).
[4] K. Haule, Phys. Rev. B 75, 155113 (2007).
[5] G. Sordi, K. Haule, and A.-M.S. Tremblay, Phys. Rev. Lett. 104, 226402 (2010).
[6] G. Sordi, K. Haule, and A.-M.S. Tremblay, unpublished (2010).

10:24AM Y1.00005 Computational Studies of Realistic Multiband Models of the Copper Oxides , CEDRIC WEBER, Rutgers University — High temperature superconductivity was achieved by introducing holes in a parent compound consisting of copper oxide layers separated by spacer layers. It is possible to dope some of the parent compounds with electrons, and their physical properties are bearing some similarities but also significant differences from the hole doped counterparts. Here, we use a modern first principles method, to study the electron doped cuprates and elucidate the deep physical reasons why their behavior is so different than the hole doped materials. We find that electron doped compounds are Slater insulators, e.g. a material where the insulating behavior is the result of the presence of magnetic long range order. This is in sharp contrast with the hole doped materials, where the parent compound is a Mott charge transfer insulator, namely a material which is insulating due to the strong electronic correlations but not due to the magnetic order. In particular, we point out that both hole and electron doped compounds are located close to the charge-transfer insulator to metal transition, and we discuss the consequences for optical and specific heat measurements done for the normal state, and additional consequences for the magnetic and superconducting orders of electron and hole doped copper oxides.

Work done in collaboration with Kristjan Haule and Gabriel Kotliar, Rutgers University.

Friday, March 25, 2011 8:00AM - 11:00AM –
Session Y2 DCMP: Topological Insulators: Transport and Interactions Ballroom A2

8:00AM Y2.00001 Quantum oscillations and Hall anomaly of surface electrons on Topological Insulators[1] , N. PHUAN ONG, Princeton University — The investigation of Topological Insulators (TI) by transport experiments is a challenge, because the surface currents cannot be well-resolved when the bulk conductance is dominant, as in most crystals. I will review the progress starting from Ca-doped Bi_2Se_3, and proceeding to Bi_2Te_3 and to Bi_2SeTe_2. Using Ca dopants in Bi_2Se_3, we succeeded in lowering the Fermi energy E_F into the bulk gap. However, in non-metallic crystals, the substantial dopant-induced disorder precluded observation of Shubnikov-de Haas (SdH) oscillations. Fortunately, E_F in undoped Bi_2Te_3 can be tuned into the gap by heat treatment. The non-metallic samples display a bulk resistivity ρ = 4-12 mΩcm at 4 K. In these crystals, weak SdH oscillations are observed below 10 K. We confirmed that these oscillations arise from a 2D Fermi Surface by tilting the magnetic field $\mathbf{H}$. From the behavior of the SdH amplitude versus temperature T and H, we infer a surface Fermi velocity v_F = 3.7-4.2 $\times 10^5$ m/s, and a high surface mobility μ = 10,000 cm^2/Vs. The high mobility of the surface electrons is confirmed by the appearance of an unusual weak-field anomaly in the Hall conductance G_{xy}. I will discuss recent progress in further lowering the bulk conductance in the new TI Bi_2Se_3, in which a Se layer is sandwiched between two Te layers in each quintuplet unit cell. In these crystals, ρ at 4 K is a factor of 1000 larger (6 Ωcm). The interesting pattern of SdH oscillations in this new system will be reported.

Collaborators: D.X. Qu, J. M. Checkelsky, Y. S. Hor, J. Xiong, R. J. Cava

[1]Supported by NSF-MRSEC DMR 0819860. High-field experiments were performed in the National High Magnetic Field Lab., Tallahassee.

8:36AM Y2.00002 Dirac Fermions in HgTe Quantum Wells , LAURENS W. MOLENKAMP, Physics Institute (EP3), Wuerzburg University — Replace this text with your abstract. Narrow gap HgTe quantum wells exhibit a band structure with linear dispersion at low energies and thus are very suitable to study the physics of the Dirac Hamiltonian in a solid state system. In comparison with graphene, they boast higher mobilities and, moreover, by changing the well width one can tune the effective Dirac massfrom positive, through zero, to negative. Negative Dirac mass HgTe quantum wells are 2-dimensional topological insulators and, as a result, exhibit the quantum spin Hall effect. In this novel quantum state of matter, a pair of spin polarized helical edge channels develops when the bulk of the material is insulating, leading to a quantized conductance. I will present transport data provide very direct evidence for the existence of this third quantum Hall effect: when the bulk of the material is insulating, we observe a quantized electrical conductance. Apart from the conductance quantization, there are some further aspects of the quantum spin Hall state that warrant experimental investigation. Using non-local transport measurements, we can show that the charge transport occurs through edge channels - similar to the situation in the quantum Hall effect. However, due to the helical character of the quantum spin Hall edge channels, inhomogeneities in the potential profile of the experimental devices have a much stronger effect on the transport properties. Moreover, the quantum spin Hall edge channels are spin polarized. We can prove this fact in split gate devices that are partially in the insulting and partly in the metallic regime, making use of the occurrence of the metallic spin Hall effect to convert the magnetic spin signal into an electrical one. Finally, I will address another aspect of Dirac Fermion physics: HgTe quantum wells at a critical thickness of 6.3 nm are zero gap systems and exhibit transport physics that is very similar to that observed over the past few years in graphene. However, zero gap HgTe wells have a higher mobility than graphene, and also have only a single Dirac valley. This makes them especially suitable to study quantum interference effects under a Dirac Hamiltonian.

9:12AM Y2.00003 Band Topology, Electron Correlations and 3D Dirac Metal in Pyrochlore Iridates , ASHVIN VISHWANATH, UC Berkeley — We study consequences of strong spin orbit interaction in a class of correlated systems. We discuss the possibility of novel phases such as a π axion insulator, protected by inversion, rather than time reversal symmetry and a gapless topological phase, the three dimensional Dirac semimetal. The latter phase has unusual surface states that take the form of 'Fermi Arcs', that cannot be realized in any two dimensional band structure. The pyrochlore iridates, (such as $Y_2Ir_2O_7$) according to LDA+U calculations and existing experimental data, are argued to be promising materials for realizing these states. This work was done in collaboration with Xiangang Wan (Nanjing U.), Sergey Savrasov (UC Davis) and Ari Turner (UC Berkeley).

9:48AM Y2.00004 General Theory of interacting Topological insulators , SHOUCHENG ZHANG, Stanford University — In this talk, I shall first briefly review the theory of topological insulators and the experimental status. I will then discuss the general theory of an interacting topological insulator, whose topological order parameter is expressed in terms of the full interacting Green function. This topological order parameter is also experimentally measurable in terms of the quantized magneto-electric effect. I shall discuss various applications of this theory to realistic materials which could realize the topological Mott insulator state.

"Topological Field Theory of Time-Reversal Invariant Insulators," Phys. Rev. B. **78**, 195424, (2008).
"General theory of interacting topological insulators," arXiv:1004.4229.
"Dynamical Axion Field in Topological Magnetic Insulators," Nature Physics **6**, 284 (2010).
"Quantum Spin Hall Effect in a Transition Metal Oxide Na2IrO3," Phys. Rev. Lett. **102**, 256403 (2009).
"Topological Mott Insulators," Phys. Rev. Lett. **100**, 156401, (2008).

10:24AM Y2.00005 Classification of Topological Insulators and Superconductors: the "Ten-Fold Way"[1] , ANDREAS LUDWIG, Dept. of Physics, University of California, Santa Barbara — We review the exhaustive ten-fold classification scheme of topological insulators and superconductors. It is found that the conventional (i.e.: "Z_2", or 'spin-orbit') topological insulator, experimentally observed in 2D ('Quantum Spin Hall') and in 3D materials, is one of a total of five possible classes of topological insulators or superconductors which exist in every dimension of space. Different topological sectors within a given class can be labeled, depending on the case, by an integer winding number, or by a "binary" Z_2 quantity. The topological nature of the bulk manifests itself through the appearance of "topologically protected" surface states. These surface states completely evade the phenomenon of Anderson localization due to disorder. Examples of the additional topological phases in 3D include topological superconductors (i) with spin-singlet pairing, and (ii) with spin-orbit interactions, as well as ^{3}He B. – The classification of topological insulators (superconductors) in d dimensions is reduced to the problem of classifying Anderson localization at the (d-1)-dimensional sample boundary which, in turn, is solved. The resulting five symmetry classes of topological insulators (superconductors) found to exist in every dimension of space correspond to a certain subset of five of the ten generic symmetry classes of Hamiltonians introduced 16 years ago by Altland and Zirnbauer in the context of disordered systems (generalizing the three well-known "Wigner-Dyson" symmetry classes). For a significant part of the phases of topological insulators (superconductors) of the classification a characterization can be given in terms of the responses of the system. For these, the responses are described by a field theory possessing a [gauge, gravitational (thermal), or mixed] anomaly. This implies that these phases are well defined also in the presence of inter-fermion interactions.

[1]Work done in collaboration with S. Ryu, A. Schnyder, A. Furusaki, and with S.Ryu, J.E. Moore. Supported by NSF DMR-0706140.

Friday, March 25, 2011 8:00AM - 11:00AM –
Session Y3 DCMP: Recent Developments in Solid 4He Ballroom A3

8:00AM Y3.00001 Dynamics, Defects and Deformation in Solid Helium[1]

, JOHN BEAMISH, University of Alberta — The shear modulus of solid ^{4}He shows remarkable softening above 100 mK, the same temperature range in which the apparent supersolid disappears in torsional oscillator experiments. We have measured helium's shear modulus and dissipation at frequencies from 0.5 to 8500 Hz. The onset temperature for softening/stiffening is broad, frequency dependent, and is accompanied by a dissipation peak - features typical of a dynamical crossover in a disordered system rather than a true phase transition. This behavior can be qualitatively explained if dislocations are mobile at high temperatures but are pinned by ^{3}He impurities below 100 mK. To better understand the role of dislocations, we have plastically deformed crystals by rapid thermal quenching and used pressure gradient measurements to study subsequent annealing. In our most recent experiments we have sheared solid helium mechanically and looked at the effect of large deformations on the helium's elastic properties.

[1]This work was supported by NSERC

8:36AM Y3.00002 New evidence of supersolidity in rotating solid helium[1]

, EUNSEONG KIM, Department of Physics, KAIST — The irrotationality of superfluid causes it to decouple form the container, leading to a reduction in the rotational inertia. This is more technically known as non-classical rotational inertia (NCRI). Although it is intuitively most natural to associate superflow only with the liquid phase, a decrease in the resonant period of a torsional oscillator (TO) was detected in solid helium below about 200 mK and interpreted as the appearance of NCRI. However, the resonant period may be also reduced for reasons other than supersolidity, such as the temperature dependence of the elastic modulus of solid helium. Unusual increase in the shear modulus with striking resemblance to those of NCRI supports the non-superfluid explanations. We superimposed dc rotation onto oscillatory measurements to distinguish between the supersolidity and classical elastic modulus change effects. We performed such simultaneous measurements of the TO and the shear modulus, and observed substantial change in the resonant period with rotational speed where the modulus remained unchanged. This contrasting behavior suggests that the decrease in the TO period is a result of supersolidity. This work is performed by collaboration with H. Choi, D. Takahashi, and K. Kono.

[1]This work is supported by the National Research Foundation through Creative Research Initiatives and Japan Society for the Promotion of Science through Grant-in-Aid for Scientific Research respectively.

9:12AM Y3.00003 Quantum plasticity and supersolidity[1]

, SEBASTIEN BALIBAR, ENS & CNRS - Paris (France) — We have discovered that, in the total absence of impurities, helium 4 crystals are anomalously soft [1]. In our opinion, this is a consequence of the quantum properties of their dislocation lines which are able to move macroscopic distances (typically a fraction of a millimeter) at high speed (several meters per second) as a response to very small applied stresses (one microbar). Moreover, this quantum plasticity appears to be closely related to another astonishing property of quantum crystals, namely their "supersolidity," that is the possible superflow of a fraction of the crystal mass through the rest which remains elastic, actually more rigid than in the normal state [2]. Very tiny traces of helium 3 impurities are sufficient to pin the dislocations below about 100 mK and destroy the quantum plasticity. By studying rotational and elastic properties of crystals with various qualities and variable helium 3 content, we are now checking that supersolidity is a consequence of matter flowing along dislocation lines but only if these dislocations are pinned by impurities.

[1] X. Rojas, A. Haziot, V. Bapst, H.J. Maris, and S. Balibar, Anomalous softening of helium 4 crystals, Phys. Rev. Lett. 105, 145302 (2010).
[2] S. Balibar, The enigma of supersolidity, Nature 464, 176 (2010).

[1]Work supported by ERC grant 2009-AdG247258-SUPERSOLID.

9:48AM Y3.00004 Mass Flow in Solid ^{4}He as Observed by Fountain Effect Measurements[1]

, ROBERT HALLOCK, University of Massachusetts Amherst, Amherst, MA 01003 — We have created an experimental cell in which solid helium is sandwiched between two Vycor rods which are each in turn in contact with reservoirs of superfluid ^{4}He [1]. Application of a temperature difference between the two reservoirs creates a thermo-mechanical effect, which causes a flux of atoms from one reservoir to the other through the solid helium, which is off the melting curve. The flux is measured to increase with falling temperature below about 650 mK, fall precipitously near 80 mK and then rise again at lower temperatures [2]. Results of these experiments as well as the behavior of solid growth will be presented and discussed in the context of recent theoretical work.

[1] M. Ray and R.B. Hallock, Phys. Rev. Letters 100, 235301 (2008); Phys. Rev. B 79, 224302 (2009).
[2] M. Ray and R.B. Hallock, Phys. Rev. Letters 105, 145301 (2010).

[1]Work done in collaboration with Michael Ray (now at Dept. of Physics, Univ. of California, Berkeley, CA); supported by NSF DMR 08-55954

10:24AM Y3.00005 Superclimb of Dislocations in Solid ^{4}He[1]

, ANATOLY KUKLOV, CSI, CUNY — Edge dislocation with superfluid core can perform *superclimb* – non-conservative motion (climb) assisted by superflow along its core. Such dislocation, with Burgers vector along the C-axis, has been found in *ab initio* simulations of *hcp* solid ^{4}He [1]. Uniform network of superclimbing dislocations can induce *isochoric compressibility* $\chi = dN/d\mu$ which is finite (in contrast to ideal solid where it vanishes) and, practically, independent of the network density. Here N is total number of atoms and μ is chemical potential [1]. Such giant response has been observed by Ray and Hallock during superfluid flow events through solid He4 [2]. Study [3] of superclimbing dislocation within the model of Granato-Lücke string, subjected to Peierls potential and to vanishing bias by μ, has found that χ exhibits wide peak in the intermediate range of temperatures (T) - above some T_p determined by Peierls energy and below $T_s \sim 0.5$K above which superfluidity of the core essentially vanishes. Non-Luttinger type behavior characterized by $\chi \sim L^b$ scaling as some power $1 < b \leq 2$ of dislocation length L is observed in the wide peak region. Biasing superclimbing dislocation by finite μ (due to a contact with liquid ^{4}He through vycor electrodes [2],[4]) can induce core roughening caused by thermally assisted tunneling of jog-antijog pairs through the barrier produced by combination of Peierls potential and the bias [5]. The threshold for this effect scales as $\mu_c \sim 1/L^a$ with some power $a \approx 1.7$. The roughening is found to be hysteretic below some temperature $T_{\rm hyst}$. At $T_{\rm hyst} < T < T_R$, with T_R determining temperature of thermal roughening, χ exhibits strong and narrow resonant peak leading to a dip in the core superfluid sound velocity. This mechanism is proposed as an explanation for a strong and narrow dip observed in critical superflow rate [4]. It is found that the dip characteristics are sensitive to the bias by μ and, therefore, this can be used as a test for the proposed mechanism. It is also predicted that the dip depth at given T should be periodic in μ with the period $\sim \mu_c$.

[1] S. G. Söyler, et. al., PRL bf 103, 175301 (2009).
[2] M. W. Ray and R. B. Hallock, PRL **100**, 235301 (2008) ; PRB **79**, 224302 (2009); PRB **81**, 214523 (2010); Phys. Rev. **B82**, 012502 (2010);
[3] D. Aleinikava, et al., JLTP, to be published;
[4] M. W. Ray and R. B. Hallock , Phys. Rev. Lett. **105**, 145301 (2010);
[5] D. Aleinikava and A.B. Kuklov, unpublished.

[1]This work was supported by NSF, grants PHY1005527 and PHY0653135,and by CUNY, grant 63071-00 41

Friday, March 25, 2011 8:00AM - 11:00AM –
Session Y4 DPOLY: Polymer Colloids: Structure, Function and Dynamics Ballroom A4

8:00AM Y4.00001 Colloidal photonic crystals: Beyond optics, beyond spheres , KOEN CLAYS, University of Leuven, Belgium — Monodisperse and symmetrically shaped colloidal particles tend to form ordered aggregates. When the particle size is in the hundreds of nanometres, such highly ordered structures exhibit fascinating optical properties, hence their name and fame as colloidal "photonic crystals" or as "photonic bandgap material", because they exhibit a forbidden energy band for photons, very much like semiconductor crystals are characterized by a bandgap for electrons. Photonic bandgap engineering is possible by a proper choice of the size and nature of the "photonic atom", and by a proper combination of different kinds of particles. The fame of monodisperse colloidal spheres as photonic atoms is largely based on the self-assembling capabilities into inherently three-dimensional photonic crystals. Colloidal photonic crystals can hence be used as an easy photonic crystal platform to demonstrate proof-of-principle for effects such as reduced local density of states for photons on their emission probability. We have induced spectral narrowing for emission from dye molecules and enhanced energy transfer between light-absorbing molecules in colloidal photonic crystals. By inserting superparamagnetic particles in the tens of nanometres range, it is possible to additionally impart magnetic properties to the photonic crystal. Tuning and enhancing Faraday rotation was possible by careful nanoscale bandgap engineering at two different nanoscales. One disadvantage of colloidal spheres for photonic crystals is the incomplete bandgap that is typical for the highly symmetrical crystal structures that are commensurable with dense packing of spheres. A number of approaches allow deviating from this paradigm towards a complete bandgap in the visible. Etching of material allows a less dense crystal, while non-spherical colloidal particles provide alternate crystal structures. Orientational ordering of such anisotropic particles in an anisotropic photonic crystal requires an additional handle on the particles, the colloidal assembly providing the positional order. Magnetism again provides this handle. Post-formation processing of crystals of positionally ordered spheres into orientationally anisotropic crystals represents another approach.

8:36AM Y4.00002 Near Wall Dynamics in Colloidal Suspensions Studied by Evansescent Wave Dynamic Light Scattering[1] , PETER R. LANG, Research Centre Juelich, Juelich, Germany — The dynamics of dispersed colloidal particles is slowed down, and becomes anisotropic in the ultimate vicinity of a flat wall due to the wall drag effect. Although theoretically predicted in the early 20th century, experimental verification of this effect for Brownian particles became possible only in the late 80s. Since then a variety of experimental investigations on near wall Brownian dynamics by evanescent wave dynamic light scattering (EWDLS) has been published. In this contribution the method of EWDLS will be briefly introduced, experiments at low and high colloid concentration for hard-sphere suspensions, and the theoretical prediction for measured initial slopes of correlation functions will be discussed. On increasing the particle concentration the influence of the wall drag effect is found to diminishes gradually, until it becomes negligible at volume fractions above $\phi > 0.35$. The effect that a wall exerts on the orientational dynamics was investigated for different kinds of colloids. Experiments, simulations and a virial expansion theory show that rotational dynamics is slowed down as well. However, the effect is prominent in EWDLS only if the particles' short axis is of the order of the evanescent wave penetration depth.

[1]The author acknowledges financial support from the EU through FP7, project Nanodirect (Grant 395 No. NMP4-SL-2008-213948).

9:12AM Y4.00003 Assembly of Dimer-Based Photonic Crystals , CHEKESHA M. LIDDELL WATSON, Department of Materials Science and Engineering, Cornell University — Recent advances in colloid synthesis to prepare monodisperse shape anisotropic particles provide the opportunity to address challenges related to structural diversity in ordered colloidal solids. In particular, computational simulations and mechanical models suggest that upon system densification nonspherical dimer colloids undergo disorder-order and order-order phase transitions to unconventional solid structures including, base-centered monoclinic crystals, degenerate aperiodic crystals, plastic crystal or rotator, etc. based on free energy minimization. The particle systems have notable analogy to molecular systems, where the shape of molecules and their packing density has been shown to critically influence structural phase behavior and lead to a rich variety of structures, both natural and synthetic. The materials engineering challenges have been in attaining sufficiently monodisperse (size uniformity) colloidal building blocks, as well as the lack of understanding and control of self-assembly processes for non-spherical colloids. This talk highlights our investigations of how particle shape programs the self-organization of colloidal structures. Methods including evaporation mediated assembly and confinement provide a platform to understand the formation of complex colloidal structures from non-spherical building blocks (silica-coated iron oxide, polystyrene, hollow silica shell). Optical property simulations for unconventional 2D and 3D structures with nonspherical particle bases will also be discussed.

9:48AM Y4.00004 Directed self-assembly of small colloidal clusters[1] , VINOTHAN MANOHARAN, Harvard University — We study the formation and structure of equilibrium colloidal clusters at small particle number ($N \sim 10$) using optical microscopy. Our experimental system consists of isolated groups of colloidal microspheres with short-ranged attractions. With non-specific depletion interactions, we observe that the number of configurations increases sharply with N. The most favorable states are those with the lowest symmetry. With specific DNA-mediated attractions, the number of states is reduced. Experiments and theoretical calculations suggest that it is possible to direct the assembly of specific structures through multiple competing DNA-mediated interactions.

[1]We acknowledge support from the National Science Foundation under grant nos. DMR-0820484, ECS-0335765, and ECCS-0709323

10:24AM Y4.00005 Convective microsphere monolayer deposition , JAMES GILCHRIST, Lehigh University — There is perhaps no simpler way of modifying surface chemistry and morphology than surface deposition of particles. Micron-sized microspheres were deposited into thin films via rapid convective deposition, similar to the 'coffee ring effect' using a similar method to that studied by Prevo and Velev, Langmuir, 2003. By varying deposition rate and blade angle, the optimal operating ranges in which 2D close-packed arrays of microspheres existed were obtained. Self-assembly of colloidal particles through a balance of electrostatic and capillary forces during solvent evaporation was revealed. These interactions were explored through a model comparing the residence time of a particle in the thin film and the characteristic time of capillary-driven crystallization to describe the morphology and microstructure of deposited particles. Co-deposition of binary suspensions of micron and nanoscale particles was tailored to generate higher-quality surface coatings and a simple theory describes the immergence of instabilities that result in formation of stripes. Optical and biomedical applications that utilize the described nanoscale control over surface morphology will also be discussed.

Friday, March 25, 2011 8:00AM - 11:00AM –
Session Y5 DCOMP DCP: Opening the Gap: Chemical Functionalization and Substitution in Graphene Ballroom C1

8:00AM Y5.00001 Magnetic Moment and Electronic Correlations in Chemically Functionalized Graphene

, JORGE SOFO, Penn State — Magnetic moments in extended systems are the result of local electronic correlations. In the case of graphene functionalized with chemisorbed atoms such as hydrogen, fluorine, or oxygen, the Anderson Model picture, where correlations in a localized state are responsible for the formation of a magnetic moment, has to be modified to properly describe the magnetic moment formation and their interactions. We use a tight-binding model with local correlations to analyze the results obtained with Density Functional Theory calculations for these systems. The model allows the treatment of local correlations beyond the mean field level and the investigations of a possible Kondo effect. We find that the Coulomb repulsion at the carbon atoms near the impurity play a crucial role in the magnetic moment formation. External doping with a gate voltage can control the nature of the binding and the formation of the magnetic moment. This effect could be observed in transport experiments as the scattering of the graphene electrons at the Fermi energy strongly depends on the structure of the defect.

8:36AM Y5.00002 A theoretical study of chemical functionalisation of graphene: graphane and graphXene

, OLLE ERIKSSON, Uppsala University — Chemical functionalisation of graphene is reported from a first principles, theoretical study [1]. The electronic structure, including band gap, of H adsorbed on graphene (i.e. graphane) is discussed in this presentation [2]. In addition, adsorption of Group VII elements on graphane (named graphXene) is also reported [3]. Similarities and differences in the chemical binding and electronic structure of graphane and graphXene are analyzed. The adsorption on graphene is found to, depending on adatoms, result in sp2 or sp3 binding, where in general the sp3 bonded systems show a bandgap. The theoretical calculations make use of both GGA functionals as well as the GW approximation. In addition to large graphene layers, theoretical analysis of functionalised graphene nano-ribbons will also be presented [4]. References:

[1] V. A. Coleman, et al.,J. Phys. D: Appl. Phys. 41,062001 (2008); S. H. M. Jafri, et al, J. Phys. D 43, 45404 (2010).
[2] S.Lebegue, et al., Phys. Rev. B 79, 245117 (2009).
[3] M.Klintenberg, et al., Phys. Rev. B 81, 85433 (2010).
[4] S. Bhandary, et al., Phys. Rev. B 82, 165405 (2010).

9:12AM Y5.00003 Gap control via graphene solid-state reactions

, BORIS I. YAKOBSON, Rice University — While a gapless dispersion law of Dirac fermions in graphene does warrant admiration, to serve as useful semiconductor graphene needs a gap. Relatively inert, it can nevertheless be induced to react. A generic outcome of a reaction, C + A -> $C_{1-x}A_x$ is a transition of some C-atoms from their sp^2- into sp^3-state, corresponding to a situation of the insulating, ultimate (mono- or few-layer) diamond slab [1]. Computations support a concept that the product of such reactions (A = H, F, O, Cl, etc.) forms a well-defined phase [2], permitting a patterning of 2D-geometries with useful properties: interconnects-nanoroads [3], quantum isles-dots [4], etc. Comparison of hydrogenation (A = H) into graphAne with fluorination (A = F) into 2D-teflon, shows the former as hindered by nucleation barrier and reversible (H-storage), in contrast to barrier-less reaction into a stable CF in the latter. *** In collaboration with F. Ding, E. Penev, M.A. Ribas, and A.K. Singh. ***

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[2] Y. Lin, et al., Phys. Rev. B, 78, 041402(R), 2008.
[3] A.K. Singh and BIY, Nano Lett., 9, 1540, 2009.
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9:48AM Y5.00004 Spin-polarized semiconductor induced by magnetic impurities in graphene[1]

, MARIA DAGHOFER, IFW Dresden — Magnetic impurities adsorbed on graphene sheets are coupled antiferromangetically via the itinerant electrons in the graphene. We study this interaction and its impact on the electrons' spectral density by use of unbiased Monte-Carlo simulations. The antiferromagnetic order breaks the symmetry between the sublattices, and a gap for the itinerant electrons opens. Our simulations show that the itinerant states below and above the gap are not dispersionless states trapped by the impurities, but are instead mobile states with a large dispersion. We compare various scenarios for the impurity distribution and find that random doping produces a standard semiconductor. If, on the other hand, all or most of the impurities are localized in the same sublattice, the spin degeneracy is lifted and the conduction band becomes spin-polarized. We also discuss the properties of edge states at edges or magnetic domain boundaries.

M. Daghofer, N. Zheng, A. Moreo; Phys. Rev. B **82**, 121405(R) (2010)

[1]Supported by the DFG under the Emmy-Noether Program, and the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. DOE.

10:24AM Y5.00005 Graphene monofluoride: a wide bandgap material derived from graphene

, JUN ZHU, Penn State University — Fluorination provides an effective way of controlling the properties of carbon materials. In this talk, I will describe our experimental and theoretical work on the synthesis, structural, electrical and optical properties of fully fluorinated graphene and graphite, i. e., graphene monofluoride CF and graphite monofluoride $(CF)_n$. $(CF)_n$ is synthesized by reacting HOPG graphite with F_2 gas at high temperature. Transmission electron microscopy and electron diffraction measurements show crystalline few-layer CF with a lattice constant 4% larger than that of graphene, in good agreement with first principle calculations. We observe the E_g and A_{1g} Raman modes of graphene monofluoride using UV Raman spectroscopy. Photoluminescence measurements of $(CF)_n$ using variable excitation wavelength (244-514 nm) and temperature (5-295 K) show several emission modes in the visible spectrum, which likely originate from mid-gap defect states. The absence of the band edge emission suggests a large band gap of greater than 5 eV. Partially fluorinated graphene fluoride exhibits non-linear, strongly insulating transport with variable-range hopping temperature dependence, consistent with the presence of localized states due to missing fluorine atoms. Highly conductive graphene can be recovered by annealing CF in Ar/H_2 at high temperature, resulting in a conductance improvement of five orders of magnitude. As a transparent and atomically thin insulator, graphene monofluoride may find its use in graphene electronics and photonics. In collaboration with: Bei Wang, Shih-Ho Cheng, Justin Sparks, Humberto Gutierrez, Ke Zou, Ning Shen, Youjian Tang, Qingzhen Hao, Awnish Gupta, Peter Eklund, Vincent Crespi, Jorge Sofo and Fujio Okino (Shinshu University, Japan). References: Cheng et al, "Reversible fluorination of graphene: towards a two-dimensional wide band gap semiconductor," Phys. Rev. B 81, 205435 (2010) Wang et al, "Photoluminescence from nanocrystalline graphite monofluoride," Appl. Phys. Lett. 97, 141915 (2010)

Friday, March 25, 2011 8:00AM - 11:00AM –

Session Y6 GMAG: Ultrafast Magnetization Dynamics: Where Are We Today? Ballroom C2

8:00AM Y6.00001 The x-ray few of femtosecond spin-orbit excitations in ferromagnets

, HERMANN DURR, SLAC — Polarized soft x-rays have been used over the past 20 years to obtain fascinating new insights into nanoscale magnetism. The separation of spin and orbital magnetic moments, for instance, enabled detailed insights into the interplay of exchange and spin-orbit interactions at the atomic level. The now available polarized soft x-ray pulses with only 100 fs duration allow us to observe the magnetic interactions at work in real time. The ultimate goal of such studies is to understand how spins may be manipulated by ultrashort magnetic field, spin polarized current or light pulses. In this talk I will focus on fs laser induced spin-orbit dynamics in 3d transition metals. Using fs x-ray pulses from the BESSY II femtoslicing facility I will show how fs excitation of the electronic system modifies the spin-orbit interaction enabling ultrafast angular momentum transfer between spin, orbital and lattice degrees of freedom.

8:36AM Y6.00002 Possibility of Nanoscale Imaging of Ultrafast Magnetization Dynamics[1]

, ANDREAS SCHERZ, SIMES, SLAC Nat. Acc. Lab., California — Understanding the microscopic mechanisms driving the magnetization dynamics on the fs time scale is of essential importance for manipulating and controlling the macroscopic state in magnetic storage devices. The demagnetization in ferromagnetic films by an ultrashort laser excitation on a time scale of a few hundred fs raised controversies about the effective path to dissipate angular momentum to the lattice, see e.g. [1]. Even more intriguing is the demonstration of all-optical magnetization reversal in ferrimagnetic compounds using circularly polarized, fs laser pulses [2]. Until only recently, the field of "Femto-magnetism" has naturally been driven by all-optical pump-probe techniques. Femtosecond time-resolved X-ray magnetic circular dichroism spectroscopy has been utilized to unambiguously determine the ultrafast quenching of spin and orbital moments after ultrashort laser excitation [3]. While all-optical pump-probe techniques allow ultrafast excitations (pump) and the study of their evolution (probe) on the macroscopic scale by use of the magneto-optical Kerr or Faraday effect, little is known about the microscopic processes on nano- and sub-nanometer length scales because of the lack of real or momentum space resolution of optical techniques. By combining resonant coherent resonant magnetic scattering with the unique high peak-brightness, short pulse structure, and fully transverse coherence of the new x-ray free-electron lasers, the dynamics of magnetic fluctuations and magnetization relaxation processes can be studied on the nanometer scale with sub-picosecond time resolution. We demonstrate the possibility of nondestructive single shot imaging of the magnetization in Co/Pd multilayers at LCLS.

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[2] Stanciu, C.D., et al., Phys. Rev. Lett. 99, 047601 (2007).
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[1]Both LCLS and the conducted research are supported by DOE-BES.

9:12AM Y6.00003 Imaging Magnetization Dynamics on the Nanoscale Using X-ray Microscopy

, GUIDO MEIER, University of Hamburg — We aim at time- and spatially resolved imaging of excitations in ferromagnetic materials such as spin waves, the motion of domain walls and the gyration of magnetic vortices and antivortices. Special emphasize is given to the interaction of electrical currents with magnetic inhomogeneities like domains walls and vortices. The spin-polarized current can give rise to a spin torque on spatially inhomogeneous magnetization configurations. With magnetic transmission X-ray microscopy we observe a current-driven oscillation of an individual domain wall on its genuine time scale. In the framework of an analytical model insight into the domain-wall motion and its characteristic damping time is gained by examination of different phase spaces [1]. Current-induced depinning of a domain wall from a pinning site depends on the temporal shape of the current pulse. Apart from resonant excitation of the wall this effect arises from an additional force on the wall due to a fast changing current. Efficient depinning is achieved for rise times smaller than the damping time of the domain wall [2]. Time-resolved X-ray microscopy is used to image the influence of alternating high-density currents on the magnetization dynamics of vortices and antivortices. They behave as two-dimensional oscillators with a gyrotropic eigenmode which can be resonantly excited by spin currents and magnetic fields [3]. It is shown that the two excitation types couple in an opposing sense of rotation in case of resonant antivortex excitation with circular-rotational currents [4]. We report on the experimental observation of purely spin-torque induced antivortex-core reversal. Financial support by the DFG via SFB 668 and via GK 1286 as well as by the City of Hamburg via the Landesexzellenzcluster Nano-Spintronics is gratefully acknowledged. The ALS is supported by the Director, Office of Science, Office of Basic Energy Sciences, of the US Department of Energy.

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9:48AM Y6.00004 Ultrafast magnetization dynamics in lanthanide ferromagnets: From bulk to surfaces[1]

, UWE BOVENSIEPEN, University of Duisburg-Essen, Faculty of Physics, Germany — The intense research on femtosecond laser-induced magnetization dynamics resulted in rich ultrafast phenomena [1]. A microscopic description of the underlying elementary processes, however, remains a challenge. Most efforts focus on the $3d$ transition metal ferromagnets and related compounds. This talk discusses recent work on the lanthanide ferromagnets Gd and Tb. Their magnetic moment is dominated by $4f$ electrons which are localized at the ion core. Their spin-lattice coupling is determined by the angular momentum of the $4f$ electrons. Using femtosecond x-ray magnetic circular dichroism at the femtosecond slicing facility at the BESSY II storage ring in Berlin, Germany, we measure the ultrafast change in the magnetic moment, which occurs on two specific timescales [2]. The faster one is 0.75 ps. It is driven by hot electrons and is identical for both lanthanides. The slower one is different for Gd (40 ps) and Tb (8 ps) due to the stronger spin-lattice coupling in Tb. The talk also discusses time-resolved non-linear optical studies on Gd(0001) and Tb(0001) surfaces [3]. We find a coherent surface phonon which is strongly coupled with the ultrafast magnetic response and pronounced differences compared to the bulk dynamics which are attributed to spin-polarized transport effects.

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[1]This work was supported by the German Federal Ministry of Education and Research through FEMTOSPEX.

10:24AM Y6.00005 Ultrafast magnetization dynamics in a system with tunable angular momentum , ANDREI KIRILYUK, Radboud University Nijmegen — Many peculiarities of the magnetization dynamics are related to the fact that a certain amount of angular momentum is associated with magnetic moment. Here the dynamics of angular momentum is studied in ferrimagnetic rare-earth – transition metal alloys, e.g. GdFeCo, where both magnetization and angular momenta are temperature dependent. Depending on their composition, such ferrimagnets can exhibit a magnetization compensation temperature TM where the magnetizations of the sublattices cancel each other and similarly, an angular momentum compensation temperature TA where the net angular momentum vanishes. At the latter point, the frequency of the homogeneous spin precession diverges. As a consequence, ultrafast heating of a ferrimagnet across its compensation points may result in a subpicosecond magnetization reversal [1]. Moreover, we have experimentally demonstrated that the magnetization can be manipulated and even reversed by a single 40 femtosecond circularly polarized laser pulse, without any applied magnetic field [2,3]. This optically induced ultrafast magnetization reversal is the combined result of laser heating of the magnetic system and circularly polarized light acting as a magnetic field with amplitudes of up to several Teslas. The direction of this opto-magnetic switching is determined only by the helicity, i.e. angular momentum, of light. This novel reversal pathway (see [4]) is shown to crucially depend on the net angular momentum reflecting the balance of the two opposite sublattices.

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Friday, March 25, 2011 8:00AM - 11:00AM –

Session Y8 FGSA FIP: Experiences and Issues for Young Physicists in the International Arena: Impact on the Future of Physics followed by Panel Discussion Ballroom C4

8:00AM Y8.00001 Impact of Visa Issues on an International Physics Graduate Student in the U.S. , AZADEH KEIVANI, Louisiana State University — More than 35 percent of the physics graduate students in the US are temporary visa holders. Many of these students work in large international collaborations and must travel abroad for research and international conferences, sometimes more than once a year. In many cases, students have to reapply for their visas in order to return to the U.S., a process that can be time-consuming and costly. Furthermore, many international students cannot leave the U.S. even in the case of an emergency because a slow visa process may mean deferring for a semester or losing financial support. Thus visa issues affect not only the scholastic life of students but also their personal lives. Finding ways to resolve these issues could positively affect the quality of graduate research by eliminating these extra hurdles to the progress of international physics graduate students.

8:20AM Y8.00002 Overcoming the Cultural Barrier: An International Physicist's Experience , J. PEDRO OCHOA, Berkeley lab — Doing experimental physics in the midst of an international community, a necessity in certain fields due to the breadth and the complexity of the projects involved, is a task that presents many advantages but also challenges. I will be reviewing some of these from the point of view of an international physicist working in China. I will also be sharing my personal experiences in overcoming the cultural barriers and in transitioning from a country that is traditionally underrepresented in science.

8:40AM Y8.00003 Life In a large scientific collaboration , RISHIRAJ PRAVAHAN — I will be talking about life in a large scientific collaboration. The dynamics of dealing with many groups, collaborating with people from various linguistic and cultural origins can be a daunting experience. However, it is exactly this diversity of culture and learning that can make it an invigorating journey. You need to find your place in terms of professional contribution as well as personal liaisons to be productive and innovative in a large work culture. Scientific problems today are not solved by one person hunched over an old notebook. It is solved by sharing computer codes, experimental infrastructure and your questions over coffee with your colleagues. An affinity to take in and impart healthy criticism is a must for productive throughput of work. I will discuss all these aspects as well as issues that may arise from adjusting to a new country, customs, food, transportation or health-care system. The purpose of the talk is to familiarize you with what I have learned through my past five years of stay at CERN and working in the ATLAS collaboration.

9:00AM Y8.00004 Perspectives from an International Female Physicist in Academia , TULIKA BOSE, Boston University — I will bring my perspective as an international physicist in academia to the discussion of issues facing international physicists. I will also talk about issues facing women physicists worldwide.

9:20AM Y8.00005 Panel Discussion: Issues Facing International Physicists and the Future of Physics , AMY FLATTEN[1], American Physical Society — The panel will discuss the challenges and key issues faced by today's young physicists, especially when participating in international collaborations.

[1]APS Director of International Affairs

Friday, March 25, 2011 8:00AM - 11:00AM –

Session Y9 DFD: Motility, Locomotion and Cellular Fluid Mechanics D220

8:00AM Y9.00001 ABSTRACT WITHDRAWN –

8:12AM Y9.00002 Coordinated Swimming: Hydrodynamic interactions between multi-flagellated bacteria , NOBUHIKO WATARI, RONALD LARSON, University of Michigan — Multi-flagellated bacteria, such as Escherichia coli, often have flagella attached at random locations to the cell body, which drive swimming behavior. To study the effect of hydrodynamic interactions on the swimming behavior, we develop a bead-spring model which represents both the body and the flagella using up to 240 Stokeslets, or hydrodynamic drag centers. These beads are bonded by 1) a spring potential, 2) a bending potential, and 3) a torsional potential to adjacent beads. This modeled bacterium swims by rotating the flagella with constant torques. We find that the number and arrangement of the flagella along the bodies of the swimmers affects how two such swimmers approach each other, when swimming either in a line, or side by side, and affects whether or not flagellar rotations are synchronized or not. We show how the flow field generated by each swimmer can be represented using a low order multipole expansion, which can capture the qualitative features of their interactions. With this simple low order expansion, simulations of hundreds or thousands of such swimmers can be carried out, allowing the effects of numbers and locations of flagella on swimming pattern formation to be captured.

8:24AM Y9.00003 Remote Powering and Steering of Self-Propelling Microdevices by Modulated Electric Field , RACHITA SHARMA, ORLIN VELEV, North Carolina State University — We have demonstrated a new class of self-propelling particles based on semiconductor diodes powered by an external uniform alternating electric field [1]. The millimeter-sized diodes floating in water rectify the applied voltage. The resulting particle-localized electroosmotic flux propels them in the direction of the cathode or the anode depending on their surface charge. These particles suggest solutions to problems facing self-propelling microdevices, and have potential for a range of additional functions. The next step in this direction is the steering of these devices. We will present a novel technique that allows on-demand steering of these self-propelling diodes. We control remotely their direction of motion by modifying the duty cycle of the applied AC field. The diodes change their direction of motion when a DC component (wave asymmetry) is introduced into the AC signal. The DC component leads to redistribution of the counterions near the diode surface. The electric field resulting from this counterion redistribution exerts a torque on the dipole across the diode, causing its rotation. Thus, the reversal of the direction of the electroosmotic flux caused by field asymmetry leads to reversal of the direction of diode motion. This new principle of steering of self-propelling diodes can find applications in MEMs and micro-robotics. [1] S. T. Chang, V. N. Paunov, D. N. Petsev, O. D. Velev, Nat Mater, 6, 235-240 (2007).

8:36AM Y9.00004 Motility of rotating flagella in viscoelastic fluids , BIN LIU, THOMAS POWERS, KENNETH BREUER, Brown University — Bacteria achieve motility by eluding the constraints of kinematic reversibility, for instance, by rotating a helical flagellum. We study experimentally the motility of the flagellum with a scaled-up model system, a motorized helical coil that rotates along its axial direction. The rotating helix is tethered on a linear stage that advances at a predetermined speed along the axial direction. A free-swimming speed is obtained when the net force on the helix is zero. In the Newtonian case, the free-swimming speed of the helix is always proportional to its rotation rate. We show how such motility is affected by the presence of the viscoelasticity of the fluid, a ubiquitous environment for living bacteria.

8:48AM Y9.00005 Electrical Control of Microtubule Translocation on Graphene , EUNJI KIM, Department of Biophysics and Chemical Biology, Seoul National University, Seoul 151-747, Korea, DONG SHIN CHOI, Department of Nano Science and Engineering, Seoul National University, Seoul, 151-747 Korea, KYUNG-EUN BYUN, Department of Physics and Astronomy, Seoul National University, Seoul, 151-747, Korea, HEEJUN YANG, JINSEONG HEO, HYUN-JONG CHUNG, SUNAE SEO, Semiconductor Devices Lab, Samsung Advanced Institute of Tech., Giheung-Gu, Yongin-Si, Gyeonggi-Do 449-712, Korea, SEUNGHUN HONG, Department of Biophysics and Chemical Biology, Seoul National University, Seoul 151-747, Korea — Motor protein systems such as a kinesin-microtubule complex play an important role in intracellular cargo transport by directly converting a chemical energy into a mechanical work. For exploiting their high energy efficiency, there have been considerable efforts to integrate them with various nanostructures to build nanoscale biodevices such as an advanced nano-transportation system. Herein, we demonstrated a successful motility assay of microtubules on a kinesin-functionalized graphene electrode which has a good transparency and conductivity. By applying a voltage bias onto the graphene electrode, we could spatially control the translocation of the microtubules. Our result clearly shows that graphene can be used not only as a good substrate for a motor-protein motility assay but also as a key component for a nano-mechanical system based on biomotors.

9:00AM Y9.00006 Swimming speed of an oscillating sheet in Newtonian and viscoelastic fluids , MOUMITA DASGUPTA, MICHAEL BERHANU, ARSHAD KUDROLLI, Clark University, HENRY FU, University of Nevada, Reno, KENNETH BREUER, THOMAS POWERS, Brown University — We discuss a mechanical experimental model of a flexible sheet swimming with a prescribed wave pattern - a Taylor swimmer - through a fluid. Our study is motivated by a need for a fundamental understanding of microorganism locomotion through non-Newtonian fluids. In order to simplify the problem, we suspend a tall flexible cylindrical sheet concentric within a cylindrical tank filled with the fluid. Torque free boundary conditions are imposed by supporting the flexible sheet and the tank with friction-free ball-bearings. A traveling wave is imposed on the sheet with a pair of rollers in the azimuthal direction. We first demonstrate a linear response in the swimming velocity of the sheet with respect to its phase velocity in a viscous Newtonian fluid. Further, we show that the analytical system is essentially two dimensional by varying the height of fluid in the tank. We then discuss measurements of swimming speed in Polyox-water mixtures as a function of wave speed. We demonstrate that the swimming speed in this viscoelastic fluid decrease relative to the Newtonian case as wave speed is increased. We will further discuss the dependence of swimming speed on Deborah number and other characteristics of the fluid.

9:12AM Y9.00007 Highly-Controllable Near-Surface Swimming of Magnetic Nanorods , BENJAMIN EVANS, Elon University, LAMAR MAIR, UNC - Chapel Hill — Directed manipulation of nanomaterials has significant implications in the field of nanorobotics, nanobiotechnology, microfluidics, and directed micro- and nano-object assembly. With this in mind, we present a simple, efficient method for the fabrication and controlled manipulation of rod-shaped micro-scaled swimmers in a low-Reynolds environment. We demonstrate fine spatial control of the swimmers' motion and we approach, capture, and manipulate a polystyrene microbead as proof of principle. The swimmers consist of 200-nm-diameter gold nanowires which are grown by electrodeposition in an AAO template. The template is removed via dissolution in NaOH, and a layer of nickel (50 nm) is subsequently evaporated onto the surface of the wires. These wires settle near the floor of an enclosed water-filled cell and are observed via optical microscopy. Rotation is induced via an external magnetic field provided by a permanent magnet. The field is rotated in a plane nearly parallel to the floor; a small tilt out-of-plane results in symmetry-breaking, with the end of the rod nearest the floor experiencing an enhanced drag coefficient due to the presence of the boundary. The imbalance in drag forces between the two ends of the rotating rod results in a net translation. We use resistive force theory to develop an analytical model which describes the motion of these swimmers and correlate this model with experimental results.

9:24AM Y9.00008 Textured boundaries and their effects on ciliary locomotion , SAIKAT JANA, Department of Engineering Science and Mechanics, Virginia Tech, SUNG YANG, Department of Nanosystems and Engineering, GIST, South Korea, SUNGHWAN JUNG, Department of Engineering Science and Mechanics, Virginia Tech — Many microorganisms in nature propel themselves by creating coordinated motion of the cilia and often interact with each other through hydrodynamic interactions. We study the behavior of these organisms near boundaries of different topography and rationalize the hydrodynamic effects involved. Various geometries like wavy, rough or solid walls are simulated using micro fabrication and their effects on the locomotory traits are observed. Finally a comprehensive discussion on the effect of different boundaries on the swimming characteristics of the organism is presented.

9:36AM Y9.00009 Motion of Elastic Microcapsules on Compliant Surfaces with Adhesive Ligands , EGOR MARESOV, GERMAN KOLMAKOV, ANNA BALAZS, University of Pittsburgh — By integrating mesoscale models for hydrodynamics, micromechanics and adhesion, we examine the fluid driven motion of elastic microcapsules on compliant surfaces. The capsules, modeled as three-dimensional fluid-filled elastic shells, represent polymeric microcapsules or biological cells. Our combined integrated Lattice Boltzmann model/Lattice spring model (LBM/LSM) approach allows for a dynamic interaction between the elastic capsule's wall and surrounding fluid. To capture the interaction between the shell and the surface, we adopt the Bell model, used previously to describe the interaction of biological cell like leukocytes rolling on surfaces under the influence of an imposed shear. The surface of the microcapsule contains receptors with an affinity to adhesive ligands of the substrate. We examine how the parameters of adhesion and rigidity of the capsules and the substrate affect movement of the capsules. The findings provide guidelines for creating smart surfaces that could regulate the microcapsules' motion.

9:48AM Y9.00010 Modelling the dynamics of colloidal nanorods in a spatially varying electric field , GREGORY RICHARDS, Dept. of Mathematical Sciences and Liquid Crystal Institute - KSU, XIAOYU ZHENG, Dept. of Mathematical Science - KSU, PETER PALFFY-MUHORAY, Liquid Crystal Institute - KSU — The behavior of anisotropic nanoparticles is of great current interest in the design of optical metamaterials. We have carried out numerical simulations to model the dynamical behavior of metallic nanorods, dispersed in an isotropic solvent, under the influence of a radially varying electric field. Diffusive and convective transport is considered both in orientation and position space. The Smoluchowski equation governing the spatial and orientational probability density function (PDF) was derived. Discretization was carried out using a finite-volume method on a mesh generated via Voronoi tesselation and regularization on the unit sphere. The time evolution of the PDF was obtained using a combination of operator splitting and a stable biconjugate gradient method. We present the results of our numerical experiments. We report interesting and anomalous behavior, where, due to the coupling of orientation and translational mobility, the applied field depopulates certain orientational states, similar to 'orientational hole burning' in nonlinear optics.

10:00AM Y9.00011 Designing self-propelling micro-swimmer that navigates in microfluidic channels , BEN BINGHAM, HASSAN MASOUD, ALEXANDER ALEXEEV, Georgia Institute of Technology — Using a fully-coupled computational approach that integrates the lattice Boltzmann model for the hydrodynamics and the lattice spring model for the micromechanics of deformable solids, we design a synthetic micro-swimmer that not only self-propels but also successfully navigates in a low Reynolds number environment of a microfluidic channel. The swimmer body consists of a responsive polymer gel that undergoes periodical swelling and shrinking. Two thin elastic flappers are attached to the opposite sides of the swimmer body. The flappers wiggle driven by swimmer body oscillations and, in this fashion, propel the micro-swimmer through its highly viscous fluid environment. Third, light sensitive flapper is attached in the front of the swimmer and serves to steer its trajectory in microchannel. When exposed to light, the steering flap bends towards the light source. We show that this swimmer can either move straight or turn in the required direction following light signals. Thus, guided by light, the micro-swimmer can successfully navigate towards the target in a microfluidic channel.

10:12AM Y9.00012 Azobenzene Crystal Shooting and Shape Behavior in the Context of Time Dependent Ginzburg-Landau Equations[1] , THOMAS SUTTER, Polymer Engineering, University of Akron, GRANG RILEY, Physics Department, Miami University, DMITRY GOLOVATY, Theoretical and Applied Mathematics, University of Akron, THEIN KYU, Polymer Engineering, University of Akron — Blends of azobenzene chromophore and diacrylate monomer show novel nucleation instability. Once a crystal nucleates near a larger growing crystal, it shoots away from the growing front. This shooting phenomenon is explained in the context of "Marangoni propulsion," an imbalance of surface energies at the leading and trailing crystal edges. A concentration gradient is established during the course of diffusion-controlled crystal growth; as the crystal front pulls azobenzene molecules in and rejects acrylate solvent molecules. Thus, crystal growth dynamics influence the concentration gradient build up at the advancing front, as well as the crystal's shape. The time dependent Ginzburg-Landau model C equation was used to simulate crystal growth using a free energy expression which combines Flory-Huggins theory of liquid-liquid demixing and the phase field free energy of crystallization. We have also established a theoretical phase diagram by self-consistently solving the free energy expression. Crystal shape and shooting character will be explained in the context of the phase diagram.

[1]We thank the donors of the American Chemical Society Petroleum Research Fund (PRF#48735-ND7).

10:24AM Y9.00013 Flagellar generated flow mediates attachment of *Giardia lamblia*[1] , JEFFREY URBACH, HAIBEI LUO, THEODORE PICOU, RYAN MCALLISTER, HEIDI ELMENDORF, Georgetown University — *Giardia lamblia* is a protozoan parasite responsible for widespread diarrheal disease in humans and animals worldwide. Attachment to the host intestinal mucosa and resistance to peristalsis is necessary for establishing infection, but the physical basis for this attachment is poorly understood. We report results from TIRF and confocal fluorescence microscopy that demonstrate that the regular beating of the posterior flagella generate a flow through the ventral disk, a suction-cup shaped structure that is against the substrate during attachment. Finite element simulations are used to compare the negative pressure generated by the flow to the measured attachment force and the expected performance of the flagellar pump.

[1]NIH grant 1R21AI062934-0

10:36AM Y9.00014 Probing the directional structure and intracellular microrheology of vascular endothelial cells , MANUEL GOMEZ-GONZALEZ, KATHRYN OSTERDAY, JULIE LI, GERARD NORWICH, JUAN LASHERAS, SHU CHIEN, JUAN CARLOS DEL ALAMO, University of California, San Diego — The magnitude of the rheological properties of cytoplasm is important because it sets the level of intracellular deformation in response to stress. The directionality is equally important because it allows the cell to modulate the stress-strain relation differently along different directions. We aim to elucidate the relation between the structural organization of the cytoplasm and the directionality of its rheological properties by 1) measuring the local orientation of fluorescently labeled intracellular filaments and 2) determining the local directions of the maximum and minimum intracellular viscosity. For this purpose, we improved current microrheology measurements by studying the drag force experienced by a microsphere in an anisotropic viscoelastic network permeated by a liquid. In the limit of strong frictional coupling between network and liquid, the flow around the sphere is modeled with a generalized Stokes equation using several viscosity parameters. We solve this equation analytically to provide new closed-form microrheology formulae relating the resistance measured experimentally to the anisotropic properties of the network. Tracking the random motion of endogenous particles in 2D and using these novel microrheology formulae we measured directional intracellular viscosities.

10:48AM Y9.00015 Non-equilibrium fluctuations of cell membranes: The effect of cytoskeletal motor activity on membrane dynamics , ROIE SHLOMOVITZ, ALEX LEVINE, UCLA, Department of Chemistry & Biochemistry — The mechanics and non-equilibrium (i.e. molecular motor-driven) fluctuation spectrum of living cells remains an open problem. In this talk, we explore the question: What can one infer about the action of endogenous motors in the cytoskeleton by observing the height fluctuations of cell membrane? To address this, we treat the cytoskeleton as a uniform elastic half-space bounded by a membrane with a finite bending modulus and driven out of equilibrium by molecular motors (i.e. myosin). These motors produce transient and stochastic contractile stresses in the elastic bulk. We first calculate the induced undulations of the membrane-bound surface due to the action of a single molecular motor. Then, making assumptions about the spectrum of motor force fluctuations, we calculate the expected non-thermal contribution to the cellular membrane fluctuations due to the action of an ensemble of such motors. We discuss extensions of this simple model to include, e.g. the effect spatially inhomogeneous coupling between the cytoskeleton and the membrane. We also mention ongoing experimental tests of these ideas.

Friday, March 25, 2011 8:00AM - 11:00AM –

Session Y10 DCMP: Electronic Structure of Surfaces and Interfaces D221

8:00AM Y10.00001 Interface structure and magnetic anisotropy of Fe/Pd(001) and Pd/Fe/Pd(001) monatomic films , TETSURO UENO, MASAHIRO SAWADA, KAZUHITO FURUMOTO, TETSURO TAGASHIRA, AKIO KIMURA, HIROFUMI NAMATAME, MASAKI TANIGUCHI, Hiroshima University — Fe and Pd are known to form $L1_0$-ordered alloy, which exhibits easy magnetization axis perpendicular to the atomic stacking plane. In order to reveal the origin of the uniaxial magnetic anisotropy in the point of view of atomic structure, we performed the experiments on bare and Pd-covered Fe monatomic films on Pd(001) surface. Interface structure analysis was done by means of intensity-voltage analysis of low-energy electron diffraction (LEED I-V), and the magnetic anisotropy was investigated by X-ray magnetic circular dichroism (XMCD). Sample fabrication and XMCD experiments were performed at HiSOR-BL14 of Hiroshima Synchrotron Radiation Center, Hiroshima University. It is revealed that the intermixing between Fe films and Pd substrate occurs at room temperature growth, and Pd-overlayer compresses the interlayer distance around Fe layer. Fe thickness dependent XMCD revealed that the spin reorientation transition from perpendicular to in-plane direction occurs in bare Fe/Pd(001) with Fe thickness increase. On the contrary, in-plane magnetic anisotropy is stable in Pd/Fe/Pd(001). We attributed the perpendicular magnetic anisotropy in Fe/Pd(001) to the $L1_0$-like interface structure which realized in this system.

8:12AM Y10.00002 Enhancement of Kondo effect through Rashba spin-orbit interactions[1] , NANCY SANDLER, MEHDI ZAREA, SERGIO ULLOA, Ohio University — The role of Rashba spin-orbit (RSO) interactions on the Kondo regime has been a topic of debate since resistivity measurements on Pt doped Cu:Mn compounds were interpreted as evidence for suppression of the Kondo effect by SO scattering. Subsequent theoretical and experimental activity has yielded conflicting results. Thus, the question: what is the role of SO interactions in the Kondo regime? remains open. To provide a definite answer we obtain an exact solution of an Anderson magnetic impurity model in a two-dimensional metallic host with RSO interactions. We show that the Hamiltonian reduces to an effective two-band Anderson model coupled to a S=1/2 impurity. An appropriate Schrieffer-Wolff transformation produces an effective 2-channel Kondo model plus a Dzyaloshiinski-Moriya (DM) interaction term. The exact solution reveals that the impurity couples to the bath with ferro- and antiferromagnetic couplings. DM interactions, that vanish at half-filling and at the Hubbard U-infinity limits, introduce an exponential increase in the value of the Kondo temperature.

[1]Supported by NSF-PIRE and MWN/CIAM.

8:24AM Y10.00003 Correlation induced charge ordering metal-insulator transition in a two-dimensional triangular lattice , R. CORTES, Univ. Complutense de Madrid, A. TEJEDA, Institut Jean Lamour, J. LOBO-CHECA, CIN2, C. DIDIOT, B. KIERREN, D. MALTERRE, Institut Jean Lamour, J. MERINO, F. FLORES, E.G. MICHEL, Univ. Autonoma de Madrid, A. MASCARAQUE, Univ. Complutense de Madrid — Mott insulators are one of the clearest examples on how electronic correlations limit the band theory. Semiconducting surfaces offer an ideal playground to study correlation effects in two dimensions. We report here a combined experimental and theoretical analysis on correlation effects in an atomically ordered reconstruction of 1/3 ML of Sn on Ge(111). This interface exhibits a Mott metal insulator transition below 30 K [1,2]. We find a novel phase between the known metallic and insulating phases, settled by electronic correlations and characterized as a charge ordering insulator (COI) that competes with the lower temperature Mott phase. We describe here the electronic mechanism behind the stabilization of the COI-phase, the role of atomic vibrations in the process, and interpret these findings on the basis of DMFT theoretical calculations. These results explain recent controversies [3] on the interpretation of the nature of the low temperature phase. [1] A. Tejeda et al. Phys. Rev. Lett. 100 (026103) 2008 [2] R. Cortes et al. Phys. Rev. Lett. 96 (126103) 2006 [3] H. Morikawa et al. Phys. Rev. B 78 (245307), 2008; S. Colonna et al., Phys. Rev. Lett. 101 (186102) 2008

8:36AM Y10.00004 Passage from Spin-Polarized Surface States to Unpolarized Quantum Well States in Topologically Nontrivial Sb Films , GUANG BIAN, University of Illinois at Urbana-Champaign, THOMAS MILLER, University of Illinois, TAI-CHANG CHIANG, University of Illinois at Urbana-Champaign, CNL TEAM — Topological insulators, which possess robust gapless surface states as a result of strong spin-orbit coupling, have attracted much interest because of their unusual surface spin structures. When such materials are reduced to ultrathin films, the spin-split surface states must connect, by analytic continuation, to quantum well states, which are spin-unpolarized in centrosymmetric systems. We report herein a combined experimental and theoretical study of this passage from polarized to unpolarized states in Sb films. Bulk Sb is semimetallic with a negative band gap; nevertheless, it shares the same topological order as $Bi_{1-x}Sb_x$ ($0.07< x< 0.2$), the first material identified as a three-dimensional topological insulator. Angle-resolved photoemission (ARPES) from Sb films, aided by first-principles calculations, shows smooth dispersion relations associated with this passage; the spin polarizations of the two states fade away, while the energy splitting is maintained through the emergence of different charge density patterns of the resulting quantum well states.

8:48AM Y10.00005 Electron-grain boundary scattering and the resistivity of nanometric metallic structures , R.C. MUNOZ, M. FLORES, G. KREMER, R. HENRIQUEZ, J.G. LISONI, L. MORAGA, S. OYARZUN, M.A. SUAREZ, Dept. of Physics, University of Chile — The resistivity of metallic structures depends on electron-grain boundary and electron-surface scattering. By tuning the grain size, we have been able to separate the contribution to the resistivity originating in electron-grain boundary scattering, from that arising in electron-surface scattering. The resistivity of gold films approximately 54 nm thick deposited onto mica substrates under high vacuum, was measured between 4 and 300 K. It exhibits a cross over, in samples where the average grain diameter $d > 38$ nm and the resistivity is determined by electron-surface plus electron-phonon scattering, to a regime where it is determined by electron-grain boundary plus electron phonon scattering , in samples where $d < 38$nm. l(300)=38 nm is the electron mean free path in the bulk at 300 K. The resistivity can described by Drude's model. It can be described as well by Mayadas's theory using the grain boundary reflectivity R *as the only adjustable parameter.* Funded by FONDECYT 1085026. **References.** R. Henriquez et al., Phys. Rev. **B82** (2010) 113409.

9:00AM Y10.00006 Atomic and Electronic Structures of the Cu2O/TiO2 Heterostructure Interface , SHUZHI WANG, BALASUBRAMANIAM KAVAIPATTI, JOEL AGER, Lawrence Berkeley National Laboratory, RAMAMOORTHY RAMESH, University of California, Berkeley, LIN-WANG WANG, Lawrence Berkeley National Laboratory, LAWRENCE BERKELEY NATIONAL LABORATORY COLLABORATION, UNIVERSITY OF CALIFORNIA, BERKELEY COLLABORATION — Earth-abundant metal oxides have great potentials in replacing Si in semiconductor solar cells and meeting the terawatt scale global energy demand. The structural and electronic properties of the heterojunction interface in oxide-based thin film solar cells, which is of great importance to the energy conversion efficiency, however, is not well understood yet. In this talk, we will present our experimental and theoretical work on the atomic and electronic structures of the interface of Cu_2O and anatase TiO_2. Despite the large lattice mismatch of 13%, Cu_2O can be grown epitaxially on TiO_2(001) in the cube-on-cube orientation by pulsed laser deposition. The interface is found to form a regular coincidence lattice of 8 Cu_2O and 9 TiO_2 unit cells in each in-plane direction. The relaxed structure of this coincidence lattice is simulated using density functional theory calculations. The local density of states along the interface is found to shift as much as 0.4 eV, depending on the local alignment of the two lattices. As a result, the valence band and conduction band edge wave functions are well separated.

9:12AM Y10.00007 Response of the Shockley surface state on Cu(111) to an external electrical field: A density-functional theory study[1] , KRISTIAN BERLAND, PER HYLDGAARD, Chalmers U. of Tech., T.L. EINSTEIN, U. of Maryland — We study the response of the Cu(111) Shockley surface state to an external electrical field E by combining a density-functional theory calculation for a finite slab geometry with an analysis of the Kohn-Sham wavefunctions to obtain a well-converged characterization. We find that the surface state displays isotropic dispersion, quadratic until the Fermi wave vector but with a significant quartic contribution beyond. We find that the shift in band minimum and effective mass depend linearly on E. Most change in electrostatic potential profile, and charge transfer occurs outside the outermost copper atoms, and most of the screening is due to bulk electrons. Our analysis is facilitated by a method used to decouple the Kohn-Sham states due to the finite slab geometry, using a rotation in Hilbert space. We discuss applications to tuning the Fermi wavelength and so the many patterns attributed to metallic surface states.

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

9:24AM Y10.00008 Measuring Transport Properties of Thin Films Under Isotropic and Anisotropic Strain Using Piezoelectric Substrates , S. WOLGAST, C. KURDAK, Department of Physics, University of Michigan, Ann Arbor, Michigan 48109, A. GAITAS, W. ZHU, PicoCal, Inc., 333 Parkland Plaza, Ann Arbor, Michigan 48103 — Thin film systems have been of great technological interest in the last few decades due to their unique properties. It is crucially important to understand transport properties of such films under strain for some applications such as in strain gauges. Piezoelectric materials have been used in the past to study the isotropic strain-dependent properties of magnetotransport devices. We have extended this technique using one of the shearing modes of a Lead Magnesium Niobate-Lead Titanate (PMN-PT) crystal poled in the <011> direction to study anisotropic strain in thin films. A double Hall Bar pattern oriented along the eigenaxes of the piezoelectric shearing mode permits the characterization of the film in both directions simultaneously. A uniform field in the piezoelectric substrate may be achieved for patterned devices by growing a metal surface surrounding the entire pattern. We will discuss how the changes in the carrier density and electron mobility associated with strain can be characterized in thin metal films deposited directly on the PMN-PT substrate.

9:36AM Y10.00009 Symmetry-induced confinement in reconstructed Au(100) , S. BENGIO, Universidad Autónoma de Madrid, Madrid, Spain, V. NAVARRO, M.A. GONZALEZ-BARRIO, R. CORTES, Universidad Complutense, Madrid, Spain, I. VOBORNIK, TASC National Laboratory, Trieste, Italy, E.G. MICHEL, Universidad Autónoma de Madrid, Madrid, Spain, A. MASCARAQUE, Universidad Complutense, Madrid, Spain — The clean reconstructed Au(100) surface was investigated by angle-resolved photoemission spectroscopy, Low Energy Electron Diffraction and Scanning Tunneling Microscopy. The reconstruction can be described as a floating, corrugated hexagonal layer on top of the bulk-terminated substrate, as in the case of Ir(100) and Pt(100) surfaces. We determine a superperiodicity of (5x26). The substrate Shockley surface state survives the reconstruction and becomes an interfacial surface state. Compelling evidence supports that the overlayer behaves as a quasi-1D system. The presence of quasi-1D states and Shockley surface states are both a consequence of a certain degree of vertical electronic confinement induced by the different symmetry of the hexagonal overlayer and the square bulk-terminated Au(100). The existence of quasi-1D states reveals a significant lateral confinement perpendicular to the atomic chains of the reconstructed Au layer.

9:48AM Y10.00010 Surface states localization induced by single adatoms at metal surfaces , SIMONA ACHILLI, Dept. Material Science, University of Milan Bicocca, MARIO ITALO TRIONI, CNR – National Research Council of Italy, ISTM — The perturbation introduced at metal surfaces by the adsorption of a single adatom affects the surface states. Due to their two dimensional character, localized bound states could result at energy lower then the pristine surface states. The extent of such a localization depends on a variety of aspects such as the attractive strength of the adatom induced potential, the adsorption distance, the nature of the surface state. We investigate this effect through a density functional theory approach that accounts for the semi-infinite character of the substrate and which reproduces the experimental surface states and the surface projected energy gap. The results obtained for different kind of adatoms (both magnetic and paramagnetic) on metal surfaces are discussed, focusing on the localization of the Shockley state and of the image states for different adsorption configurations. The spin splitting of the localized bound state will be also analyzed for magnetic adatoms.

10:00AM Y10.00011 Structure, Morphology and SRF Characteristics of Superconducting Niobium Thin Films on Ceramic Substrates , DOUGLAS BERINGER, Department of Physics, The College of William and Mary, WILLIAM ROACH, CESAR CLAVERO, Department of Applied Science, The College of William and Mary, ROSA ALEJANDRA LUKASZEW, Professor of Physics and Applied Science, The College of William and Mary, CHARLES REECE, Director of Institute for SRF Science and Technology, Jefferson Lab, INSTITUTE FOR SRF SCIENCE AND TECHNOLOGY, JEFFERSON LAB COLLABORATION — The need to improve superconducting thin film coatings for radio frequency (SRF) cavities used in linear accelerators has inspired recent niobium thin film research. To better understand the SRF properties in thin film niobium, correlated studies of structure, surface morphology and SRF performance are examined. Recent work on epitaxial growth of niobium on insulating ceramic substrates — a-plane sapphire and MgO (001) — anticipates Superconducting / Insulating / Superconducting (SIS) multilayer structures, which have been proposed as a means to achieve higher field gradients in SRF cavities, overcoming the intrinsic SRF limitations of bulk niobium. A fundamental study correlating structure, morphology and SRF superconducting properties of niobium thin films is an imperative first step towards realizing next generation SRF materials.

10:12AM Y10.00012 The Electronic Structure and Properties of Different Surface Terminations of Li2B4O6 Single Crystal , IHOR KETSMAN, University of Nebraska -Lincoln, YAROSLAV LOSOVYJ, Louisiana State University, VOLODYMYR ADAMIV, YAROSLAV BURAK, Institute of Physical Optics, Lviv, Ukraine, DAVID WOOTEN, JAMES PETROSKY, JOHN MCCLORY, Air Force Institute of Technology, Wright Patterson Air Force Base, OH, USA, PETER DOWBEN, University of Nebraska -Lincoln — The electronic structure of the(100) and (110) surfaces of Li2B4O6 single crystal was investigated by combined angle- resolved photoemission and inverse photoemission spectroscopies. The obtained results are in a qualitative agreement with the available model bulk band structure calculations.Together with some common features, they reveal clear differences between the two surfaces. For both of them the observed dispersion of the conduction band is much greater than that of valence band and both surfaces are of n-type, though the feature is more pronounced for (100) surface, which, on the whole, is more polar. However, the (110) surface demonstrates much more sofisticated properties exhibiting, in particular, the true surface states and complicated temperature and time dependent photovoltaic charging behaviour. For this surface, in the temperature range of(80-280)K, the off-axis pyroelectric effect was observed with strongly temperature dependent currents in the <110> direction and much smaller pyroelectric coefficient than that measured in the <001> direction.

10:24AM Y10.00013 Correlated electron effects in low energy alkaline earth ion scattering , XIAOXIAO HE, JORY YARMOFF, Department of Physics & Astronomy, University of California, Riverside — The spin correlations of many electrons can lead to emergent phenomena that cannot be extrapolated from the behavior of independent electrons. The role of such multi-electron processes in charge exchange during atom-surface collisions remains a challenging and unsolved problem. Two prior independent theoretical investigations predicted that when a projectile has a single unpaired electron or hole, this localized spin impurity would induce a Kondo resonance at the Fermi energy leading to a mixed-valent state in the metal conduction band. The occupancy of this sharp state would be a strong function of the surface temperature, which would cause an anomalous temperature dependence of the neutralization probability in a scattering experiment. We demonstrate such dependence for low energy Sr^+ scattered from clean polycrystalline gold. This unusual temperature dependence is amplified when the metal work function is reduced by embedding Sr atoms into the material.

10:36AM Y10.00014 ABSTRACT WITHDRAWN –

10:48AM Y10.00015 ABSTRACT WITHDRAWN –

Friday, March 25, 2011 8:00AM - 11:00AM –

Session Y13 GSNP DFD: Granular Materials I D225/226

8:00AM Y13.00001 ABSTRACT WITHDRAWN –

8:12AM Y13.00002 Homogeneous linear shear of a two dimensional granular system , JOSHUA A. DIJKSMAN, JIE REN, ROBERT P. BEHRINGER, Duke University — Using a novel shear device, we experimentally study the response of dry granular materials to quasi-static shear. Our apparatus is capable of creating linear strain profiles over the entire width of the two dimensional shear cell. By eliminating the usual tendency of granular shear to localize in non-uniform shear bands, we can study the poorly understood nature of granular flows in great detail. We employ photo elastic particles, fluorescent labelling and high resolution imaging to obtain information about particle positions, rotation and inter particle forces. We discuss our results in the context of the jamming scenario and also look at various measures capable of elucidating the physics of dense granular flows.

8:24AM Y13.00003 Constitutive relations for granular fluid of smooth inelastic hard spheres, to Burnett order , VINAY GUPTA, MEHEBOOB ALAM, JNCASR, Bangalore, India — In the framework of kinetic theory for dilute granular gases, we have generalized the work of Sela & Goldhirsch (1998) by including body force (gravity) term in the Boltzmann equation. In order to derive the constitutive relations for flows of smooth inelastic hard spheres in three dimensions, the Boltzmann equation is perturbatively solved by performing generalized Chapman-Enskog (double expansion) in two small parameters, the Knudsen number and the degree of inelasticity. We have derived the constitutive relations till Burnett order (up to second order in small parameters). In this talk I would like to present the methodology for obtaining the constitutive relations.

Ref: Sela, N. & Goldhirsch, I. 1998 Hydrodynamic equations for rapid flows of smooth inelastic spheres, to Burnett order. *J. Fluid Mech.* **361**, 41–74.

8:36AM Y13.00004 Random to ordered granular sphere packings through cyclic shear , ANDREEA PANAITESCU, ANKI REDDY, ARSHAD KUDROLLI, Clark University — We investigate the structure of a dense granular packing submitted to quasi-static cyclic shear deformations using a fluorescent liquid refractive index matching method. This technique allows us to obtain the three dimensional position of 1mm glass spheres in the bulk during each cycle. The granular packing is observed to evolve towards crystallization over hundreds of thousands of shear cycles and the packing fraction is correspondingly observed to increase from loose packing fraction, 0.59, to above random close packing, 0.634. The appearance and the propagation of the crystalline order was studied using the orientational order metric, Q_6. In the early stages of nucleation the particles belonging to the nucleating crystallites are predominantly in hexagonal close packed configuration. When the packing volume fraction approaches a value close to random close packing, a rapid increase of the global Q_6 and the number of particles with local face centered cubic order is observed. Following the evolution of the crystallites, we find the critical nuclei size to be between 10-50 particles, surprisingly consistent with transitions observed with thermal elastic frictionless spheres. A detailed description of the crystalline clusters and their development will be presented.

8:48AM Y13.00005 Shearbanding Instability and Patterns in Granular Shear Flows , PRIYANKA SHUKLA, MEHEBOOB ALAM, J.N.Centre for Advanced Scientific Research, Bangalore — When a (dense) granular material is sheared in shear-cell experiments, shearing remains confined to a narrow localized zone ("shearband") near the moving boundary. Such shear-banding has also been realized in the molecular dynamics simulations of granular plane Couette flow for a range of densities (even without gravity) in the rapid flow regime. In this talk I will present the shear-banding instability of granular shear flow via an order parameter equation.

[1] Weakly nonlinear theory of shear-banding instability in granular plane Couette flow: analytical solution, comparison with numerics and bifurcation, Priyanka Shukla and Meheboob Alam, Journal of Fluid Mechanics 2010, **665**, p. 1-50.
[2] Landau-type order parameter equation for shear banding in granular Couette flow, Priyanka Shukla and Meheboob Alam, Physical Review Letters, **103**, 068001, 2009.
[3] Universality of shear-banding instability and crystallization in sheared granular fluid, Meheboob Alam, Priyanka Shukla and Stefan Luding, Journal of Fluid Mechanics, **615**, p. 293-321, 2008.

9:00AM Y13.00006 Shearing granular media: from elasticity to compaction , JEAN-FRANCOIS METAYER, MPI for Dynamics and Self-Organization, Bunsenstr. 10, 37073 Göttingen, ELIE WANDERSMAN, MARTIN VAN HECKE, University of Leiden, MATTHIAS SCHRÖTER, MPI for Dynamics and Self-Organization, Bunsenstr. 10, 37073 Göttingen — A granular system is able to behave like a solid (a sand pile for example) or like a liquid depending on the deformation imposed on the material. Using rheometry measurements we investigate the response of a granular bed to an imposed deformation or an imposed stress as a function of its packing fraction. We observed different regimes: elastic and plastic behaviors, flow regime and finally compaction. The dependence of these regimes on the packing fraction and on the pressure allows us to delineate the phase diagram of granular media.

9:12AM Y13.00007 Microscopic rearrangements and macroscopic stress fluctuations in dense emulsion flow , DANDAN CHEN, KENNETH W. DESMOND, ERIC R. WEEKS, Emory University — One characteristic of dense granular materials is they can resist small stresses but start to flow under large stresses. During granular flow, the stress exerted on the boundaries of the flow can have large fluctuations. These fluctuations are thought to originate from internal rearrangements and from changes of force chains; however, the connection between these internal microscopic changes and the macroscopic influences seen at the boundaries is not yet clear. We experimentally study the shear flow of oil-in-water emulsion droplets in a Hele-Shaw cell with a hopper shape. Due to the thinness of the Hele-Shaw cell, the droplets are deformed into quasi-2D pancakes, somewhat analogous to soft photoelastic disks. As droplets approach the hopper exit, they shear past one another and droplets are forced to rearrange. We focus on a typical plastic rearrangement called T1 event, where local four particles have neighbor exchanges. Simultaneously, we use the deformation of the droplets to determine the interdroplet forces, which also change as the sample is sheared. These forces fluctuate over large regions as expected. Our analysis of this emulsion system shows a direct and local relationship between microscopic T1 rearrangements and macroscopic stress ?uctuations.

9:24AM Y13.00008 Flow and Sedimentation of particulate suspensions in Fractures[1] , TAK SHING LO, JOEL KOPLIK, Levich Institute and Department of Physics, City College of CUNY — Suspended particles are commonly found in reservoir fluids. They alter the rheology of the flowing liquids and may obstruct transport by narrowing flow channels due to gravitational sedimentation. An understanding of the dynamics of particle transport and deposition is, therefore, important to many geological, enviromental and industrial processes. Realistic geological fractures usually have irregular surfaces with self-affine structures, and the surface roughness plays a crucial role in the flow and sedimentation processes. Recently, we have used the lattice Boltzmann method to study the combined effects of sedimentation and transport of particles suspended in a Newtonian fluid in a pressure-driven flow in self-affine channels, which is especially relevant to clogging phenomena where sediments may block fluid flows in narrow constrictions of the channels. The lattice Boltzmann method is flexible and particularly suitable for handling irregular geometry. Our work covers a broad range in Reynolds and buoyancy numbers, and in particle concentrations. In this talk, we focus on the transitions between the "jammed" and the "flow" states in fractures, and on the effects of nonuniform particle size distributions.

[1]Work supported by DOE and NERSC.

9:36AM Y13.00009 Dilation of Granular Packings of Spheres and Non-Spherical Particles under Shear , ABIGAIL POLIN, BEZ LADERMAN, CHRISTOPHER PEEL, JOHN R. ROYER, PAUL M. CHAIKIN, New York University — A parallelepiped shear cell is used to experimentally measure the dilation of particles prepared at different initial volume fractions from relatively loose assemblies to densely packed ones. The samples consist of spherical marbles, plastic ellipsoids and tetrahedral dice at the centimeter scale and specially prepared particles at the millimeter scale. Under quasi-static shear, loosely packed samples compact while densely packed particles dilate, as in previous studies. For small shear amplitudes, both the dilation and compaction of the tetrahedral packings is significantly larger than that of spheres.

9:48AM Y13.00010 Dynamic crystallization in granular flow[1] , ALINE HUBARD, MARK D. SHATTUCK, The City College of New York — We explore dynamic crystallization in simulations of two dimensional (2D) inelastic frictional hard disks as a model for granular materials. Previous simulations and experiments show formation of hexagonal structures in quasi-2D systems under vibration, rotation, and shearing. In experiments of a uniform but non-equilibrium steady-state (UNESS) under constant pressure the gas-crystal transition shows all of the classic signs of a first-order sublimation phase transition including discontinuous change in density, rate dependent hysteresis, and an equation of state consistent with sublimation. We use molecular dynamics to simulate steady shear under a variety of boundary conditions to determine a dynamic equation of state in the in the density range of the crystallization transition. We compare the dynamic equation of state with that found in non-flowing UNESS experiments, simulations, and theory.

[1]Funding: National Science Foundation DMR-0934206, CBET-0968013.

10:00AM Y13.00011 The path to fracture: dynamics of broken-link networks in granular flows , MARK HERRERA, University of Maryland, SHANE MCCARTHY, STEVEN SLOTTERBACK, MICHELLE GIRVAN, WOLFGANG LOSERT, University of Maryland — Capturing the dynamics of granular flows on intermediate length scale can often be difficult. We propose the broken-links network as a new tool to study fracture at the intermediate scale. Using experimental data on the 3D tracks of all particles in a region, we calculate the dynamically evolving broken-links network and observe a second-order, percolation-like phase transition in the formation of the giant component as links are broken. We implement a velocity gradient model of link breakages and find that the model demonstrates a faster growth of the giant component than the data. Surprisingly, the broken-links network formed in the model is also more highly clustered than our empirical observations.

10:12AM Y13.00012 Hockey night in phase space , KIRI NICHOL, Leiden University, KAREN DANIELS, North Carolina State University — In order to explore the possibility of developing a statistical mechanics for dissipative ensembles, we have performed an experiment in which we track the translational and rotational velocities of pucks on an air hockey table. The pucks are driven by bumpers at the boundaries and are bidisperse to prevent crystallization. At packing fractions of 60% we find that the system distributes rotational and translation energy according to the equipartition theorem. However, as the packing fraction increases, the ratio of rotational energy to translational energy also increases to a value larger than predicted by equipartition. The translational and angular velocity distributions are approximately exponential and the distributions of the translational velocity are the same for both large and small particles. In contrast, the distribution of the angular velocities is broader for the small particles than for the large.

10:24AM Y13.00013 Rotational statistics in dense granular flows of smooth cylindrical particles , JEFFREY OLAFSEN, JACOB JANTZI, Department of Physics, Baylor University — We report the results of an experiment to investigate the dissipation in the rotational degree of freedom for smooth cylindrical particles in a dense, driven granular flow. The flow is studied in a rotating drum of radius R = 30 cm for particles of radius r = 0.635 cm while the cell is rotated at speeds between 0.25 and 0.75 Hz. The 2D geometry of the experimental design allows for the measurement of two translational degrees of freedom as well as the rotation of the disks within the driven flow. The rotational velocity statistics demonstrate non-Gaussian behavior as well as a significant amount of energy being dissipated within the flow via the tangential friction between the particles. The results of this experiment are significant in that many driven granular experiments use smooth cylindrical or spherical particles to investigate granular dynamics, but the contribution from the rotational degrees of freedom are often unmeasured. A novel imaging technique is used to extract both the translational and rotational velocity statistics to a high degree of precision in the entire cell during the experiment.

10:36AM Y13.00014 ABSTRACT WITHDRAWN –

10:48AM Y13.00015 Size Segregation of Granular Materials , ANURAG TRIPATHI, D.V. KHAKHAR, Indian Institute of Technology Bombay — Segregation of granular materials due to size difference while flowing/energized is a very well known but poorly understood phenomena. Despite of some good understanding of the mechanism of size segregation, predictive models for size segregation are not available. Size segregation of binary granular mixtures flowing over inclined plane is studied by means of DEM simulations. Buoyant force acting on trace particles of a bigger size is obtained by varying the density of the trace particles rising/sinking in the granular flow. We show that moderately big trace particles of same density as that of the light particles tend to rise because of higher buoyancy forces than the weight of the trace particles. For very big trace particles of same density, however, the buoyant force becomes smaller than the weight of the particles causing the particles to settle down. Drag force on the trace particle is found to be given by Stokes' law. Friction drag is found to almost $10 - 12\%$ of the weight of the trace particles. Incorporating the Stokes' law and balancing the segregation and diffusion flux of big particles, we are able to predict the number fraction of the big particles in terms of viscosity and diffusivity for moderately dilute binary mixture of different size particles. The proposed theory is tested against DEM simulation results and very good agreement has been found with the simulation results.

Friday, March 25, 2011 8:00AM - 11:00AM –

Session Y14 GSNP: Focus Session: Statistical Mechanics of Complex Networks II D227

8:00AM Y14.00001 Universal features of dynamic small-world networks , THOMAS STONE, Husson University, SUSAN MCKAY, University of Maine — In a dynamic small-world contact network, an individual has fixed short range links within its local neighborhood and time-varying stochastic long range links outside of that neighborhood. The probability of a long range link occurring (p, in analogy with the standard small-world rewiring parameter) is a measure of the mobility of the population. In this study we investigate the epidemic to non-epidemic phase transition that occurs in a susceptible-infected-recovered (SIR) disease spreading model located on this type of dynamic network. We first derive the finite-valued critical mobility p_c and find excellent agreement with numerical simulations. Close to p_c the outbreak size scales as $(p\text{-}p_c)^\beta$ since it is a continuous transition; we find that β is near 2, but varies as a function of the infectivity and recovery rates. At the critical point our study shows that the distribution of outbreak sizes scales as $\sim N^{-\alpha}$ with $\alpha = 1.5 \pm 0.03$. We compare these critical exponents to those found in related small-world and dynamic small-world networks and comment on potential universality.

8:12AM Y14.00002 Robustness and dynamics of networks of coupled modules , JAMES BAGROW, YONG-YEOL AHN, Northeastern University, SUNE LEHMANN, Technical University of Denmark — Many systems, from power grids and the internet, to the brain and society, can be modeled using networks of coupled overlapping modules. The elements of these networks perform individual and collective tasks such as generating and consuming electrical load or transmitting data. We study the robustness of these systems using percolation theory: a random fraction of the elements fail which may cause the network to lose global connectivity. We show that the modules themselves can become isolated or uncoupled (non-overlapping) well before the network falls apart. This has important structural and dynamical consequences for these networks and may explain how missing information hides pervasive overlap between communities in real networks.

8:24AM Y14.00003 Explosive Percolation in the Human Protein Homology Network , HERNAN ROZENFELD, APS, LAZAROS GALLOS, HERNAN MAKSE, CCNY — We study the explosive character of the percolation transition in a real-world network. We show that the emergence of a spanning cluster in the Human Protein Homology Network (H-PHN) exhibits similar features to an Achlioptas-type process and is markedly different from regular random percolation. The underlying mechanism of this transition can be described by slow-growing clusters that remain isolated until the later stages of the process, when the addition of a small number of links leads to the rapid interconnection of these modules into a giant cluster. Our results indicate that the evolutionary-based process that shapes the topology of the H-PHN through duplication-divergence events may occur in sudden steps.

8:36AM Y14.00004 ABSTRACT WITHDRAWN –

9:12AM Y14.00005 Power Spectrum of the Finite Kuramoto Model , DAVID MERTENS, RICHARD WEAVER, University of Illinois at Urbana-Champaign — We study the synchronization of oscillators in the finite Kuramoto model, a simple model for coupled phase oscillators that exhibits a phase transition. The usual self-consistent approach used in studying the Kuramoto model gives a prediction for the distribution of modified frequencies that includes a Dirac delta at the synchronized frequency and a depletion of nearby frequencies. For finite systems, the prediction adequately describes the distribution of frequencies averaged over very long durations, but the accompanying power spectrum of the order parameter looks very different. The sharp peak at the synchronization frequency has a finite width and oscillators that are otherwise entrained manage to occasionally escape. The resulting harmonics of these escaped oscillators leads to a power spectrum with an exponential drop-off from the peak, rather than the originally predicted depletion.

9:24AM Y14.00006 Recruitment dynamics in adaptive social networks , MAXIM SHKARAYEV, LEAH SHAW, College of William and Mary, IRA SCHWARTZ, Naval Research Lab — We model recruitment in social networks in the presence of birth and death processes. The recruitment is characterized by nodes changing their status to that of the recruiting class as a result of contact with recruiting nodes. The recruiting nodes may adapt their connections in order to improve recruitment capabilities, thus changing the network structure. We develop a mean-field theory describing the system dynamics. Using mean-field theory we characterize the dependence of the growth threshold of the recruiting class on the adaptation parameter. Furthermore, we investigate the effect of adaptation on the recruitment dynamics, as well as on network topology. The theoretical predictions are confirmed by the direct simulations of the full system.

9:36AM Y14.00007 The spread of opinion on co-evolving networks[1] , PRAMESH SINGH, S. SREENIVASAN, G. KORNISS, B. K. SZYMANSKI, RPI — We discuss a model of opinion formation in co-evolving networks. In realistic scenarios, the network constantly changes structure favoring connections between similar individuals (homophily). Here we allow the opinions to co-evolve with the reorganization of links in the network. This dynamical nature of the network impedes the spreading of opinions. We study how this resistance to the spread can be overcome and consensus can be achieved by randomly distributing a few committed agents (-nodes that are not influenceable in their opinions). In this model adjacent nodes influence each other if they are similar on at least Q attributes, where Q is the influence threshold. Nodes will rewire their existing links if they are not similar enough. We demonstrate through simulations that in the absence of committed agents, time to reach consensus in opinions diverges exponentially with system size N. However, as committed agents are added, beyond a small value of committed fraction, the consensus time becomes a slowly varying function of N. (Ref- F. Vazquez et al. - Phys. Rev. E76, 046120 -2007)

[1]supported in part by ARL and ONR

9:48AM Y14.00008 Network resilience to real-world disasters: Eyjafjallajökull and 9/11 , OLIVIA WOOLLEY, Northwestern University, CHRISTIAN THIEMANN, DANIEL GRADY, DIRK BROCKMANN, Northwestern University — We investigate the resilience of the the world-wide air transportation network (WAN) to the 9/11 terrorist attacks and the recent eruption of the volcano Eyjafjallajökull. Although both disasters caused wide-spread disruption, the number of airports that were closed and the volume of interrupted traffic were well below the percolation threshold predicted by the classical theory. In order to quantify and visualize network deformation before breakdown, we introduce a framework based on the increase in shortest-path distance and homogenization of shortest-path structure. These real-world disasters are a new type of disruption because the removal of all vertices (airports) is geographically compact. Our framework incorporates the dual perspective of individual airports and geopolitical regions to capture how the impact interacts with the sub-network structure.We find that real-world events have an impact signature which is qualitatively different from that of random or high-centrality attacks. Furthermore, we find that the network is more resilient to the 9/11 disaster, although it removed more airports and traffic than the volcanic ash-cloud. This is due to the network roles of Europe and North America. We discuss how regional roles influence resilience to a region's removal.

10:00AM Y14.00009 Stochastic Moment Equations - Case Closed , BARUCH BARZEL, Northeastern university, OFER BIHAM, The Hebrew University — Reaction networks frequently appear in many natural systems, such as chemistry, biology and ecology. The modelling of these networks is commonly based on rate equations models, incorporating the law of mass action kinetics. However, when the system is microscopic, it becomes governed by fluctuations, the law of mass action kinetics no longer applies, and the rate equations fail. To obtain an accurate description of microscopic reaction networks, one must refer to stochastic methods based on the master equation. The problem is that the number of equations rises exponentially with the number of species, rendering the treatment of the master equation infeasible. Moment equations are known to be more efficient, however the equations are not closed, and become prohibitively complicated when moments of high order are included. In this talk we present the binomial moment equations. The binomial moments are linear combinations of the ordinary moments related to the population size of the reactive species. They capture the essential combinatorics of the reaction processes reflecting their stoichiometric structure. This leads to a simple and transparent form of the equations, allows a highly efficient and surprisingly simple truncation scheme and enables the inclusion of moments up to any desired order. The result is a set of equations that enables an equation-based stochastic analysis of reaction networks under a very broad range of conditions.

10:12AM Y14.00010 Using a Projector to Control BZ Drops: Attractor Selection by Pattern Entrainment , NATHAN TOMPKINS, HECTOR GONZALEZ OCHOA, IRVING EPSTEIN, SETH FRADEN, Brandeis University — An emulsion consisting of drops in the 100μm diameter range containing the Belousov-Zhabotinsky (BZ) oscillatory chemicals can interact via diffusive inhibition and can be thought of as coupled phase oscillators. For weak coupling, a 2-D hexagonal lattice of these drops naturally develop regions of attractor states of sequential oscillations with phase differences of plus/minus $2\pi/3$ much like the 2D anti-ferromagnetic Heisenberg spin model. An untrained system of these oscillators will develop unstable regions of both attractors that grow and compete. We use photo-initiated inhibition to optically entrain the system with a projected $+2\pi/3$ pattern in an attempt to force the system into the $+2\pi/3$ attractor state. However, both the left and right handed variants of the $2\pi/3$ attractor are present in the entrained system. Defining an order parameter $e^{i3\phi}$ allows for a quantitation of the purity of the $2\pi/3$ attractor state in the final system.

10:24AM Y14.00011 Complexity facilitates perturbation of a coherent dynamical process , MALGORZATA TURALSKA, University of North Texas, ELVIS GENESTON, La Sierra University, PAOLO GRIGOLINI, University of North Texas — We discuss the influence of perturbation on networks of globally coupled three state stochastic oscillators. When coupled, the system shows intermittent behavior characterized by a waiting time distribution which reveals both inverse power-law and coherent dynamical properties. Specifically, we compare the results of perturbation realized with a periodic signal to those obtained using perturbation provided by a matching system. We find that the SNR (signal-to-noise ratio) does not depend on the frequency of the perturbing signal. We also observe that the second approach results in higher values of SNR. We discuss how those findings cannot be explained by either classical or statistical resonance theory. With the help of the fluctuation-dissipation theorem [1] we determine the role of the scaling dynamics in the system under investigation.

[1] Aquino G., Bologna M., Grigolioni P., West B.J., PRL 105, 040601 (2010)

10:36AM Y14.00012 Coupled Oscillations in a 1D Emulsion of Belousov-Zhabotinsky Droplets[1] , SETH FRADEN, JORGE DELGADO, NING LI, MARCIN LEDA, HECTOR GONZALEZ-OCHOA, IRVING EPSTEIN, Brandeis University — We experimentally and computationally study the dynamics of interacting oscillating Belousov-Zhabotinsky (BZ) droplets of $\sim$120 μm diameter separated by perfluorinated oil and arranged in a one-dimensional array (1D). The coupling between BZ droplets is dominated by inhibition and is strongest at low concentrations of malonic acid (MA) and small droplet separations. A microfluidic chip is used for mixing the BZ reactants, forming monodisperse droplets by flow-focusing and directing them into a hydrophobized 100 μm diameter capillary. For samples composed of many drops and in the absence of well defined initial conditions, the anti-phase attractor, in which adjacent droplets oscillate 180° out of phase, is observed for strong coupling. When the coupling strength is reduced the initial transients in the phase difference between neighboring droplets persist until the BZ reactants are exhausted. In order to make quantitative comparison with theory, we use photosensitive Ru(bipy)$_3^{2+}$-catalyzed BZ droplets and set both boundary and initial conditions of arrays of small numbers of oscillating BZ droplets with a programmable illumination source. In these small collections of droplets, transient patterns decay rapidly and we observe several more complex attractors, including ones in which some adjacent droplets are in-phase.

[1]This work was supported by the National Science Foundation (CHE-0615507 and MRSEC DMR-0820492).

10:48AM Y14.00013 Quarantine generated phase transition in epidemic spreading , MARK DICKSION, Boston University, CECILIA LAGORIO, F. VAZQUEZ, L. BRAUNSTEIN, P.A. MACRI, M.V. MIGUELES, S. HAVLIN, H.E. STANLEY — We study the critical effect of quarantine on the propagation of epidemics on an adaptive network of social contacts. For this purpose, we analyze the susceptible-infected-recovered (SIR) model in the presence of quarantine, where susceptible individuals protect themselves by disconnecting their links to infected neighbors with probability w, and reconnecting them to other susceptible individuals chosen at random. Starting from a single infected individual, we show by an analytical approach and simulations that there is a phase transition at a critical rewiring (quarantine) threshold w_c separating a phase ($w < w_c$) where the disease reaches a large fraction of the population, from a phase ($w >= w_c$) where the disease does not spread out. We find that in our model the topology of the network strongly affects the size of the propagation, and that w_c increases with the mean degree and heterogeneity of the network. We also find that w_c is reduced if we perform a preferential rewiring, in which the rewiring probability is proportional to the degree of infected nodes.

Friday, March 25, 2011 8:00AM - 11:00AM –

Session Y15 GMAG DMP FIAP: Focus Session: Spins in Semiconductors - Spin Currents IV

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8:00AM Y15.00001 Electrically-generated electron spin polarization for non-reciprocal integrated photonic devices , CHRISTOPHER TROWBRIDGE, BENJAMIN NORMAN, VANESSA SIH, University of Michigan — Electron spin polarization based photonic devices offer promising advantages over current technologies. Spin orbit coupling allows for an all-electrical means of control over light in semiconductor waveguides. Electrically generated spin polarization results in a circular dichroism near the absorption edge which results in non-reciprocal Faraday rotation. We investigate the requirements for manipulating light in semiconductor waveguides using electrically-generated spin polarization. Ultimately, device performance will be limited by the magnitude of achievable Faraday rotation, birefringence, and absorption. We show that one can limit birefringence by appropriate waveguide design and that substantial Faraday rotation is accessible sufficiently far below the band edge for material absorption to be minimal.

8:12AM Y15.00002 Spin Control of Drifting Electrons using Local Nuclear Polarization in Ferromagnet-Semiconductor Heterostructures[1]

, M.E. NOWAKOWSKI, G.D. FUCHS, S. MACK, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106, N. SAMARTH, Department of Physics and Materials Research Institute, The Pennsylvania State University, University Park, PA 16802 — We demonstrate a spatially-confined magnetic field gate to modulate the Larmor frequency of an optically-injected spin ensemble drifting down a GaAs channel [1]. The gate is activated either optically or electrically and polarizes GaAs nuclear spins at the interface between a lithographically-defined MnAs island and the channel via the ferromagnetic proximity polarization effect. We measure the rotation angle of the spin ensemble as it emerges from the polarized region using time-resolved Kerr rotation. The ensemble's spin rotation angle can be tuned by up to 5π radians as the spins travel over 30 μm by controlling the nuclear field strength and adjusting the drift velocity.

[1] M.E. Nowakowski, et. al., Phys. Rev. Lett. 105, 137206 (2010)

[1]Work supported by ONR and NSF.

8:24AM Y15.00003 Large and Small Signal Analyses of Spin Modulation in Lasers

, CHRISTIAN GOTHGEN, JEONGSU LEE, RAFAL OSZWALDOWSKI, IGOR ZUTIC, SUNY at Buffalo — We have developed a set of rate equations for semiconductor spin-lasers that contain spin-polarized carriers (electrons and holes) in the active region due to spin-polarized (electrical or optical) injection. Previous studies consider the steady-state regime [1-5], showing advantages of the spin-lasers over its conventional counterparts such as threshold reduction and enhanced emission intensity [6]. We suggest a further improvement of spin lasers under dynamical operation. We use both large and small signal analyses to show that the spin-polarized injection can lead to an enhanced bandwidth and desirable switching properties of spin-lasers. Supported by ONR, AFOSR, NSF-ECCS CAREER.

[1] J. Rudolph et al., Appl. Phys. Lett. 82, 4516 (2003).
[2] M. Holub et al., Phys. Rev. Lett. 98, 146603 (2007).
[3] S. Hovel et al., Appl. Phys. Lett. 92, 041118 (2008).
[4] C. Gothgen, R. Oszwaldowski, A. Petrou, I. Zutic, Appl. Phys. Lett. 93, 042513 (2008).
[5] I. Vurgaftman et al., Appl. Phys. Lett. 93, 031102 (2008).
[6] J. Lee, W. Falls, R. Oszwaldowski, and I. Zutic, Appl. Phys. Lett. 97, 041116 (2010).

8:36AM Y15.00004 Mapping between Quantum-Dot and Quantum-Well Spin-Lasers

, JEONGSU LEE, RAFAL OSZWALDOWSKI, CHRISTIAN GOTHGEN, IGOR ZUTIC, SUNY at Buffalo — It has been demonstrated that performance of semiconductor lasers with a quantum-well (QW) active region can be improved by injecting spin-polarized carriers [1-3]. Their rate-equation models have been developed [4-5], however, description of a quantum-dot (QD) spin-laser, demonstrated recently [6], is more complicated [7]. Here, we present a method which allows to employ the simple QW rate equations to study the QD spin-lasers. With this method, one can easily extract QW-like parameters such as differential gain, gain compression factor and time constants. This effort is worthwhile, because the QW spin-laser rate equations have exact analytical solutions, unlike their QD counterparts [7]. Supported by US ONR, AFOSR, DOE-BES, and NSF-ECCS CARRER. [1] J. Rudolph et al., Appl. Phys. Lett. 82, 4516 (2003). [2] M. Holub et al., Phys. Rev. Lett. 98, 146603 (2007). [3] S. Hovel et al., Appl. Phys. Lett. 92, 041118 (2008). [4] C. Gothgen, R. Oszwaldowski, A. Petrou, I. Zutic, Appl. Phys. Lett. 93, 042513 (2008). [5] I. Vurgaftman et al., Appl. Phys. Lett. 93, 031102 (2008). [6] D. Basu et al., Appl. Phys. Lett. 92, 09119 (2008). [7] R. Oszwaldowski, C. Gothgen, and I. Zutic, Phys. Rev. B 82, 085316 (2010).

8:48AM Y15.00005 High frequency dynamics and output polarization of a spin laser

, PALLAB BHATTACHARYA, University of Michigan, Ann Arbor, DIPANKAR SAHA, Indian Institute of Technology Bombay, DEBASHISH BASU, University of Michigan, Ann Arbor — The dynamic characteristics of a spin laser have been studied theoretically and experimentally. Calculations with the coupled carrier and photon rate equations show that the small signal modulation bandwidth of the preferred polarization mode is enhanced due to spin injection. The large signal modulation characteristics show temporally separated relaxation oscillations corresponding to the two polarization modes. More importantly, it is shown that an output polarization of 100% can be obtained, with appropriate biasing conditions, irrespective of the degree of spin injection. This is experimentally verified in a quantum dot spin-vertical cavity surface emitting laser (spin VCSEL), where an output polarization of $\sim$ 60% is measured with a 5-6% carrier spin polarization in the active region.

9:00AM Y15.00006 Consequences of spin transport in heterogeneous environments

, VIDYA BHALLAMUDI, Department of Electrical and Computer Engineering, The Ohio State University, ANDREW BERGER, Department of Physics, The Ohio State University, DOMINIC LABANOWSKI, Department of Electrical and Computer Engineering, The Ohio State University, DAVID STROUD, P. CHRIS HAMMEL, Department of Physics, The Ohio State University — Understanding behavior of spins in spatially varying environments such as magnetic fields, spin lifetime and gyromagnetic ratio is very important for real spintronic devices [1]. We present here numerical solutions of the spin diffusion equation in such situations. We show that local magnetic fields can be useful as an imaging tool for spin properties such as spin lifetime. It can also complicate the interpretation of experimental results in the case of spin injection from a ferromagnet into a semiconducting channel through a rough interface [1,2].

[1] S.P.Dash et.al, Electrical creation of spin polarization in silicon at room temperature, Nature 462, 491-494
[2] V.P. Bhallamudi et.al, Spin transport and imaging opportunities in inhomogeneous environments, arXiv:1010.3747v1 [cond-mat.mes-hall]

9:12AM Y15.00007 Robust Level Coincidences in the Subband Structure of Quasi 2D Systems[1]

, R. WINKLER, Northern Illinois University and Argonne National Lab , L.Y. WANG, Y.H. LIN, C.S. CHU, National Chiao Tung University, Hsinchu, Taiwan — Recently, level crossings in the energy bands of crystals have been identified as a key signature for topological phase transitions. In general, three independent parameters must be tuned appropriately to bring two quantum levels into degeneracy. Using realistic models we show that for Bloch electrons in a crystal the parameter space controlling the occurrence of level coincidences has a much richer structure than anticipated previously. In particular, we identify cases where level coincidences depend on only two independent parameters thus making the level coincidences robust, i.e., they cannot be removed by a small perturbation of the Hamiltonian compatible with the crystal symmetry. We consider HgTe/CdTe quantum wells as a specific example. (See arXiv:1011.xxxx)

[1]Work supported by Taiwan NSC (Contract No. 99-2112-M-009-006) and a MOE-ATU grant. Work at Argonne supported by DOE BES under Contract No. DE-AC02-06CH11357.

9:24AM Y15.00008 Anomalous spin-resolved point-contact transmission of holes due to cubic Rashba spin-orbit coupling

, STEFANO CHESI, University of Basel, GABRIELE GIULIANI, LEONID ROKHINSON, Purdue University, LOREN PFERIFFER, KEN WEST, Princeton University — We present experimental and theoretical evidence for the crossing at finite wave vector of the two lowest one-dimensional spin-split subbands in quantum point contacts fabricated from two-dimensional hole gases with strong spin-orbit interaction. We derive the existence of such crossing point from a two-dimensional spin-orbit interaction with a cubic momentum dependence, appropriate for asymmetric quantum wells. This phenomenon provides an explanation for the anomalous sign of the spin polarization filtered by the point contact, as observed in magnetic focusing experiments. Anticrossing in the one-dimensional spin subbands is introduced by a magnetic field parallel to the channel or an asymmetric potential transverse to it. Controlling the magnitude of the spin-splitting affords a novel mechanism for inverting the sign of the spin polarization.

9:36AM Y15.00009 Energy Spectra and Spin Properties of Electrons in Spin-Orbit Superlattice Quantum Wires[1] , VANITA SRINIVASA, JEREMY LEVY, University of Pittsburgh — We calculate the energy spectra of electrons in quantum wires with spatially uniform and modulated spin-orbit coupling. The effects of Rashba spin-orbit coupling arising from asymmetric confinement in perpendicular and lateral directions with respect to the plane containing the wire are considered. We investigate the resulting interplay of strong lateral confinement, a periodic one-dimensional superlattice potential, and spin-orbit coupling in two orthogonal directions. The implications for the spin-dependent properties of electrons confined within these quantum wires are discussed. A potential realization of such systems within narrow nanowires at the interface of $LaAlO_3/SrTiO_3$ heterostructures is also described.

[1]This work is supported by NDSEG, an Andrew Mellon Fellowship, NSF (DMR-0704022), and ARO MURI (W911NF-08-1-0317).

9:48AM Y15.00010 Unexpected Anisotropy of Electron g-factor in GaAs/AlGaAs(110) Quantum Well , YANG JI, SKLSM, Institute of Semiconductors, CAS — Semiconductor spin qubit is a promising candidate for solid state quantum computation. A lot of effort has been devoted to study spin dynamics in semiconductors ever since a revival of research interest in this field in the late 1990s. Spin lifetime longer than 1ns at room temperature has been discovered in GaAs/AlGaAs(110) quantum wells (QW) as a result of the absence of a predominant spin scattering mechansim (DP mechanism), which also leads to a strong anisotropy of electron spin decoherence in such QWs, with the spin lifetime of spins along the growth direction 10 times bigger than that of spins perpendicular to the growth direction. However, not much is known about the (an)isotropy of spin-related processes in the (110) QW plane, despite that it may offer useful information about spin relaxation. Utilizing a time-resolved Kerr rotation (TRKR) system with a rotatable in-plane magnetic field, we studied the spin processes in GaAs/AlGaAs (110) QWs and found an unexpected anisotropy of electron g-factor in such QWs. The g-factor as measured with the magnetic field along the [1-10] axis is some 10% larger than that along the [001] axis. Such a strong anisotropy is not only unexpected for QWs, but also much bigger than that found in InGaAs/GaAs quantum dots. An explanation for these results is still in demand but it may give some hints to improve our understanding of spin dephasing mechanisms in semiconductors.

10:00AM Y15.00011 High Resolution Magneto-Optic Measurements in GaAs using a Sagnac Interferometer , ALEXANDER FRIED, Stanford — The Sagnac Interferometer is a tool which measures the Polar Kerr effect–a direct indicator of magnetism. Using 820 nm light from a superluminescent diode, we probe GaAs structures and measure the Kerr angle with sub-microradian resolution. By utilizing diffraction limited optics and a piezoelectric scanner, we also achieve high spatial resolution. Our measurements are performed at cryogenic temperatures and offer a way to measure the Spin Hall Effect in the DC regime along with other forms of magnetic order.

10:12AM Y15.00012 Temperature-dependent spin- and phase coherence measured via h/e and h/2e quantum oscillations in resistance of mesoscopic ring arrays in an InAs 2DES , R.B. LILLIANFELD, R.L. KALLAHER, J.J. HEREMANS, Virginia Tech, W. VAN ROY, G. BORGHS, IMEC- Belgium — We investigate electron spin- and phase coherence in an array of quasi-ballistic InAs quantum well mesoscopic rings through observation of Aharonov-Bohm h/e oscillations (AB) and Altshuler-Aronov-Spivak h/2e oscillations (AAS). The temperature dependence of the AAS oscillations is characterized through a single effective coherence length, $L_{\rm eff}$, following the formalism of Douçot and Rammal, from which the phase coherence length, L_ϕ and the spin coherence length as limited by spin-orbit interaction, $L_{\rm SO}$, are extracted. AB oscillations are also present, and can be separated from AAS by Fourier transformation. We contrast the AAS method of extracting the coherence lengths with analysis of the AB oscillation amplitudes. Previous studies have examined L_ϕ from AB signals in single ballistic rings, or by using AAS amplitudes in large networks, or have observed AB and AAS in single rings with spin-orbit interaction. Here the presence of both AB and AAS in an array with spin-orbit interaction allows for study of both L_ϕ and $L_{\rm SO}$, and enables direct juxtaposition of different quantum coherence phenomena as means for measuring coherence lengths (DOE DE-FG02-08ER46532).

10:24AM Y15.00013 Weak Antilocalization and Spin-Orbit Coupling in InAlN/AlN/GaN Heterostructures , H. CHENG, C. KURDAK, Department of Physics, University of Michigan, Ann Arbor, MI, 48109, J.H. LEACH, M. WU, H. MORKOC, Department of Electrical and Computer Engineering, Virginia Commonwealth University, Richmond VA, 23284 — Spin-orbit coupling is investigated by magnetotransport and weak antilocalization (WAL) measurements in $In_xAl_{1-x}N$/AlN/GaN heterostructures in the carrier density ranges extending from 1.22×10^{13} cm^{-2} to 1.41×10^{13} cm^{-2} and from 1.99×10^{13} cm^{-2} to 2.15×10^{13} cm^{-2}. By combining the data from AlGaN/AlN/GaN samples, we find that the spin-orbit field is not a constant at high carrier densities and the electron spin-splitting energies show a deviation from linear behavior with Fermi wavefactor. However, the spin-splitting energies extracted from WAL oscillations, even in this high carrier density regime, were found to be much smaller than the previous reports based on Shubnikov-de Haas (SdH) measurements. We will discuss how the nonuniformities in the carrier density can lead to beating features in SdH oscillations, which can then be misinterpreted as large spin-splitting energies. This finding may resolve the long-standing discrepancy between the WAL and SdH results.

10:36AM Y15.00014 Spin Coulomb Drag in the Hubbard Chain[1] , PEDRO SCHLOTTMANN, Florida State University — The spin Coulomb drag is the decay of the spin current in a metal as a consequence of the Coulomb interaction between up- and down-spin carriers and is a distinctive feature of spin- polarized transport. The current of majority spins can induce a current of minority spin carriers via the transresistivity. This friction reduces the current but does not change the spin- polarization.[2] We calculate the critical exponents of the resistivity for up- and down-spin electrons and the transresistivity for the spin-polarized Hubbard chain with nonmagnetic impurities within the Kubo formalism using (1) bosonization techniques[3] and (2) the Bethe ansatz solution and conformal invariance.[4] The charge-spin separation in 1D is strictly valid only in the absence of spin-polarization. Due to the Luttinger liquid properties the temperature dependence of the transport correlation functions follow power laws of T with non-universal exponents. A large spin polarization is more favorable for a sustained spin current than a small magnetization.

[1]Work supported by the Department of Energy under grant DE-FG02-98ER45707.
[2]I. D'Amico and G. Vignale, Phys. Rev. B **62**, 4853 (2000).
[3]P. Schlottmann, Phys. Rev. B **80**, 205110 (2009).
[4]P. Schlottmann, Phys. Rev. B **82**, 075103 (2010).

10:48AM Y15.00015 Spin Texture in a Cold Exciton Gas , ALEXANDER HIGH, AARON HAMMACK, JASON LEONARD, SEN YANG, LEONID BUTOV, UC San Diego, TOMAS OSTATNICKY, Charles University, Prague, ALEXEI KAVOKIN, University of Southhampton, ARTHUR GOSSARD, UC Santa Barbara — We report on the observation of a spin texture in a cold exciton gas in a GaAs/AlGaAs coupled quantum well structure. The spin texture is observed around the rings in the exciton emission pattern. The observed phenomena include: a ring of linear polarization, a vortex of linear polarization with polarization perpendicular to the radial direction, an anisotropy in the exciton flux, a skew of the exciton fluxes in orthogonal circular polarizations and a corresponding four-leaf pattern of circular polarization, and a periodic spin texture. These phenomena emerge when the exciton gas is cooled below a few Kelvin.

Friday, March 25, 2011 8:00AM - 11:00AM –

Session Y16 GMAG DMP: Focus Session: Spins in Carbon-Based Materials – Magnetoresistance, Magneto-Electric Effect D173

8:00AM Y16.00001 Quantum Linear Magnetoresistance and Extraordinary Magnetoresistance in Graphene , ADAM FRIEDMAN, US Naval Research Laboratory — Graphene, a single atomic layer of hexagonally arranged carbon atoms, presents the optimal platform to study rarely-observed magnetoresistance (MR) effects because of its temperature-independent mobility and linear band structure with zero band gap. Linear magnetoresistance (LMR), which is characterized as a large, non-saturating linear MR, is one such unusual effect. Normally, the resistance of a conductor in an applied magnetic field increases quadratically with field and then saturates at a relatively low value. Models that explain LMR behavior have been proposed that include both quantum and classical origins, but most systems studied thus far can be explained by a purely classical model. However, we find that quantum LMR is observed in multilayer epitaxial graphene grown on SiC at temperatures as high as 300 K and with a magnitude greater than 200% at 12 Tesla (T). In addition, a phenomenon closely related to classical LMR called extraordinary magnetoresistance (EMR) and characterized by even larger MR, can be realized in metal-shunted graphene devices. Here, due to the different magnetic-field-dependent resistances of the metallic shunt, graphene, and shunt-graphene interface, current flows easily through the shunt in zero and low magnetic field, while in high magnetic field, more current flows around the shunt and is redistributed in the graphene. Devices made from chemical vapor deposition (CVD) graphene grown on copper and transferred to a SiO_2/Si substrate with Ti/Au shunts display gate-tunable longitudinal MR of $\sim$600% at 12 T and also show promise for use as Hall sensors. Graphene magnetoresistance devices have many possible applications including magnetic field sensors and magnetic read-heads. In contrast with the many proposed electronic uses for graphene, which necessitate the creation of a band-gap, graphene magnetoresistance devices that exploit LMR or EMR provide a use for as-grown or deposited graphene.

8:36AM Y16.00002 Frequency dependence of organic magnetoresistance[1] , FUJIAN WANG, JAMES RYBICKI, RAN LIN, KENT HUTCHINSON, JIA HOU, MARKUS WOHLGENANNT, University of Iowa — Organic magnetoresistive (OMAR) devices show a large enough magnetoresistive response (typically 10%) for potential applications as magnetic field sensors. However, applications often require sensing high frequency magnetic fields, and the examination of the frequency-dependent magnetoresistive response is therefore required. Analysis of time constants that limit the frequency response may also shed light on the mechanism behind the OMAR effect, because different OMAR mechanisms occur at different time scales In our experiments, the AC magnetic field is supplied by a coil with a ferrite core which is driven by a function generator The AC magnet shows a frequency response that is almost flat up to 1MHz. We found that the OMAR frequency limit is about 10 kHz for a typical organic semiconductor device and at least 100 kHz for devices made from a doped polymer film. We also performed capacitance and conductance vs. frequency measurements to understand the origin of the observed limit frequencies.

[1]This work was supported by Army MURI under GrantNo. W911NF-08-1-0317 and NSF under Grant No. ECS 0725280.

8:48AM Y16.00003 Room Temperature Ferromagnetic Polymer and the Correlated Anomalous Magnetoresistance Phenomenon[1] , JINSONG HUANG, University of Nebraska Lincoln, BIN YANG, JEFFREY SHIELD — Organic magnetoresistance (OMAR) has been observed in organic semiconductor devices where resistance can change in a relatively small external magnetic field at room temperature. Since a weak magnetic field is involved, the hyperfine interaction (HFI) is employed to explain OMAR in the reported literatures. None of these issues consider the magnetic properties of the organic semiconductors themselves. However, the we recently discovered that polymer semiconductors, such as poly(3-hexylthiophene) P3HT, can have room temperature (RT) ferromagnetic properties in their crystalline phase and when mixed with phenyl-C61-butyric acid methyl ester (PCBM). Here, we will report the possible correlation between the ferromagnetic property of the P3HT:PCBM and anomalous OMAR phenomenon including the anisotropic and hysteretic OMAR behavior. The magnetic property of the polymer including the anisotropic and photo induced change of magnetism will be also discussed to explore the possible mechanism of the room temperature ferromagnetism.

[1]This work is partially supported by the NSF MRSEC program at University.

9:00AM Y16.00004 Magnetic fringe field control of electronic transport in an organic film[1] , MARKUS WOHLGENANNT, FUJIAN WANG, University of Iowa, FERRAN MACIA, ANDREW KENT, New York University, MICHAEL FLATTE, University of Iowa — Random nuclear hyperfine fields in organic materials dramatically affect electronic transport properties such as the electrical (photo)conductivity and electroluminescence. The influence of these nuclear hyperfine fields can be overwhelmed by a uniform external applied magnetic field. As a result, in applied magnetic fields of about 10mT the kinetics of exciton formation, bipolaron formation, and carrier hopping are all modified, leading to changes in room-temperature electrical transport properties in excess of 10 % in many materials. Here we demonstrate a new method of controlling the electronic transport in an organic film, using the spatially-varying magnetic fringe fields of an unsaturated ferromagnetic electrode. The effect of these magnetic fringe fields is hysteretic, anisotropic, and depends sensitively on the distance of the organic material from the ferromagnetic electrode; all these effects appear in the magnetic-field dependences of electronic transport in these films. Such structures, which do not rely on spin injection or spin-valve behavior, may provide a simple approach to integrating magnetic metals and organics for hybrid spintronic devices.

[1]This work was supported by Army MURI Grant No. W911NF-08-1-0317

9:12AM Y16.00005 Spin-Boson Theory of Organic Magnetoresistance , CHANG-QIN WU, Department of Physics, Fudan University, Shanghai 200433 — The discovery of room-temperature, low-field magnetoresistance (MR) in organic light-emitting devices was one of major achievements of spintronics in the last decade. Compared to its inorganic counterpart, a sizable organic MR (OMR) is relatively easy to be obtained, showing extensive potential in magnetically controlled applications. Yet, after years of intense research, a comprehensive understanding of this magnetic field effect out of these nonmagnetic materials is still lacking. In this work, we present a spin-boson theory for magnetotransport in organic semiconducting materials, on the basis of a coupling between charge carriers' spin and a local bosonic environment, which is shown to be an irreducible ingredient in understanding of the anomalous OMR. Among those compose this environment triplet excitons play a basic role. The incoherent hopping rate between molecules is calculated to give out the basic behavior of OMR. The underlying mechanism is revealed from the calculation of entanglement, represented by the von Neumann entropy, between the carrier's spin and bosons. We also obtain the dependence of OMR on both of the bias voltage and the spin-boson coupling. The results obtained from the theory are in good agreement with experiments.

9:24AM Y16.00006 Electronic and transport properties of Cobalt-based valence tautomeric molecules and polymers , YIFENG CHEN, Department of Physics, North Carolina State University, ARRIGO CALZOLARI, Istituto Nanoscienze CNR-NANO-S3, MARCO BUONGIORNO NARDELLI, Department of Physics, North Carolina State University — The advancement of molecular spintronics requires further understandings of the fundamental electronic structures and transport properties of prototypical spintronics molecules and polymers. Here we present a density functional based theoretical study of the electronic structures of Cobalt-based valence tautomeric molecules Co^{III}(SQ)(Cat)L $Co^{II}(SQ)_2$L and their polymers, where SQ refers to the semiquinone ligand, and Cat the catecholate ligand, while L is a redox innocent backbone ligand. The conversion from low-spin Co^{III} ground state to high-spin Co^{II} excited state is realized by imposing an on-site potential U on the Co atom and elongating the Co-N bond. Transport properties are subsequently calculated by extracting electronic Wannier functions from these systems and computing the charge transport in the ballistic regime using a Non-Equilibrium Green's Function (NEGF) approach. Our transport results show distinct charge transport properties between low-spin ground state and high-spin excited state, hence suggesting potential spintronics devices from these molecules and polymers such as spin valves.

9:36AM Y16.00007 Spin polarized transport properties of impurity induced Carbon nanostructures , SERKAN CALISKAN[1], Fatih University, MEHMET CANTURK, Atilim University — We study spin polarized transport on structures consisting of Carbon wires including impurities. We perform first principle calculations on these structures using the nonequilibrium Green Function formalism combined with the density functional theory. The different impurity induced Carbon nanostructures are found to depend strongly on the geometrical disorder. Through the conductance, transmission spectra, density of states and current-voltage characteristics the numerical results of spin polarized calculations are discussed.

[1]Corresponding (Presenting) Author

9:48AM Y16.00008 Spin transport in organic semiconductor single crystals , H.-JAE JANG, Semiconductor Electornics Div. NIST & Dept. of Physics, Wake Forest Univ., OLEG KIRILLOV, KURT PERNSTICH, Semiconductor Electornics Div. NIST , WILLIAM RIPPARD, Electromagnetics Div. NIST, KATELYN P. GOETZ, OANA D. JURCHESCU, Dept. of Physics, Wake Forest Univ., DAVID GUNDLACH, MARIONA COLL BAU, BRAD R. CONRAD, CHRISTINA HACKER, CURT A. RICHTER, Semiconductor Electornics Div. NIST — Organic semiconductors have been attracting much attention as potential spin transport media due to their weak spin-orbit and hyperfine interactions that promise long spin lifetimes. However, to date most studies have focused on amorphous, or polycrystalline thin-film based organic semiconductors. In addition, short transport distances equal to or less than a couple of hundred nanometers have been measured despite the prediction of long spin transport distance. We have investigated spin injection and transport in high purity single-crystal organic semiconductors, especially rubrene(5,6,11,12-tetraphenylnaphthacene). We will present and discuss our experimental results obtained in both vertical and lateral transport geometries. Great care is needed to understand and avoid possible spurious effects in these studies.

10:00AM Y16.00009 Correlation of electric polarization and magnetic ordering in cobalt chloride thiourea , EUNDEOK MUN, National High Magnetic Field Laboratory (NHMFL), Los Alamos National Lab (LANL), Los Alamos, NM, JASON WILCOX, JAMIE MANSON, Department of Chemistry and Biochemistry Eastern Washington University Cheney, WA 99004 USA, BRIAN SCOTT, MPA-MC, Los Alamos National Lab (LANL), Los Alamos, NM, PAUL TOBASH, ERIC BAUER, VIVIEN ZAPF, MPA-CMMS, Los Alamos National Lab (LANL), Los Alamos, NM — The coupling between electricity and magnetism in magneto-electric multiferroics has been intensively investigated in a wide range of transition metal oxides. Recently the material classes have been extended to organo-metallic insulators (sometimes known as metal-organic frameworks or molecular magnets) such as $NiCl_2$-4[$SC(NH_2)_2$], which provides a new arena for designing magneto-electric multiferroics. We have grown single crystals of cobalt chloride thiourea, $CoCl_2$-n[$SC(NH_2)_2$], which forms two different crystal structures with n = 2 and 4. The compound $CoCl_2$-2[$SC(NH_2)_2$] has a triclinic crystal structure with strong magnetic anisotropy and $\sim$ 3 μ_B/Co ion, indicating **S** = 3/2 Co spins, and the compound $CoCl_2$-4[$SC(NH_2)_2$] has a tetragonal structure with almost no magnetic anisotropy and 1 μ_B/Co ion, indicating **S** = 1/2 Co spins. We will present details of the magnetic field-induced electric polarizations and magnetic properties of these compounds.

10:12AM Y16.00010 Magneto-electric multiferroic behavior in a metal-organic framework , VIVIEN S. ZAPF, National High Magnetic Field Lab, Los Alamos National Lab, Los Alamos, NM, PINAKI SENGUPTA, Nanyang Technological University, Singapore, CRISTIAN BATISTA, Theoretical Division, Los Alamos National Lab, FARZANA NASREEN, NHMFL, LANL and New Mexico State University, FREDERIK WOLFF-FABRIS, NHMFL, LANL, now at Dresden Hochfeld Labor, ARMANDO PADUAN-FILHO, Universidade de Sao Paulo — We will discuss strong magneto-electric coupling in the metal-organic compound $NiCl_2$-4$SC(NH_2)_2$(also known as a metal-organic framework or molecular magnet). Magneto-electric multiferroic behavior is traditionally investigated in transition-metal oxides, however we are expanding the field to metal-organics, which are designable materials with soft lattices and electrically polar organic elements. In this material we observe a magnetic field-induced change in the electric polarization of 50 $\mu C/m^2$ driven by ordering of the Ni S = 1 spins. We can model it in terms of a combination of exchange striction and crystal electric fields, and Quantum Monte Carlo simulations of these effects provide an excellent fit to the data. We find that the induced electric polarization is a sum of $<S_z^2>$ and the nearest neighbor correlation function $<S_i$ dot $S_j>$ The presence of electrically polar thiourea molecules [$SC(NH_2)_2$] amplifies the effect of small magnetically induced crystal distortions on the electric polarization.

10:24AM Y16.00011 Manipulating singlet-triplet equilibrium in organic biradical materials , O. GUNAYDIN-SEN, J. FOSSO-TANDE, P. CHEN, J.L. WHITE, J.L. MUSFELDT, University of Tennessee, R.J. HARRISON, University of Tennessee and Oak Ridge National Laboratory, T.L. ALLEN, P.M. LAHTI, University of Massachusetts, J. CHERIAN, T. TOKUMOTO, S. MCGILL, National High Magnetic Field Laboratory — We investigated the tunability of the singlet-triplet equilibrium population in 1,4-phenylenedinitrene via magneto-optical spectroscopy. Both temperature- and magnetic field-induced spectral changes in this organic biradical are sensitive to magnetic energy scales, specifically the spin gap, demonstrating the important interplay between charge, and magnetism in this system. These measurements also establish the value of local-probe photophysical techniques for extraction of magnetic properties data in systems where a traditional Curie law analysis has intrinsic limitations. *This work is supported by the National Science Foundation.

10:36AM Y16.00012 Reversible mechanism for spin crossover in transition-metal cyanides , MUKUL KABIR, KRYSTYN J. VAN VLIET, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA — Spin transitions generally occur in compounds of octahedrally coordinated $3d$ transition metal ions. These transitions can be induced by external perturbations such as light, heat, pressure, magnetic field, and chemical substitution. Transition metal cyanides are one such material, which exhibit *reversible* spin transition while perturbed with light at T <10 K. Here we report the first-principles (DFT+U) study of anhydrated $KCoFe(CN)_6$. We find that the complete spin transition from the low spin ground sate ($S = 0$) to a high spin ($S = 2$) state takes place due to intra-atomic and inter-atomic charge transfers in two steps. In the first step a d-electron is transferred from Fe to Co through cyanide ligand, which is followed by the d-electron rearrangement in the Co. This spin transition is strongly correlated with the internal lattice, and we find as large as 10% extension of the Co−N bond via a Jahn-Teller active (tetragonally distorted) lattice in the intermediate spin ($S = 1$) state. The calculated energy required for this transition is in agreement with experiments. We further predict that this spin transition in such materials can be induced, and further tuned, by external pressure to enable realization of such reversible transitions at ambient temperatures.

10:48AM Y16.00013 Psuedo-entanglement between nuclear spins in photoexcited functionalized fullerenes , VASILEIA FILIDOU, STEPHANIE SIMMONS, University of Oxford, HARRY L. ANDERSON, University of Oxford, G. ANDREW D. BRIGGS, ARZHANG ARDAVAN, University of Oxford, STEVEN KARLEN, University of Chicago, FELICIANO GIUSTINO, JOHN J.L. MORTON, University of Oxford — Optically excited triplet electron spins can be used to polarise, manipulate, couple and measure nuclear spins. Here we present photoexcited pulsed magnetic resonance experiments for the characterization of functionalized fullerene structures with homo and hetero nuclear spins. We use density functional theory in order to predict the hyperfine interaction between the photoexcited triplet and various nuclear spins in the structure, and then use magnetic resonance (ENDOR) to investigate these values experimentally. In addition to the hyperfine coupling strength, we measure the relevant relaxation rates and initial hyperpolarisation of the triplet in order to understand the possible degree of entanglement of nuclear spins through the optically excited mediator spin. We measure an increased nuclear-nuclear coupling in the presence of the triplet which permits fast nuclear controlled-NOT gates.These operations, in conjunction with the transfer of electron polarisation to the nucleus, allow the demonstration of nuclear-nuclear pseudo-entanglement, measured using quantum state tomography.

Friday, March 25, 2011 8:00AM - 11:00AM –

Session Y18 GMAG DMP: Focus Session: Low D/Frustrated Magnetism - More Frustrated Magnets D172

8:00AM Y18.00001 Field-induced thermal transport in BEC antiferromagnets[1] , SASHA CHERNYSHEV, UC Irvine, CRISTIAN BATISTA, LANL — Recent experiments in BEC quantum magnets exhibit a dramatic evolution of the thermal conductivity of these materials in magnetic field. By considering various relaxation mechanisms of bosonic excitations in the vicinity of the BEC quantum-critical point at finite temperature we provide a detailed explanation of several unusual features of the data. We identify the leading impurity-scattering interaction and demonstrate that its renormalization due to quantum fluctuations of the paramagnetic state compensates the related mass renormalization effect. This explains the enigmatic absence of the asymmetry between the two critical points in the low-T thermal conductivity data, while such an asymmetry is prominent in many other physical quantities. The observed characteristic "migration" of the peak in thermal conductivity away from the transition points as a function of temperature is explained as due to a competition between an increase in the number of heat carriers and an enhancement of their mutual scattering. An important role of the three-boson scattering processes within the ordered phase of these systems is also discussed. Other qualitative and quantitative features of the experiment are clarified and the future directions are sketched.

[1]supported by the DoE

8:12AM Y18.00002 Investigation of the magnetic susceptibility of the disordered BEC system $NiCl_{0.85}Br_{0.15}$-4SC$(NH_2)_2$ at ultralow-temperatures , LIANG YIN, CHAO HUAN, JIAN-SHENG XIA, NEIL SULLIVAN, University of Florida, VIVIEN ZAPF, LANL, ARMANDO PADUAN-FILHO, Universidade de Sao Paulo, RONG YU, Rice University, TOMMASO ROSCILDE, ENS Lyon — We report measurements of the magnetic susceptibility of a disordered BEC system of magnons for single crystals of $NiCl_{0.85}Br_{0.15}$-4SC$(NH_2)_2$ (with 15% Cl atoms replaced by Br). $NiCl_{0.85}Br_{0.15}$-4SC$(NH_2)_2$ is a potential candidate for a Bose glass (BG) phase of the spins adjacent to a region of Bose-Einstein condensation (BEC). The BG to BEC phase is the bosonic analog of a metal-insulator transition for fermions. The measurements were carried out for temperatures down to 1mK and for applied magnetic fields up to 14.5T. The results show that the critical fields H_c do not obey the conventional 3D universality class for a BEC, $H_c(T) - H_c(0) \sim T^{\alpha}$, where $\alpha = 1.5$ [1]. The values of α changes from $\alpha = 0.52$ for T $>$ 300 mK to $\alpha = 0.91$ for T $<$ 250 mK and then again at 70$\sim$90mK to $\alpha = 0.48$ for T$<$ 70 mK, indicating a crossover to possible BG behavior.

8:24AM Y18.00003 Bose-Einstein Condensation in Han Purple - a NMR Study[1] , RAIVO STERN, NICPB, Tallinn, Estonia, STEFFEN KRÄMER, MLADEN HORVATIC, CLAUDE BERTHIER, LNCMI, Grenoble, France, IVO HEINMAA, ENNO JOON, NICPB, Tallinn, Estonia, TSUYOSHI KIMURA, Osaka University, Japan — NMR study of the two quasi-2D coupled spin-1/2 dimer compound, $BaCuSi_2O_6$ (Han Purple) [1], is presented. $T_{\rm BEC}$ varies as $(H - H_{c1})^{2/d}$, where d is the dimensionality of the system, and H_{c1} the critical field which closes the gap. $BaCuSi_2O_6$ was claimed to exhibit an reduction of d from 3D to 2D at low T [2]. However, due to a structural transformation at 90 K, different intradimer exchange couplings and different gaps ($\Delta_{\rm B}/\Delta_{\rm A}$=1.16) exist in every second plane along the c axis [3]. In our first NMR experiments [3], we have shown that the population of bosons in the B planes $n_{\rm B}$ was much smaller than $n_{\rm A}$, but finite in the field range $\Delta_{\rm A}/g\mu_{\rm B} < H < \Delta_{\rm B}/g\mu_{\rm B}$ where $n_{\rm B} = 0$ is expected in a naive model of uncoupled planes. Recently, a new model has been presented [4] which takes into account both frustration and quantum fluctuations. This leads to a non-zero population $n_{\rm B}$ of *uncondensed* bosons in the B plane, increasing quadratically with $(H - H_{c1})$, as compared to the linear dependence of $n_{\rm A}$. We compare our new NMR results to these predictions. [1] M. Jaime *et al.*, PRL **93**,087203 (2004). [2] S. E. Sebastian *et al.*, Nature **441**, 617 (2006). [3] S. Krämer *et al.*, PRB **76**, 100406(R) (2007). [4] N. Laflorencie and F. Mila, PRL **102**, 060602 (2009).

[1]Euromagnet II and Estonian Science Foundation.

8:36AM Y18.00004 Magnetic neutron scattering of a Prussian blue analogue photomagnet[1] , D.M. PAJEROWSKI, Dept. Phys. and NHMFL, Univ. Florida and NCNR-NIST, E.S. KNOWLES, Y.M. CALM, M.W. MEISEL, Dept. Phys. and NHMFL, Univ. Florida, M.J. ANDRUS, J.E. GARDNER, D.R. TALHAM, Dept. Chem., Univ. Florida, V.O. GARLEA, S.E. NAGLER, NSSD-ORNL — Since the discovery of photoinduced magnetism in cobalt hexacyanoferrate (CoFe) Prussian blue analogues (PBAs) in 1996,[1] there have been many, multifarious studies that elucidated the nature of the photoeffect. However, the magnetization in CoFe has proven difficult to model quantitatively using macroscopic data due to the presence of multiple magnetic species, magnetic bistability, superexchange, and unquenched orbital angular momentum. To investigate the ordered magnetization directly, we have studied dueterated powders of CoFe using unpolarized and polarized neutron diffraction, and observed magnetic neutron scattering for the first time in this compound. A model for the magnetic structure based upon neutron diffraction, elemental analysis, infrared spectroscopy, and macroscopic magnetization will be presented.
[1] O. Sato, et al., Science 272, 704 (1996).

[1]Supported, in part, by NSF DMR-0701400 (MWM), DMR-1005581 (DRT), and DMR-0654118 (NHMFL). Research at ORNL was sponsored by the Scientific User Facilities Division, BES, DOE.

8:48AM Y18.00005 Photoinduced Magnetism in Nanoscale Heterostructures of Prussian Blue Analogues*

E.S. KNOWLES, D.M. PAJEROWSKI, M.W. MEISEL, Dept. Phys. and NHMFL, Univ. Florida, M.F. DUMONT, A. GUIET, D.R. TALHAM, Dept. Chem., Univ. Florida, A. GOMEZ, S.W. KYCIA, Dept. Phys., Univ. Guelph — Nanometer-scale cubic heterostructures of two Prussian blue analogues, ferromagnetic $K_jNi_k[Cr(CN)_6]_l{\cdot}nH_2O$ (**A**) with $T_c \sim 70$ K and photo-active ferrimagnetic $Rb_aCo_b[Fe(CN)_6]_c{\cdot}mH_2O$ (**B**) with $T_c \sim 20$ K, have been studied.[1] These samples exhibit a persistent photoinduced decrease in magnetization at temperatures up to $T_c \sim 70$ K of the **A** constituent, resembling results from analogous **ABA** heterostructured films.[2] This net decrease suggests that the photoinduced structural transition in the **B** layer generates a strain-induced decrease in the magnetization of the **A** layer, similar to a pressure-induced decrease previously observed in the pure **A** material.[3] Core-shell and core-shell-shell configurations **AB**, **BA**, **ABA**, and **BAB** have been characterized by TEM, FTIR, XRD, and SQUID magnetometry.

*Supported, in part, by NSF DMR-0701400 (MWM) and DMR-1005581 (DRT), NSERC, CFI, the NHMFL, and the State of Florida.

[1]M. F. Dumont *et al.*, Inorg. Chem., submitted.
[2]D. M. Pajerowski *et al.*, J. Am. Chem. Soc. **132**, 4058 (2010).
[3]M. Zentková *et al.*, J. Phys.: Condens. Matter **19**, 266217 (2007).

9:00AM Y18.00006 Structural and Magnetic Interplay in Molecule-based Magnets with Photocontrollable Properties[1]

Y.M. CALM, E.S. KNOWLES, D.M. PAJEROWSKI, A.M. ZIEGLER, M.W. MEISEL, Dept. Phys. NHMFL, Univ. Florida, H. PHAN, M. SHATRUK, Dept. Chem., Florida State Univ., M.J. ANDRUS, M.F. DUMONT, D.R. TALHAM, Dept. Chem., Univ. Florida — Understanding the cooperative effects, such as electron-lattice interactions, in molecule-based magnetic coordination complexes possessing photoinduced phase transitions is an important step to being able to rationally tune the variables governing the process.[2] Specifically, variable temperature FTIR spectroscopy and magnetometry have been used to explore the temperature and photocontrollable spin transitions in Co-Fe Prussian blue analogues, $A_jCo_k[Fe(CN)_6]_\ell \cdot nH_2O$, where A is an alkali ion, and in new Fe spin-crossover complexes. By studying nanoparticles[3] and heterostructures,[4] the data provide insight into the roles played by restricted lattice geometries and strain-pressure effects.

[1]Supported by NSF DMR-0701400 (MWM), CHE-0911109 (MS), DMR-1005581 (DRT), DMR-0851707 (UF Physics REU for AMZ), and DMR-0654118 (NHMFL).
[2]H. Watanabe *et al.*, Phys. Rev. B **79** (2009) 180405.
[3]M.F. Dumont *et al.*, Inorg. Chem., submitted.
[4]D.M. Pajerowski *et al.*, J. Am. Chem. Soc. **132** (2010) 4058.

9:12AM Y18.00007 Interplay between charge fluctuations and magnetic order in a stacked triangular-Kagome lattice : Applications to FeCrAs

JEFFREY RAU, HAE YOUNG KEE, University of Toronto — The recently studied antiferromagnet FeCrAs [Wu et al, EPL, 85 17009 (2009)] exhibits a surprising combination of experimental signatures, with Fermi liquid like specific heat but resistivity showing strong non-Fermi liquid character. From the material properties we motivate a minimal model for the low energy degrees of freedom, and study its properties using slave-rotor mean field theory. Using this approach we find a variety of exotic phases and propose that the features of FeCrAs can be qualitatively explained by a spin liquid proximate to a metal-insulator transition.

9:24AM Y18.00008 Giant Anomalous Hall Effect in (Ba,Sr)$T_{2+x}Ru_{4-x}O_{11}$ (T=Fe,Co,Mn) Ferrites[1]

LANCE DELONG, LARYSA SHLYK, University of Kentucky — Hexagonal R-type ferrites (Ba,Sr)$T_{2+x}Ru_{4-x}O_{11}$ are promising spintronic materials that exhibit collinear ferrimagnetic order at unusually high critical temperatures $T_C \leq 490$ K for Fe-bearing compositions, and an in-plane, "all-in/all-out" order at T_C's $<<$ 300 K due to frustrated antiferromagnetic interactions within the Kagome basal plane in metallic Co or Mn compositions. A strong, nonmonotonic field dependence of the anomalous Hall effect is observed in metallic ferrites, which is generated by non-zero scalar spin chirality and the Berry phase acquired by carriers moving in the "topologically nontrivial" spin background of the Kagome plane. The FM semiconductor $BaFe_{3.4}Ru_{2.6}O_{11}$ (T_C = 440 K) exhibits a giant Hall resistivity = 77 $\mu\Omega$-cm at 300 K, with a low-temperature sign change and monotonic field dependence that are consistent with a strong Berry phase curvature (gauge field) acquired by carriers in momentum space.

[1]Research supported by U.S. DoE Grant No. DE-FG02-97ER45653

9:36AM Y18.00009 Coexistence of ferromagnetic and antiferromagnetic orders in Ba-doped cobalt perovskites studied by neutron scattering[1]

HUIBO CAO, Oak Ridge National Laboratory, FANGWEI WANG, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, CAS, VASILE GARLEA, Oak Ridge National Laboratory, ARSEN GUKASOV, Centre de Saclay, DSM/IRAMIS/Laboratoire Léon Brillouin, CEA, ZHAOHUA CHENG, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, CAS — Cobalt-containing oxide compounds have attracted a great deal of interest in recent years due to the variety of magnetic and electrical properties. We performed single crystal neutron diffraction on 6T2 at the LLB in France and the HB3A four-circle diffractometor at the HFIR of ORNL. The Ba-doped cobalt perovskite ($La_{0.8}Ba_{0.2}CoO_3$) crystal was measured in the temperature range of 2-250 K. At temperature $T < 200$ K, a set of ferromagnetic peaks ($k_1 = 0$) onsets and then antiferromagnetic peaks with k_2* = (1/2 0 1/2) and (0 0 3/2) join in at $T < 100$ K. Both ferromagnetic and antiferromagnetic peaks saturate at $T \approx 40$ K. By refining the peaks collected for k_1 and k_2 sets, magnetic structures were determined.

[1]This research is supported by UT Battelle, LLC, Contract DE-AC05-00OR22725 for U.S. D.O.E., and the National Basic Research Program of China (973 Program, 2010CB833102).

9:48AM Y18.00010 Density matrix renormalization group study of optical conductivity in the one-dimensional Mott insulator Sr_2CuO_3

SHIGETOSHI SOTA, TAKAMI TOHYAMA, Yukawa Institute for Theoretical Physics, Kyoto University — We examine the optical conductivity of Sr_2CuO_3 by using zero and finite temperature dynamical density matrix renormalization group (DMRG) methods. Employing a Hubbard- Holstein model containing Holstein-type coupling of electron to the Einstein phonons, we reproduce both the Mott-gap excitation and phonon-assisted spin excitation observed experimentally [1,2] by using the dynamical DMRG method combined with a regulated polynomial expansion [3]. We find a parameter set describing Sr_2CuO_3. Furthermore, by using a low- temperature dynamical DMRG method which is recently developed by present authors [4], we examine the temperature effect of the Mott-gap excitation to clarify the effect of optical phonons on spectral shape at finite temperatures. We find that the presence of phonons induces the enhancement of the width of an excitonic peak in the optical conductivity. [1] M. Ono, K. Miura, A. Maeda, H. Matsuzaki, H. Kishida, Y. Taguchi, Y. Tokura, M. Yamashita, and H. Okamoto, Phys. Rev. B **70**, 085101 (2004). [2] H. Suzuura, H. Yasuhara, A. Furusaki, N. Nagaosa, Y. Tokura: Phys. Rev. Lett. **76**, 2579 (1996). [3] S. Sota and M. Itoh, J. Phys. Soc. Jpn. **76**, 054004 (2007). [4] S. Sota and T. Tohyama, Phys. Rev. B **78**, 113101 (2008).

10:00AM Y18.00011 A Compton scattering study of the magnetic structure of $NbFe_2$, THOMAS HAYNES, University of Bristol, UK, MATTHEW BUTCHERS, JONATHAN DUFFY, University of Warwick, UK, STEPHEN DUGDALE, University of Bristol, JONATHAN TAYLOR, SEAN GIBLIN, ISIS Facility, RAL, UK, JUDE LAVEROCK, Boston University, CLAUDIA UTFELD, University of Bristol, ROSS STEWART, ISIS Facility, RAL, UK — $NbFe_2$ displays a diverse phase diagram over a narrow compositional range, possibly due to close proximity to a Quantum Critical Point. The ground state of $NbFe_2$ has been the subject of a number of recent theoretical investigations [1,2], but for near-stoichiometric compositions its exact nature remains ambiguous. We have probed the low temperature magnetic structure by performing Magnetic Compton Scattering (MCS) measurements on polycrystalline $Nb_{1+y}Fe_{2-y}$ samples with $y = -0.02, 0.00$ and 0.03. MCS is able to measure how the magnetic electrons within a sample are distributed in momentum space, and can be a useful tool for resolving site-specific contributions to the spin moment. The interpretation of these measurements was aided by electronic structure calculations, which favour a ferrimagnetic ground state. The results are presented with reference to the possible presence of spin fluctuations.

[1] Subedi and Singh, PRB **81**, 024422 (2010)
[2] Tompsett et al, PRB **82**, 155137 (2010)

10:12AM Y18.00012 Impurity-entanglement in dimerized spin chains , ANDREAS DESCHNER, ERIK SORENSEN, McMaster University — To quantify the entanglement caused by an impurity in an $S = \frac{1}{2}$ dimerized $J_1 - J_2$ quantum spin chain, several different entanglement-measures have been utilized. We present the results of variational calculations of the impurity entanglement entropy as well as the negativity for a chain with an impurity attached at one end. We compare the results for both of these measures.

10:24AM Y18.00013 On the low-temperature behavior of a geometrically frustrated Heisenberg antiferromagnet[1] , STEFAN SCHNABEL, D.P. LANDAU, U. of Georgia — The thermodynamic behavior of the Heisenberg antiferromagnet on the kagome lattice and the effects of its geometrical frustration are widely understood [1]. At low temperatures planar spin configurations due to multiple zero-modes (so-called Weathervane loops) are favored entropically. These modes occur when spin clusters are bounded by spins pointing in a similar direction, so that the cluster spins revolve freely around this direction. However, it remains unclear if with decreasing temperature the number of these modes continues to increase and if this eventually leads to a highly ordered $\sqrt{3}\times\sqrt{3}$ state. In order to investigate this system we applied the simulated tempering method, combined with the Heatbath algorithm for single spins and a Metropolis loop-flip Monte Carlo move. We examined the thermodynamic properties for temperatures $\frac{k_B T}{J} \geq 10^{-6}$; and found that once the planar state is attained, the out-of-plane excitations are reduced with decreasing temperature but no further order is established. Hence, the prevailing spin structure represents a temperature independent entropy maximum where any entropy gain produced by additional zero modes is neutralized by an entropy loss in the Weathervane loop structure.

[1] J. N. Reimers and A. J. Berlinsky, Phys. Rev. B **48**, 9539 (1993).

[1]Research supported by NSF.

10:36AM Y18.00014 Topological phases and quenches in spin-ladder systems , SMITHA VISHVESHWARA, WADE DEGOTTARDI, Univ. of Illinois at Urbana-Champaign, DIPTIMAN SEN, Indian Institute of Science — We show that a ladder version of Kitaev's honeycomb model can be directly mapped to a one-dimensional p-wave superconducting system. The ladder system is characterized by Z_2 vortices at every unit cell; the presence of vortices is encoded in the sign of the local chemical potential in the p-wave system. Compared to recently studied phases in topological superconductors, we show that certain vortex patterns in this ladder system can result in new topological phases and can alter the universality classes for associated phase transitions. We discuss the effect of performing time-dependent quenches in these new phases.

10:48AM Y18.00015 Multi-spin exchange model for a quantum spin liquid on the honeycomb lattice , YI-FEI WANG, Zhejiang Normal Univ. and California State Univ. Northridge, DONNA SHENG, California State Univ. Northridge, CHANG-DE GONG, Zhejiang Normal Univ. — Recently, a possible quantum spin liquid (QSL) state has been found through quantum Monte Carlo studies of Hubbard model on the honeycomb lattice. The obtained QSL does not show long range correlation of any known type, which has a finite spin gap and a short range dimer-dimer correlation pattern resembling the short range resonant-valence-bond (RVB) state. Given the intensive current interest in such an exotic QSL, it is natural and timely to ask a question: what is the effective spin model to capture the essential low-energy physics near this QSL region? We report here a comparative numerical study based on finite-size exact diagonalizations (ED) of the Hubbard model, and a multi-spin exchange model with two-, four- and six-spin exchange terms. The latter model is derived from the strong coupling expansion of the former one. Through extensive ED calculations of low-energy spectra and ground-state correlation functions of both models, we try to establish connections between them, especially near the QSL region. Furthermore, the phase diagram of the multi-spin exchange model is explored in details.

Friday, March 25, 2011 8:00AM - 11:00AM –

Session Y20 DMP FIAP GERA: Focus Session: Thermoelectric Materials: Chalcogenides and 1D/2D Systems D168

8:00AM Y20.00001 Resonant Energy Levels and the Thermoelectric Figure of Merit[1] , JOSEPH P. HEREMANS, Ohio State University, Dept of Mechanical Engineering, and Dept. of Physics — Distortions of the electronic density of states are a potent mechanism to increase the thermopower and ZT of thermoelectric semiconductors. Band-structure engineering approaches will be reviewed that can be used to do this, namely quantum size effects, hybridization effects in strongly correlated electron systems, and resonant impurity levels. The properties of known resonant impurities for PbTe, SnTe, Bi_2Te_3 and GaSb will also be reviewed. They can increase the thermoelectric power through 2 mechanisms, (1) the increase in density of states, and (2) resonant scattering. The first increases the thermopower in a nearly temperature-independent way; the second results in an electron energy filtering effect that increases the thermopower, but only at cryogenic temperatures where the electron-phonon interactions are weaker. An analysis of the thermomagnetic tensor components makes it possible to dissociate the two contributions experimentally.

[1]In collaboration with Y. Gao, C.M. Jaworski, A. Chamoire, H. Jin and M. Nielsen, work supported by AFOSR, DOE, NSF

8:36AM Y20.00002 The Effect of Sintering on the Thermoelectric Properties of Chemically Synthesized Nano-Bulk $Bi_{2-x}Sb_xTe_3$, J.S. DYCK, S. DORROH, Physics Dept., John Carroll University, B.D. MAO, J.W. WANG, C. BURDA, Chemistry Dept., Case Western Reserve University — Considerable research effort has gone into improving the performance of traditional thermoelectric (TE) materials such as $Bi_{2-x}Sb_xTe_3$ through a variety of nanostructuring approaches. Bottom-up, chemical approaches have the potential of producing very small nanoparticles ($<$ 50 nm) with narrow size distributions and controlled shape. For this study, nanocrystalline powder of $Bi_{2-x}Sb_xTe_3$ with x = 0 – 1.5 has been synthesized using a ligand- assisted chemical method, and consolidated into bulk pellets with cold pressing followed by sintering. These materials have the interesting property that a wide range of carrier concentrations are accessible through different Bi/Sb ratios, with low values of x being n-type and higher values becoming p-type. In this work, we present the thermoelectric transport measurements from 6 – 300 K as a function of sintering temperature, and a beneficial effect is found. The samples are also characterized by Hall effect, XRD, and compositional analysis. We will present results on the structure-property relations, and discuss strategies for optimization of this class of TE materials for high performance.

8:48AM Y20.00003 Coherent Phase Stability of IV-VI Rocksalt Semiconductor Alloys[1] , JEFFREY DOAK, CHRIS WOLVERTON, Northwestern University — The creation of nanoscale precipitates via phase separation provides a mechanism for decreasing the lattice thermal conductivity of some bulk thermoelectric materials. The IV-VI semiconductor alloy systems may phase separate by either a spinodal decomposition or nucleation and growth mechanism. To better understand these phase transformations, we use first-principles density functional theory (DFT) calculations to investigate the coherent and incoherent phase stability of a series of IV-VI rocksalt semiconductor alloys (IV=Pb, Sn, Ge and VI = S, Se, Te). We use mixing enthalpies derived from calculations of special quasirandom structures (SQS), along with coherency strain energies to model the thermodynamic driving forces for incoherent and coherent phase separation. By fitting these inputs to a sub-regular mixing enthalpy model and including an ideal mixing entropy term, we calculate incoherent and coherent phase diagrams. We show the incorporation of coherency strain energies cause large depressions of the coherent spinodals for each system. The depressions are large enough that at realistic processing temperatures, the dominant precipitation mechanism of phase separation is nucleation and growth.

[1]Supported by the Center for Revolutionary Materials for Solid State Energy Conversion, an EFRC funded by the US DOE, Office of BES

9:00AM Y20.00004 Electronic structure of PbTe doped with K and Na[1] , MAL-SOON LEE, S. D. MAHANTI, Michigan State University — PbTe is a well-known thermoelectric which shows excellent thermoelectric performance (for both p- and n-type) in the temperature range between ambient and 600°C. Thermopower (S) of PbTe can be enhanced with proper doping. Hermann *et al.* have found the figure of merit ZT=1.5 at 773 K with 2 % Tl doping in PbTe. They ascribe this to the enhancement of the density of states (DOS) caused by Tl-induced resonance level in the valence band. This is in agreement with the *ab initio* studies of Ahmad *et al.*, who also found an enhanced DOS associated with K defects in PbTe. Recently Androulakis *et al.* have looked for resonant states in the valence band associated with Na/K impurities in PbTe. Although they observe an increase in power factor at high temperature, they do not find any evidence of resonant states. We have reexamined this issue by carrying out detailed band structure calculations in the presence of K and Na defects in PbTe using 64-atom supercells. The question of the existence of resonant states and the origin of the enhanced DOS near the valence band maximum will be discussed.

[1]This work was supported by the US Department of Energy, Office of Basic Energy Sciences as part of an Energy Frontier Research Center.

9:12AM Y20.00005 Ho Doped Bi_xSb_y Nanopolycrystalline Alloys[1] , K.C. LUKAS, G. JOSHI, DEZHI WANG, Z.F. REN, C.P. OPEIL — Department of Physics, Boston College, Chestnut Hill, Massachusetts, 02467. Bismuth-Antimony alloys have been shown to have high ZT values below room temperature, especially for single crystals. For polycrystalline samples, impurity doping and magnetic field have proven to be powerful tools in the search for understanding and improving thermoelectric performance. Nanopolycrystalline Bi_xSb_y doped with 1 and 3% Ho were prepared by ball milling and dc hot pressing technique. Electrical resistivity, Seebeck coefficient, thermal conductivity, carrier concentration, mobility, and magnetization are measured in a temperature range of 5-350 K and in magnetic fields up to 9 Tesla. The effects of Ho doping on the thermoelectric properties of Bi_xSb_y in magnetic field will be discussed.

[1]D.O.E. Energy Frontier Research Center Grant (S3TEC), at Massachusetts Institute of Technology

9:24AM Y20.00006 Thermoelectric properties of Quintuple Layer Bi_2Te_3[1] , ROGER LAKE, FERDOWS ZAHID, University of California Riverside — Motivated by recent experimental results,[2] we derive the thermoelectric parameters of a Bi_2Te_3 film of one quintuple layer thickness. Our results show approximately ten times increase in the figure of merit (ZT) for the thin film (ZT = 7.2) compared to that for the bulk (ZT = 0.68). The large enhancement in ZT results from the change in the distribution of the valence band density of modes brought about by the quantum confinement in the thin film. Our theoretical model uses ab initio electronic structure calculations as implemented in the VASP software package combined with a Landauer approach for calculating the linear-response transport coefficients. We employ two fitting parameters: a rigid shift of the conduction and valence bands to match the known bulk bandgap (i.e. a 'scissors operator'), and an energy independent electron mean free path for the phonon scattering inside the device. With these two fitting parameters, our results show excellent agreement with the known experimental values for bulk Bi_2Te_3.

[1]Supported by the MARCO Center FENA

[2]D. Teweldebrhan, V. Goyal and A. A. Balandin, Nano Lett. 10, 1209 (2010); D. Teweldebrhan, V. Goyal, M. Rahman, and A. A. Balandin, Appl. Phys. Lett. 96, 053107 (2010); Y. Zhang et al., Nat. Phys. 6, 584 (2010).

9:36AM Y20.00007 Phase diagram of thermoelectric Bi2S3-Bi2Se3-Bi2Te3 system , WEISHU LIU, QINYONG ZHANG, QIAN ZHANG, Boston College, BO YU, GANG CHEN, ZHIFENG REN, Boston College, BOSTON COLLEGE TEAM, MIT TEAM — It is well known that the highest ZT value, at an optimized carrier concentration, is mainly determined by a material parameter $\beta = \mu(m^*/m0)3/2/\kappa lat$, where $\mu(m^*/m0)3/2$ and κlat are the weighted carrier mobility and lattice thermal conductivity, respectively. In order to explore some new compositions in Bi2S3-Bi2Se3-Bi2Te3 system, we propose a compositional thermoelectric phase diagram (TPD), including weighted carrier mobility, lattice thermal conductivity, and material parameter, for the 1% copper doped Bi2S3-Bi2Se3-Bi2Te3 solid solution fabricated by MA-HP method. Here, the $\mu(m^*/m0)3/2$ and κlat values could be deduced from the measured electrical resistivity, Seebeck coefficient, and thermal conductivity. The alloying effect on the thermoelectric phase diagram will be discussed from varying atomic size, chemical bond, lattice structure, etc.

9:48AM Y20.00008 Exploration of effects of various impurities in Bismuth and its extension to Bismuth-Antimony alloys[1] , HYUNGYU JIN, KATHERINE WHITEHOUSE, Department of Mechanical Engineering, The Ohio State University, JOSEPH HEREMANS, Department of Mechanical Engineering and Department of Physics, The Ohio State University — While Te and Se are known donors and Pb and Sn known acceptors in elemental bismuth, little is known about other possible dopants. The effect of various impurities on thermoelectric properties of elemental bismuth is investigated here. Impurities investigated encompass the transition metals, group III and IV elements, and the chalcogens. The thermoelectric power, electrical resistivity and Hall coefficients of Bi samples doped with these impurities are measured from room temperature to 2K. Indium is found to be an acceptor, which is surprising because it is mostly trivalent. A calculation of the band structure subsequently performed at the AGH University of Science and Technology in Cracow reveals that In gives an excess density of states in the valence band. This finding in elemental Bi is extended to the case of bismuth-antimony alloys which have superior thermoelectric efficiency at cryogenic temperatures.

[1]This work is funded by MURI FA9550-10-1-0533.

10:00AM Y20.00009 Thermoelectric properties of Sn1-xEuxTe , YIBIN GAO, JOSEPH HEREMANS, the Ohio State University — SnTe has potential in thermoelectric application for intermediate temperature [1]. However, the figure of merit ZT of SnTe is limited because that it always has a high hole concentration owing to Sn vacancies. As a result, the Seebeck coefficient of SnTe is low and it is very difficult to get SnTe to the optimized doping level required to get a good figure of merit. SnTe also has heavy valence band close to the light valence band edge. We know from theoretical calculations that degenerate bands are preferable than bands separated by an energy difference for thermoelectric application. EuTe has a much higher band gap than SnTe. Recent results [2] show that in Sn1-xEuxTe films prepared by hot-wall epitaxy, the direct L-point bandgap first closes with x, and then opens. In this presentation, we report on the synthesis of bulk Sn1-xEuxTe samples, and report on their Seebeck coefficient, Hall coefficient, resistivity and thermal conductivity. A simplified model is proposed to explain the experimental data. The results confirm the results of the previous study, and point towards the possibility of finding a high-ZT formulation in these compounds. The work is supported by ZTPlus.

[1] V. P. Vedeneev et al., Semiconductors, 32, 241 (1998)
[2] Akihiro Ishida et al., J. Appl. Phys. 107, 123708 (2010)

10:12AM Y20.00010 Incipient Ferroelectricity in Thermoelectric Lead Telluride[1] , EMIL BOZIN, Brookhaven National Laboratory, CHRISTOS MALLIAKAS, Northwestern U, PETROS SOUVATZIS, THOMAS PROFFEN, Los Alamos National Laboratory, NICOLA SPALDIN, ETH Zurich, MERCOURI KANATZIDIS, Northwestern U, SIMON BILLINGE, Brookhaven National Laboratory, Columbia U — PbTe, is the parent compound of currently the most important thermoelectric (TE) materials in applications just above room temperature [1]. It has an anomalously low thermal conductivity resulting in a rather high TE figure of merit. Our neutron total scattering and atomic pair distribution function analysis shows the existence of a novel paraelectric state at and above room temperature. However, on cooling the structural dipoles do not order, but disappear resulting in an undistorted rock-salt ground-state. We suggest that new thermoelectrics should be sought among materials that, like PbTe [2], are close to a ferroelectric instability.

[1] Z.H. Dughaish, Physica B v.322, pp205 (2002).
[2] E.S. Bozin et al, Science (to be published).

[1]US Department of Energy, Division of Basic Energy Sciences

10:24AM Y20.00011 Enhancement of thermoelectric figure-of-merit in a wide temperature range in $In_4Se_{3-x}Cl_y$ bulk crystals , JONG-SOO RHYEE, Kyung Hee University, KYUNGHAN AHN, KYU HYOUNG LEE, Samsung Advanced Institute of Technology, JI HOON SHIM, Pohang University of Science and Technology, JAE HOON KIM, Yonsei University, KYUNG HEE UNIVERSITY TEAM, SAMSUNG ADVANCED INSTITUTE OF TECHNOLOGY COLLABORATION, POHANG UNIVERSITY OF SCIENCE AND TECHNOLOGY COLLABORATION, YONSEI UNIVERSITY COLLABORATION — Recently, we proposed that the charge density wave is a new pathway for high thermoelectric performance in bulk crystalline materials [1,2]. Through the quasi one-dimensional lattice distortion (Peierls distortion) in In_4Se_{3-x} bulk single crystals, we have achieved a high thermoelectric figure-of-merit ZT of 1.48 at 705 K. From the Boltzman transport calculation, it was confirmed that the reported ZT could be further increased if we could increase the chemical potential of the In_4Se_{3-x} crystals. Here we report the significant increase of ZT over a wide temperature range from 50 °C to 425 °C by chlorine doping in the In_4Se_{3-x}, which comes from the improvement of crystal quality and increase of chemical potential, resulting in the power factor enhancement and the thermal conductivity reduction.

[1] J.-S. Rhyee et al., J. Appl. Phys. **105**, 053712 (2009).
[2] Jong-Soo Rhyee et al., Nature (London) **459**, 965 (2009).

10:36AM Y20.00012 Thermoelectricity in the ultra-thin limit[1] , JAYAKANTH RAVICHANDRAN, PIM ROSSEN, VINCENT WU, University of California, Berkeley, ARUN MAJUMDAR, Department of Energy, R. RAMESH, University of California, Berkeley — Hicks and Dresselhaus [1] predicted an enhanced thermoelectric power factor due to quantum confinement. In the past, superlattices have been employed to demonstrate this effect but the results have remained controversial. Sustained efforts on surface termination and treatment of single crystalline oxide substrates has enabled growth of high quality thin films using techniques like pulsed laser deposition and molecular beam epitaxy. In this work, we explore the nature of thermoelectric response for ultra thin layers ($\sim$ 1 – 100 nm) of model thermoelectric oxides such as doped $SrTiO_3$ and $Bi_2Sr_2Co_2O_y$grown by pulsed laser deposition. Thermopower, resistivity and Hall measurements were carried out as a function of thickness to understand the role of quantum confinement and other extraneous effects like surface depletion etc. on the thermoelectric response. References: [1] L.D. Hicks and M. S. Dresselhaus, Phys. Rev. B, 47, 12727 (1993).

[1]This work was supported by the Division of Materials Sciences and Engineering, Department of Energy.

10:48AM Y20.00013 Zero-dimensional nanostructured material with metallic bismuth nanoparticles: a new route for thermoelectrics , ROLAND BENOIT, MONA TREGUER, CNRS, MARIE-LOUISE SABOUNGI — The thermoelectric figure of merit ZT has so far not exceeded the value ZT=3 need to compete with mechanical energy conversion systems. However, theoretical work has shown that it is possible to reach values of ZT higher than this. One of the most promising routes is nanostructured materials, which offer the opportunity to tailor physical properties such as electrical and heat transport, due to the effects of electron filtering and phonon confinement. Dresselhaus *et al. (ref.?)* were among the first to show that 2D and 1D structures are capable of reaching ZT values higher than 2. The thermoelectric materials of current interest are in the form of nanotubes, nanodots and, more generally, superlattices composed of a matrix and nanoparticles. In our work we synthesize a periodic network of bismuth nanoparticles in a matrix of mesoporous SiO_2. We find that in this form bismuth transforms from a rhombohedral to a cubic structure, with improved filtering of electrons and phonons.

Friday, March 25, 2011 8:00AM - 10:48AM –

Session Y21 GIMS: High Magnetic Field Measurements, Novel sensors, and Neutron Diffraction

8:00AM Y21.00001 Stand alone experimental setup for measurements of magnetoresistance tensor by dc reversal technique[1] , ALEXEY SUSLOV, NHMFL-FSU, Tallahassee, Florida 32310, USA — Several years ago Keithley Instruments, Inc. created a combination of a Current Source and a Nanovoltmeter (Model 6221 and Model 2182A, respectively) for low level transport measurements. That nanovoltmeter/ current source combination was designed for measurements of *one* voltage only. Proposed are the setups assembled from several nanovoltmeter/current source pairs which allow to measure simultaneous *several* voltages associated with the same current. The setups utilize specific wiring and a unique triggering sequence. Several milliseconds delays incorporated into triggering sequence secure stable triggering and proper data flow. The delays might be assured by selection of specific time parameters in the current sources and nanovoltmeters. The setups allow utilizing the built-in functions of the devices. Tested setups consisted of up to four pairs, allowing measurements of up to four voltages.[2] Application of the setups to simultaneous measurements of magnetoresistance tensor components will significantly simplify the experiment, increase precision, and decrease consumption of resources.

[1]NHMFL is supported by NSF DMR-0084173, the State of Florida, and the DOE.
[2]A. V. Suslov, Rev. Sci. Instrum. 81, 075111 (2010).

8:12AM Y21.00002 High Magnetic Field Characterization of Cu-Sn Alloys for Distortion-free MRI Probes[1] , M.K.A. PEPRAH, E.S. KNOWLES, M.W. MEISEL, Dept. Physics and NHMFL, Univ. Florida, G.W. ASTARY, T.H. MARECI, Dept. Biochem. and Molecular Biology, Univ. Florida, C.R. FISHER, R.L. STEWART, M.V. MANUEL, Dept. Mat. Sci. and Engineering, Univ. Florida — For a wide-range of reasons, magnetic resonance imaging (MRI) of brain activity is now exploiting miniturized electrodes and cannulas. However, common construction materials such as stainless steel cause significant distortion of the MRI signals.[2] With the goal of developing brain-susceptibility-matched electrodes and cannula for distortion-free MRI in fields up to 11 T, we have investigated the magnetic properties of a spectrum of Cu-Sn alloys. The results of various characterization studies, including SQUID magnetometry up to 7 T and MRI studies up to 11 T, will be reported and related to the stoichiometric composition of the Cu-Sn solutions. Extensions to device development and other metal alloy combinations will be discussed.

[1]Supported by NSF DMR-0701400 (MWM), NSF DMR-0654118 (NHMFL), and NIH R01-NS063360 (THM).
[2]F.M. Martinez-Santiesteban *et al.*, Phys. Med. Biol. **52** (2007) 2073.

8:24AM Y21.00003 Addressing signal recovery challenges in pulsed field environment[1] , FEDOR BALAKIREV, YOSHIMITSU KOHAMA, MOAZ ALTARAWNEH, ROSS MCDONALD, MARCELO JAIME, ALBERT MIGLIORI, CHARLES MIELKE, LANL — We review approaches to recovering weak electric signals in the challenging environment of pulsed magnetic fields implemented at the National High Magnetic Field Laboratory Pulsed Field Facility (NHMFL-PFF). Recent technique developments including AC-specific heat measurements at sub-kelvin temperatures, nanosecond-scale resistivity measurements, as well as customized instrumentation and computer-assisted signal detection using Field Programmable Gate Arrays will be discussed.

[1]Work at NHMFL-LANL is performed under the auspices of the National Science Foundation, Department of Energy and State of Florida.

8:36AM Y21.00004 The National High magnetic Field Laboratory Pulsed Field Facility. An overview of high field magnet operations and scientific techniques[1] , JON BETTS, NHMFL-PFF Los Alamos National Laboratory — The National High magnetic Field Laboratory – Pulsed Field Facility (NHMFL-PFF) is the home to the pulsed field user facility which routinely delivers 85T pulses for user science using a 1.4GW motor generator. The facility also houses a 60T shaped waveform magnet, 65T short pulse and 50T mid pulse capacitor driven magnets. Many techniques are available to users including, Transport, magnetization, calorimeter and cantilever techniques. I will describe the facilities and the measurement techniques available to users.

[1]There work at the NHMFL-PFF was carried out under the auspices of the NSF, DOE and State of Florida.

8:48AM Y21.00005 Extreme Material Physical Properties and Measurements above 100 tesla[1] , CHARLES MIELKE, NHMFL-PFF (LANL) — The National High Magnetic Field Laboratory (NHMFL) Pulsed Field Facility (PFF) at Los Alamos National Laboratory (LANL) offers extreme environments of ultra high magnetic fields above 100 tesla by use of the Single Turn method as well as fields approaching 100 tesla with more complex methods. The challenge of metrology in the extreme magnetic field generating devices is complicated by the millions of amperes of current and tens of thousands of volts that are required to deliver the pulsed power needed for field generation. Methods of detecting physical properties of materials are essential parts of the science that seeks to understand and eventually control the fundamental functionality of materials in extreme environments. De-coupling the signal of the sample from the electro-magnetic interference associated with the magnet system is required to make these state-of-the-art magnetic fields useful to scientists studying materials in high magnetic fields. The cutting edge methods that are being used as well as methods in development will be presented with recent results in Graphene and High-Tc superconductors along with the methods and challenges.

[1]National Science Foundation DMR-Award 0654118

9:00AM Y21.00006 Sub 100 nm ballistic sensors for ultra high spatial resolution magnetic field detection , A.M. GILBERTSON, L.F. COHEN, Imperial College, M. FEARN, T. ASHLEY, QinetiQ, S.A. SOLIN, University of Washington in St. Louis, A. KORMÁNYOS, C.J. LAMBERT, Lancaster University — There is an ongoing drive to develop non-invasive magnetic field sensors with ultra high spatial resolution (UHSR) of 100 nm or less for numerous applications.[1,2] Conventional field sensors e.g. based on the Hall effect, rely on diffusive transport, where high mobility III-V semiconductors offer the best field sensitivity ($T/Hz^{0.5}$).[2] For UHSR, the critical dimensions of the device must be reduced below the mean free path where transport is ballistic, and the detection properties are not preserved, e.g. the Hall response can be suppressed and/or nonlinear. We report sub 100 nm sensors utilizing the negative bend resistance of InSb/InAlSb ballistic structures at elevated temperatures.[3] These devices exhibit an enhanced responsivity that is tunable by geometric design and extremely attractive for the detection of ultra small magnetic fields. Our smallest device studied to date has an active sensor area of 35 x 35 nm^2, and a sensitivity of 0.87 $\mu T/Hz^{0.5}$ at 100 K. The performance and detection properties are reviewed with respect to state-of-the-art technologies.
[1]P. Manandhar, Nanotechnol. 20, 355501 (2009). [2]A. Sandhu, Microelectron. Eng. 73, 524 (2004). [3]A. M. Gilbertson, et al., Submitted to Appl. Phys. Letts. (2010).

9:12AM Y21.00007 dc SQUIDs as displacement detectors for embedded micromechanical resonators , SAMIR ETAKI, Delft University of Technology, MENNO POOT, yale, KOJI ONOMITSU, HIROSHI YAMAGUCHI, NTT basic research laboratories, HERRE VAN DER ZANT, Delft University of Technology — Superconducting quantum interference devices (SQUIDs) can detect tiny amounts of magnetic flux and are also used to study macroscopic quantum effects. We employ a dc SQUID as a linear detector of the displacement of an embedded micromechanical resonator with femtometer sensitivity. We have also measured the backaction of the dc SQUID on the resonator, where the resonance frequency and damping of the resonator can be tuned with bias current and applied magnetic flux. The backaction can tune the resonator from strongly damped to self-sustained oscillation and may be used to cool the resonator.

9:24AM Y21.00008 A Novel Ambient Operating Force and Acceleration Detector , MING YIN, Benedict College, SC 29204, HUAIZHOU ZHANG, MICHAEL WESCOTT, YEUNCHEOL JEONG, JAMES GAMBREL, TIMIR DATTA, Univ of South Carolina, SC 29208 — An investigation to develop a novel accelerometer capable of operating under ambient conditions without any cryogenics is in progress in our laboratory. In this device the proof mass comprises of magnetic or diamagnetic materials. This mass is freely suspended in stable equilibrium under gravity by the combined actions of magnetic attraction and repulsion forces. Stability is achieved along all three Cartesian axes even at zero frequency. For highly dynamical onboard platforms, realtime nulling by active control at high-frequency is desirable. A description of prototypes and measurements will be discussed. Sensitivity in the $\sim$ 0.1ngal regime to both kinematic and gravitational accelerations and $\sim$ pN force resolution is observed. Our initial results including (i) detection of tidal changes in the gravitational background, (ii) seismic tremors, (iii) Fourier analysis of time displacement data and (iv) design considerations for enhanced sensitivity and improved performance will be presented. Several scientific and technological implications will be suggested.

9:36AM Y21.00009 Driving electronics for a z-positioner in a new SPM design.[1] , LEUJEN CHEN, SEONG HEON KIM, ALEX DE LOZANNE, Department of Physics, University of Texas at Austin — We use a modified Pan-type walker as the z coarse approach mechanism in our new SPM design. We developed new electronics for driving and exercising the walker with the main circuit consisting of six 12V relays. Connecting the relays in series produces a timing cascade due to the mechanical delay in each relay. The traditional slow linear ramp has been replaced with the charge and discharge behavior of the RC circuits, where C is the capacitance of the piezolelectric plates. Initial tests with a 6Hz frequency input showed 10 nm step size and a 3 millimeter range. A single 555 timer serves as our frequency generating source. A highly stabilized square wave can be generated in its monostable mode, with the output frequency determined by two external resistors and a capacitor. We also replace the high voltage supply with a voltage quadrupler circuit that is compact and inexpensive, with 64V and 128V DC output in the final configuration.

[1]Supported by NSF DMR-0923231

9:48AM Y21.00010 A unique 30 Tesla single-solenoid pulsed magnet instrument for x-ray studies[1] , ZAHIRUL ISLAM, Advanced Photon Source, Argonne National Laboratory, DANA CAPATINA, JACOB RUFF, RITESH DAS, APS, ANL, HIROYUKI NOJIRI, Institute for Materials Research, Tohoku University, YASUO NARUMI, IMR, TU — We present a dual-cryostat pulsed-magnet instrument at the Advanced Photon Source (APS) with unique capabilities. The dual-cryostat independently cools the solenoid (Tohoku design) using liquid nitrogen and the sample using a closed-cycle refrigerator, respectively. Liquid nitrogen (LN) cooling allows a repetition rate of seven minutes for peak fields of 30 Tesla. The system is unique in that the LN cryostat incorporates a double-funnel vacuum tube passing through the solenoid's bore preserving the entire angular range allowed by the magnet. This scheme is advantageous in that it allows the applied magnetic field to be parallel to the scattering plane complementing typical split-pair magnets with fields normal to the scattering plane. Performance of the coils along with preliminary x-ray diffraction and spectroscopic studies will be presented.

[1]Use of the APS is supported by the U. S. DOE, Office of Science, under Contract No. DE-AC02-06CH11357. The work was supported in part by ICC-IMR, Tohoku University.

10:00AM Y21.00011 Applications of superconducting trapped field magnets for x-ray scattering experiments[1] , R.K. DAS, Z. ISLAM, J.P.C. RUFF, J.C. LANG, Argonne National Lab, R.P. SAWH, R. WEINSTEIN, University of Houston — Two long standing problems in x-ray and neutron scattering studies in applied magnetic fields are, 1) limited optical access and 2) practical impossibility to apply magnetic field parallel to x-ray (neutron) momentum transfer. In order to overcome these obstacles we have developed an application of Type-II superconducting magnets. In this approach, a small and thin plate-like single crystal sample is mounted on the surface of a melt-textured superconductor (SC). The SC is magnetized by cooling it from temperature above its superconducting critical temperature (T_c) in an applied magnetic field. Below T_c, magnetic flux gets trapped inside the SC disk after the removal of the external magnetic field. The SC disk acts as a permanent magnet with applied field normal to the flat surface of the disk providing unrestricted optical access to the entire hemisphere allowing a magnetic field parallel to the x-ray momentum transfer.

[1]Use of the APS is supported by the DOE, Office of Science, under Contract No. DE-AC02-06CH11357.

10:12AM Y21.00012 ABSTRACT WITHDRAWN –

10:24AM Y21.00013 Efficient conversion of ^{3}He(n,tp) and ^{10}B(n,α^7Li) reaction energies into far-ultraviolet radiation by noble gas excimers , PATRICK P. HUGHES, MICHAEL A. COPLAN, University of Maryland, ALAN K. THOMPSON, ROBERT E. VEST, National Institute of Standards and Technology, CHARLES W. CLARK, Joint Quantum Institute, National Institute of Standards and Technology and University of Maryland — Previous work[1,2]showed that the ^{3}He(n,tp) reaction in a cell of ^{3}He at atmospheric pressure generated tens of far-ultraviolet (FUV) photons per reacted neutron. Here we report amplification of that signal by factors of 1000 when noble gases are added to the cell. Calibrated filter-detector measurements show that this large signal is due to noble-gas excimer emissions, and that the nuclear reaction energy is converted to FUV radiation with efficiencies of up to 30%. Our results have been placed on an absolute scale through calibrations at the NIST SURF III Synchrotron and Center for Neutron Research.[3] We have also seen large neutron-induced FUV signals when the ^{3}He gas in our system is replaced with a ^{10}B film target; an experiment on substituting ^{3}He with BF_3 is underway. Our results suggest possibilities for high-efficiency, non-^{3}He neutron detectors as an alternative to existing proportional counters. [1]A. K. Thompson, *et al., J. Res. Natl. Inst. Stand. Technol.* **113**, 69 (2008) [2]M. A. Coplan, A. K. Thompson and C. W. Clark, U.S. Patent No. 7,791,045 (2010) [3]P.P. Hughes, *et al.,* arXiv:1009.4707 (*Appl. Phys. Lett.* in press, 2010)

10:36AM Y21.00014 First Results from the Triple-axis Spectrometer at OPAL , SERGEY DANILKIN, MOHANA YETHIRAJ, THOMAS SAERBECK, FRANK KLOSE, Australian Nuclear Science and Technology Organization — The thermal triple-axis spectrometer TAIPAN is the first instrument for inelastic scattering at Australian research reactor OPAL. TAIPAN started operation in February 2009 and is in full user service since November 2010. The instrument can operate with variable incident or final energies and has a secondary spectrometer with a single detector. Presently the PG (002) double-focusing monochromator and analyzer are in use. The incident energy range on the TAIPAN is from $\sim$ 5 meV up to $\sim$ 100 meV with neutron flux at sample position of $\sim 10^8 \mathrm{n/cm^2/s}$ [1]. First experiments were performed with superionic conductor $Cu_{2-x}Se$ [2]. The measurements reveal a presence of soft mode in addition to the flat optic-like phonon branch. The DFT calculations show that unstable soft mode is related to ordering of Cu atoms followed by $\alpha - \beta$ phase transition at a lower temperature. The evolution of the magnetic structure with temperature in magnetically modulated $FePt_3$ thin film was investigated in the diffraction mode of TAIPAN. The results show that the film fabricated by modulation of the chemical order parameter consists of a magnetic FM/AFM superlattice in single-crystalline $FePt_3$ [3]. [1] S.A. Danilkin et al., Neutron News, 20 (2009) 37; [2] S.A. Danilkin et al., J. Phys. Soc. Jpn. 79 (2010) Suppl. A, 25; [3] T. Saerbeck et al., Phys. Rev. B 82 (2010) 134409.

Friday, March 25, 2011 8:00AM - 11:00AM –
Session Y22 DCMP: Ferroelectric and Structural Phase Transitions D163

8:00AM Y22.00001 Magnetic and magnetoelectric excitations in multiferroic $BiFeO_3$, DIYAR TALBAYEV, Yale University, STUART A. TRUGMAN, ANTOINETTE J. TAYLOR, Los Alamos National Laboratory, SEONGSU LEE, SANG-WOOK CHEONG, Rutgers University — Ferroelectric antiferromagnet $BiFeO_3$ combines ferroelectricity with an antiferromagnetic order at room temperature. A control of its magnetic state by voltage has been demostrated both in bulk and in thin film $BiFeO_3$. The distortion of the cubic perovskite lattice leads to two effects through the Dzyaloshinski-Moriya magnetic interaction: the ferroelectric distortion results in the observed incommensurate spiral spin structure, and the rotation of oxygen octahedra with alternating sense on neighboring Fe ions results in a local canting of spins. We present a terahertz spectroscopic study of magnetic excitations in $BiFeO_3$. We interpret the observed spectrum of long-wavelength magnetic resonance modes in terms of the normal modes of the material's spiral antiferromagnetic structure. We find that the modulated Dzyaloshinski-Moriya interaction and the local spin canting lead to a splitting of the out-of-plane resonance modes. We also assign one of the observed absorption lines to an electromagnon excitation that results from the magnetoelectric coupling between the ferroelectric polarization and the spiral magnetic structure of $BiFeO_3$.

8:12AM Y22.00002 Size-dependent infrared phonon modes and ferroelectric phase transition in $BiFeO_3$ nanoparticles[1] , PENG CHEN, XIAOSHAN XU, CHRISTOPHER KOENIGSMANN, ALEXANDER C. SANTULLI, STANISLAUS S. WONG, JANICE L. MUSFELDT, University of Tennessee — One emergent property of ferroelectric nanoparticles is the sized-induced structural distortion to a high-symmetry paraelectric phase at small particle sizes. Finite length scale effects can thus be advantageously employed to elucidate ferroelectric transition mechanisms. In this work, we combine infrared spectroscopy with group theory and lattice dynamics calculations to reveal the displacive nature of the ferroelectric transition in $BiFeO_3$, a room temperature multiferroic. Systematic intensity and frequency trends in selected vibrational modes show that the paraelectric phase is $Pm\bar{3}m$ and the lowest frequency A_1 feature is the soft mode that drives the first order transition. Finite length scale effects are also evident in the electronic structure with a red shifted band gap in nanoscale $BiFeO_3$ compared with that of the rhombohedral film, a result that can impact the development of ferroelectric photovoltaics and oxide- based electronics. Taken together, these findings demonstrate the foundational importance of size effects for enhancing the rich functionality and broad utility of transition metal oxides.

[1]This work is supported by the U.S. Department of Energy.

8:24AM Y22.00003 Remarkably robust ferroelectric state in multiferroic $Mn_{1-x}Zn_xWO_4$, B. LORENZ, R.P. CHAUDHURY, Y.Q. WANG, Y.Y. SUN, C.W. CHU[1], Dept. of Physics and TCSUH, Univ. of Houston, Houston, TX 77204-5002, F. YE, H.A. MOOK, Neutron Scattering Science Division, ORNL, Oak Ridge, TN 37831, J.A. FERNANDEZ-BACA, Dept. of Physics and Astronomy, Univ. of Tennessee, Knoxville, TN 37996 — Zinc doping in $Mn_{1-x}Zn_xWO_4$ is equivalent to the removal of Mn spins and a dilution of the magnetic system. The multiferroic (ferroelectric) phase of $MnWO_4$ is stabilized through Zn substitution and the low-temperature commensurate phase (up-up-down-down phase) is completely suppressed at a Zn concentration of more than 5%. The magnetic and ferroelectric phases as well as the multiferroic properties are studied through magnetic, heat capacity, polarization, and neutron scattering experiments. The multiferroic phase is remarkably stable and it still exists for Zn substitution levels up to and above 50%. At low doping (2%) the incommensurate helical and the commensurate low-T phases coexist. External magnetic fields do lift the phase degeneracy and stabilize either one of the two ground states, depending on the direction of the field.

[1]also at: LBNL, Berkley, CA 94720

8:36AM Y22.00004 Ferroelectricity in $CaTiO_3$ Single Crystal Surfaces and Thin Films and Probed by Nonlinear Optics and Raman Spectroscopy , EFTIHIA VLAHOS, TOM LUMMEN, RYAN HAISLMAIER, SAVA DENEV, CHARLES BROOKS, The Pennsylvania State University, MICHAEL BIEGALSKI, Oak Ridge National Lab, DARRELL SCHLOM, Cornell University, CARL-JOHAN EKLUND, KARIN RABE, Rutgers University, CRAIG FENNIE, Cornell University, VENKATRAMAN GOPALAN, The Pennsylvania State University — Bulk $CaTiO_3$ has a centrosymmetric point group and is *not* polar or ferroelectric. However, we present surprising results that show highly regular polar domains in single crystals of $CaTiO_3$. Confocal Second Harmonic Generation (SHG) and Raman imaging studies were carried out on perovskite $CaTiO_3$ crystal surfaces. They reveal large, crystallographic polar domains at room temperature, with in-plane polarization components delineated by twin walls. SHG analysis indicates that the highest symmetry of the polar surface is m(space group Pc) with polarization in the m plane. In addition, we present results of the polar domain structure imaged before and after the application of an external electric field. Finally, we present the SHG studies of $CaTiO_3$ thin films grown using reactive Molecular Beam Epitaxy (MBE); these films are predicted by theory to be ferroelectric and are shown experimentally, both with SHG and in-plane dielectric measurements, to be ferroelectric for temperatures less than $\sim$150 K with group symmetry *mm*2.

8:48AM Y22.00005 Phase transitions in relaxors as seen by neutron scattering , SEVERIAN GVASALIYA, Laboratorium für Festkörperphysik, ETH Hönggerberg, Zürich, Switzerland, ROGER COWLEY, Clarendon Laboratory, Physics Department, Oxford University, UK, SERGEY LUSHNIKOV, Ioffe Physico-Technical Institute, St Petersburg, Russia, BERTRAND ROESSLI, Laboratory for Neutron Scattering, Paul Scherrer Institut, Villigen PSI, Switzerland, GELU-MARIUS ROTARU, Empa, Laboratory for Protection and Physiology, St Gallen, Switzerland — Relaxors have a broad temperature and frequency-dependent peak in the dielectric permittivity that is not necessarily linked to a structural phase transition. A model relaxor is $PbMg_{1/3}Nb_{2/3}O_3$ (PMN) doped with $PbTiO_3$ (PT). We report neutron studies of the low-energy spectra of (1-x)PMN-xPT crystals. Apart from phonons which do not show a soft mode, there are two components of the diffuse scattering: one is quasi-elastic (QE) and the other static. The energy width of the QE scattering decreases as the peak of the susceptibility is approached. The static component behaves like an order parameter. In the crystals that become ferroelectric it is maximal at the ferroelectric phase transition, but in PMN it steadily increases on cooling. We discuss previously reported and new results in terms of a random-field model of the cubic crystal.

9:00AM Y22.00006 ABSTRACT WITHDRAWN –

9:12AM Y22.00007 Elastic collapse and avalanche criticality near a Mott transition[1] , J.L. SMITH, D.J. SAFARIK, J.C. LASHLEY, Los Alamos, E.K.H. SALJE, Cambridge, C.P. OPEIL, Boston College, P.S. RISEBOROUGH, Temple University — We study some dynamic aspects of a Mott transition in a rare-earth alloy $Ce_{0.90}Th_{0.10}$ by resonant-ultrasound spectroscopy (RUS), electrical-transport, and thermal-expansion measurements. In the temperature range spanning the first-order transition, we observe a stiffening of the elastic response that is associated with a continuous front propagation ($e.g.$ solitons). A defining characteristic of a mixed phase regime, slow scanning rates (0.01 K/min) show these solitons to be superimposed with jerks and avalanches in all three data sets: RUS, resistivity, and thermal expansion data. Analysis of the avalanche data give power law distributions with critical exponents $P(E) = E^n$ for energy, in the case of thermal expansion data and length, in the case of electrical transport data.

[1]Work performed under the auspices of the U.S. Dept. of Energy.

9:24AM Y22.00008 Calculated temperature dependence of elastic constants and phonon dispersion of hcp and bcc beryllium[1] , STEVEN HAHN, Ames Laboratory and Iowa State University, SERGIU ARAPAN, Uppsala University, BRUCE HARMON, Ames Laboratory and Iowa State University, OLLE ERIKSSON, Uppsala University — Conventional first principle methods for calculating lattice dynamics are unable to calculate high temperature thermophysical properties of materials containing modes that are entropically stabilized. In this presentation we use a relatively new approach called self-consistent *ab initio* lattice dynamics (SCAILD) to study the hcp to bcc transition (1530 K) in beryllium. The SCAILD method goes beyond the harmonic approximation to include phonon-phonon interactions and produces a temperature-dependent phonon dispersion. In the high temperature bcc structure, phonon-phonon interactions dynamically stabilize the N-point phonon. Fits to the calculated phonon dispersion were used to determine the temperature dependence of the elastic constants in the hcp and bcc phases.

[1]Work at the Ames Laboratory was supported by the Department of Energy-Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

9:36AM Y22.00009 Influence of the Magnetic State on the Chemical Order-Disorder Transition Temperature in Fe-Ni Permalloy , MARCUS EKHOLM, Linköping University, Sweden, HELENA ZAPOLSKY, Université de Rouen, France, ANDREI RUBAN, Royal Institute of Technology, Sweden, IRYNA VERNYHORA, DENIS LEDUE, Université de Rouen, France, IGOR ABRIKOSOV, Linköping University, Sweden, LINKÖPING UNIVERSITY, SWEDEN TEAM, UNIVERSITÉ DE ROUEN, FRANCE TEAM, ROYAL INSTITUTE OF TECHNOLOGY, SWEDEN TEAM — In magnetic alloys, the effect of finite temperature magnetic excitations on phase stability below the Curie temperature is poorly investigated, although many systems undergo phase transitions in this temperature range. In this study [1], we consider random Ni-rich Fe-Ni alloys, which undergo chemical order-disorder transition approximately 100 K below their Curie temperature, to demonstrate from *ab-initio* calculations that deviations of the global magnetic state from ideal ferromagnetic order due to temperature induced magnetization reduction have a crucial effect on the chemical transition temperature. We propose a scheme where the magnetic state is described by partially disordered local magnetic moments, which in combination with Heisenberg Monte-Carlo simulations of the magnetization allows us to reproduce the transition temperature in good agreement with experimental data. [1] Ekholm et al., Phys. Rev. Lett. 105:167208 (2010)

9:48AM Y22.00010 Structural and magnetic properties of Ni_2MnGa from first-principles , VAMSHI KATUKURI, BURAK HIMMETOGLU, MATTEO COCOCCIONI, CEMS University of Minnesota — Ni_2MnGa is the prototype magnetic shape-memory alloy. In this work we use ab-initio calculations to characterize structural and magnetic transitions and to identify possible strategies to tune them towards the same critical point. To this aim both the austenite and the martensite phases of the Ni_2MnGa alloy are studied with particular attention to the electronic factors controlling their stability and the onset of the structural transition. Our results indicate that, in spite of its metallic character, electronic correlations play an important role in determining the behavior of this compound and, in particular, the entity (and sign) of the deformation accompanying the transition from the austenite phase to the martensite one. The vibrational properties of the austenite phase are also studied and structural instabilities (soft modes) are investigated as possible signatures of intermediate "modulated" structures.

10:00AM Y22.00011 ABSTRACT WITHDRAWN –

10:12AM Y22.00012 Origin of "aging" in shape-memory alloys , XIANGDONG DING, Los Alamos National Laboratory, JUNKAI DENG, Xi'an Jiaotong University,China, TURAB LOOKMAN, AVADH SAXENA, Los Alamos National Laboratory, XIAOBING REN, National Institute for materials science, Japan — For more than half a century it has been widely observed that a majority of shape-memory alloys exhibit a gradual change in physical properties with time in the martensitic phase, and this is referred to as "aging." However, its microscopic mechanism has remained controversial due to lack of experiments that can probe atomic level processes. We clarify the atomic mechanism for how shape memory alloys "age" in time using a combination of molecular dynamics and Monte-Carlo simulations. Through analysis of the atomic configurations during aging, we find that the observed phenomenon is associated with a gradual change in the short range order of point defects so that the defect short range order tends to adopt the same "symmetry" as the crystal symmetry of the host martensite lattice. The results provide atomic-level evidence for the symmetry-conforming short-range order model, and may provide new insight into how to control aging to design aging-free shape memory alloys. Reference: 1). J. Deng, X. Ding, T. Lookman, et al, Physical Review B , **81**, 220101(R), 2010 2). J. Deng, X. Ding, T. Lookman, et al, Physical Review B, **82**,184101, 2010 3). J. Deng, X. Ding, T. Lookman, et al, Applied Physics Letters, **97**,171902, 2010

10:24AM Y22.00013 Microstructure from ferroelastic transitions using strain pseudospin clock models in two and three dimensions , TURAB LOOKMAN, Los Alamos National Laboratory, ROMAIN VASSEUR, Ecole Normale Superieur, Paris, SUBODH SHENOY, School of Physics, University of Hyderabad — We show how microstructure can arise in first-order ferroelastic structural transitions, in two and three spatial dimensions, through a local mean-field approximation of their pseudospin Hamiltonians, that include anisotropic elastic interactions. Such transitions have symmetry-selected physical strains as their order parameters, with Landau free energies that have a single zero-strain "austenite" minimum at high temperatures, and spontaneous-strain "martensite" minima of structural variants at low temperatures. The total free energy also has gradient terms, and power-law anisotropic effective interactions, induced by "no-dislocation" St Venant compatibility constraints. In a reduced description, the strains at Landau minima induce temperature dependent, clocklike Hamiltonians, with strain- pseudospin vectors S pointing to discrete values including zero. We study elastic texturing in five such first-order structural transitions through a local mean-field approximation of their pseudospin Hamiltonians, that include the power-law interactions. The local mean-field solutions in 2D and 3D yield or oriented domain- wall patterns as from continuous-variable strain dynamics, showing the discrete- variable models capture the essential ferroelastic texturings.

10:36AM Y22.00014 Symmetry breaking in amorphous solids undergoing martensitic phase transformation - a relation to Landau's theory , MICHAEL FISCHLSCHWEIGER, Materials Center Leoben Forschung, EDUARD OBERAIGNER, University of Leoben, Institute of Mechanics — Martensitic phase transformation can be classified as displacive solid -solid phase transformations, where the symmetry of the high temperature phase (austenite) breaks when phase transformation occurs. The martensitic phase (low temperature phase) and its variants are products of symmetry breaking in solids. Based on a quasiparticle statistical mechanics approach the canonical free energy of a representative solid volume element consisting of several quasiparticles (representative mole number) can be derived. The symmetry breaking order parameter of the system is the total strain which is an ensemble mean value in the statistical mechanics concept. In the current theory the order parameter is a macroscopic strain in a sense that the representative volume element stands for the macroscopic level, whereas the lattice parameter changes are considered in the hamiltonian definition of each quasiparticle. Computational results of the developed theory correspond to experimentally observed phenomena in materials undergoing martensitic phase transformation. The present study is focusing the region nearby the phase transformation and shows how the developed theory for describing symmetry breaking and order parameter changes correspond to Landau's phenomenological theory of phase transitions.

10:48AM Y22.00015 Probing driven first order structural transitions with resistivity noise , U. CHANDNI, ARINDAM GHOSH, Indian Institute of Science — We study the avalanche-mediated driven first order structural transition in nickel titanium shape memory alloys with time-dependent fluctuations in electrical resistivity. Higher order statistics of the fluctuations, or noise, has been used as a kinetic detector of the underlying two stage athermal phase transition. We have found that the non-gaussian component of the higher order statistics carries significant information about the transition parameters and is coupled to the microscopic origin of the phase transition. The results can be explained with a model based on three competing time scales dependent on avalanche relaxation, thermal fluctuations and drive rate. The transition temperature was found to decrease with increasing drive rate indicative of the increased possibility of the system being driven towards the athermal limit. Moreover, the magnitude of the non-gaussian component is found to have signatures of the extent of correlations in the system and hence a viable tool to detect any overlap of avalanches in space or time. The study establishes noise as a sensitive tool to probe the kinetics of driven structural transitions which can be exploited in a variety of other systems. References: U. Chandni et. al, Phys. Rev. Lett. 102, 025701 (2009) U. Chandni and A. Ghosh, Phys. Rev B. **81**, 134105 (2010)

Friday, March 25, 2011 8:00AM - 10:36AM –
Session Y23 DCMP: Superconductivity: Proximity Effects D165

8:00AM Y23.00001 Supercurrent-Induced Magnetization Dynamics , JACOB LINDER, Department of Physics, NTNU, TAKEHITO YOKOYAMA, Department of Physics, Tokyo Institute of Technology — We investigate supercurrent-induced magnetization dynamics in a Josephson junction with two misaligned ferromagnetic layers, and demonstrate a variety of effects by solving numerically the Landau-Lifshitz-Gilbert equation. In particular, we demonstrate the possibility to obtain supercurrent-induced magnetization switching for an experimentally feasible set of parameters, and clarify the favorable condition for the realization of magnetization reversal. These results constitute a superconducting analogue to conventional current-induced magnetization dynamics and indicate how spin-triplet supercurrents may be utilized for practical purposes in spintronics.

8:12AM Y23.00002 Superfluid Densities in Superconducting/Ferromagnetic (Nb/NiV/Nb) Heterostructures , MICHAEL HINTON, BRIAN PETERS, ADAM HAUSER, Ohio State University, JULIA MEYER, OSU & INAC/SPSMS, CEA, FENGYUAN YANG, THOMAS LEMBERGER, Ohio State University — Superfluid density measurements allow us to probe the superconducting structure of thin films below T_c with remarkable detail. They yield information not only of the inherent robustness of the superconducting state, but also about the homogeneity of the sample and possible "hidden" transitions at temperatures lower than the initial T_c. For this reason multiple transitions in superconducting heterostructures are revealed to us. We use superfluid density measurements on $Nb/Ni_{0.95}V_{0.05}/Nb$ trilayers to study the interplay between two superconducting films separated by the destructive proximity effects of a ferromagnet. We show there are trilayers with strong coupling, which produces a single transition, that become decoupled to the point of separation into two transitions as the ferromagnetic layer thickness increases. We discuss the difficulties in observing the second transition in σ_1, while obvious in λ^{-2}.

8:24AM Y23.00003 Magnetic-state-controlled proximity effect across high-T_C superconductor/ferromagnetic interfaces.[1] , C. VISANI, C. DERANLOT, R. BERNARD, K. BOUZEHOUANE, J. BRIATICO, J.E. VILLEGAS, Unité Mixte de Physique CNRS/Thales, 1 avenue A. Fresnel, 91767 Palaiseau, France — We have investigated the electronic density of states of a ferromagnet (F: a Co/Pt superlattice) in contact with a c-axis YBCO film. This was done by measuring the current-perpendicular-to-plane differential conductance across vertical junctions of area down to 6 μm^2, which were fabricated using optical lithography and ion etching. We have found salient features of the leakage of the superconducting order parameter into the F layer, such as a zero-bias conductance peak which can be modulated by the magnetic state of the ferromagnet. We discuss the possibility of triplet superconducting correlations induced in the F layer as the origin of this behavior.

[1]Work supported by RTRA "Triangle de la Physique" "SUPRASPIN" and ANR "Superhybrids-II."

8:36AM Y23.00004 Long-Range Superconducting Proximity Effect in Template-Fabricated Single-Crystal Nanowires[1] , WENHAO WU, Texas A&M University, HAIDONG LIU, Intel Corporation, ZHIYUAN WEI, ISABEL SCHULTZ, Texas A&M UNiversity — We study a superconducting proximity effect observed in single-crystal nanowires of Zn, Sn, and Pb of length up to 60 μm. These nanowires are electrochemically deposited into the pores of anodic aluminum oxide membranes and polycarbonate membranes. Using an *in situ* self-contacting method, single nanowires are electrically contacted on both ends to a pair of macroscopic film electrodes of Au, Sn, or Pb pre-fabricated on both surfaces of the membranes. Superconductivity in the nanowires is strongly suppressed when Au electrodes are used. When electrodes having higher superconducting transition temperatures are used, the nanowires become superconducting at the transition temperatures of the electrodes. Microscopy analyses of the structure and the chemical composition of the nanowires will be presented. Measurements of sample resistance and $I-V$ characteristics at various temperatures and magnetic fields will also be presented. Furthermore, the effects of the length, the diameter, and the residual resistance ratio of the nanowires on the proximity induced superconductivity will be analyzed and discussed.

[1]Supported by NSF DMR-0551813 and DMR-0606529.

8:48AM Y23.00005 Radiative Interband Transition of Cooper Pairs in a Semiconductor , I. SUEMUNE, Y. ASANO, H. SASAKURA, C. HERMANNSTAEDTER, J.-H. HUH, Hokkaido Univ, K. TANAKA, Hamamatsu Photonics, T. AKAZAKI, NTT BRL, R. INOUE, H. TAKAYANAGI, Tokyo Univ of Science, H. KUMANO, Hokkaido Univ — Interactions of photons and superconductors have been a hot topic for superconducting (SC) qubit operations. The relevant photon energies were limited below the superconducting gap of superconductors, that is, microwave frequencies. The possibility of electron Cooper-pair interactions with photons with much higher energies was discussed theoretically [1]. In this talk we will demonstrate that Cooper pairs penetrated into a semiconductor from an adjacent superconductor by the proximity effect play a major role in interband radiative recombinations in the semiconductor experimentally. SC Nb electrodes were formed on an InGaAs/InP light emitting diode (LED) and electroluminescence (EL) around 1.55um was observed from a slit formed on the surface Nb electrode. EL was drastically enhanced below the Nb SC critical temperature (T_c) of ∼8K [2]. The reduction of radiative recombination lifetime consistent with the observed EL enhancement was observed below T_c[3]. These results are well explained with the theory [1]. We will discuss the possibility of generating entangled photon pairs based on this new scheme. [1] Y. Asano et al., PRL 103 (2009) 187001. [2] Y. Hayashi et al., Appl. Phys. Express 1 (2008) 011701. [3] I. Suemune et al., APEX 3 (2010) 054001.

9:00AM Y23.00006 Robustness of Majorana modes and minigaps in a spin-orbit-coupled semiconductor-superconductor heterostructure , LI MAO, CHUANWEI ZHANG, Department of Physics and Astronomy, Washington State University — We study the robustness of Majorana zero energy modes and minigaps of quasiparticle excitations in a vortex by numerically solving Bogoliubov-deGennes equations in a heterostructure composed of an *s* -wave superconductor, a spin-orbit-coupled semiconductor thin film, and a magnetic insulator. This heterostructure was proposed recently as a platform for observing non-Abelian statistics and performing topological quantum computation. The dependence of the Majorana zero energy states and the minigaps on various physics parameters (Zeeman field, chemical potential, spin-orbit coupling strength) is characterized. We find the minigaps depend strongly on the spin-orbit coupling strength. In certain parameter region, the minigaps are linearly proportional to the *s*-wave superconducting pairing gap Δ_s, which is very different from the Δ_s^2 dependence in a regular *s*- or *p*-wave superconductor. We characterize the zero energy chiral edge state at the boundary and calculate the STM signal in the vortex core that shows a pronounced zero energy peak. We show that the Majorana zero energy states are robust in the presence of various types of impurities. We find the existence of impurity potential may increase the minigaps and thus benefit topological quantum computation.

9:12AM Y23.00007 Topological superconductivity and Majorana fermions in half-metal / superconductor heterostructure[1] , SUK BUM CHUNG, HAI-JUN ZHANG, XIAO-LIANG QI, SHOUCHENG ZHANG, Stanford University — A half-metal is by definition spin-polarized at its Fermi level and therefore was conventionally thought to have little proximity effect to an s-wave superconductor. Here we show that if there is spin-orbit coupling at the interface between a single-band half-metal and an s-wave superconductor, $p_x + ip_y$ superconductivity would be induced on the half-metal. This can give us topological superconductor with a single chiral Majorana edge state. We show that two atomic layers of CrO_2 or CrTe gives us the single-band half-metal and is thus a candidate material for realizing this physics.

[1]This work is supported by DOE under contract DE-AC02-76SF00515, the Sloan Foundation, and NSF under grant number DMR-0904264

9:24AM Y23.00008 Superconducting proximity effects of Pb nano-islands[1] , JUNGDAE KIM, GREGORY FIETE, HYOUNGDO NAM, ALLAN MACDONALD, CHIH-KANG SHIH, Department of Physics, The University of Texas at Austin, Austin, Texas 78712 — Superconductivity in systems with spatial dimensions smaller than the coherence length has been the subject of intense interest for decades. We systematically address how superconducting nano-islands interact each other via a detailed scanning tunneling microscopy/spectroscopy (STM/STS). By measuring the spatial mapping of the local superconducting gap, an intriguing lateral proximity effect is observed in an island containing regions of different thicknesses and different superconducting strength which shows a gradual but evident change of local superconductivity at the thickness boundary. This must be due to a lateral proximity effect caused by the tunneling of Cooper pairs with different binding energies across the boundary. We were also able to experimentally determine a proximity length. When an island is smaller than the proximity length, it is found that superconductivity within the island is rather uniform, indicating the rigidity of the order parameter on the scale of proximity length.

[1]NSF grant DMR-0906025, CMMI-0928664, Welch Foundation F-1672, and Texas Advanced Research Program 003658-0037-2007

9:36AM Y23.00009 S -N-S junction formed by graphene with lead (Pb) contacts , IVAN BORZENETS, Duke University, ULAS COSKUN, University of Illinois , GLEB FINKELSTEIN, Duke University — We fabricate lead (Pb) contacts to graphene that allow us to observe supercurrent in the Pb-graphene-Pb structure up to temperatures of ∼3K. The measured critical current is much smaller than a naive expectation based on calculations for a superconductor-insulator-superconductor (S-I-S) junction. Hysteresis is seen in the switching current despite the fact that the junction is made to be overdamped. The behavior of the Pb-graphene-Pb structure is qualitatively explained by considering it as an S-N-S junction.

9:48AM Y23.00010 Switching and retrapping behavior in graphene proximity-effect superconducting junctions , MATTHEW BRENNER, ULAS COSKUN, ALEXEY BEZRYADIN, University of Illinois Physics — Since the pioneering work by R. Holm and W.Meissner [Z. Physik. 86, 787 (1933)], who observed zero resistance in SNS pressed contacts, many manifestations of the superconducting proximity effect have been reported. Recently it was shown that when closely spaced superconducting leads are placed on graphene, the proximity effect is induced and a supercurrent can flow between the electrodes. Here we fabricate graphene proximity-effect junctions (GPJ) and compare them to Josephson junctions (JJ). As the bias current is increased to near the critical current, a thermal escape from the washboard potential can occur driving the junction into the runaway voltage state. The standard deviation of the switching current is measured as a function of temperature and compared to the thermal and quantum escape models for JJs. We find that the temperature dependence of the standard deviation of switching currents of graphene proximity junctions is qualitatively different from the well-studied behavior of the insulator-based JJs. Possible reasons will be discussed.

10:00AM Y23.00011 Interface Engineering of Thin Film Superconductor Heterostructures[1] , CHENDONG ZHANG, Department of Physics, UT Austin; Institute of Physics, CAS, JISUN KIM, JUNGDAE KIM, HYOUNGDO NAM, Department of Physics, UT Austin, HONGJUN GAO, Institute of Physics, CAS, CHIH-KANG SHIH, Department of Physics, UT Austin — Thin film superconductivity is a subject with great scientific and technological importance. The previous works demonstrated that the superconductivity exits in extreme two-dimensional lead film with a thickness of only two atomic layers. Most strikingly, the Tc is only slightly suppressed from the bulk value. However, when the film is pseudomorphically strained, the Tc is suppressed further, implying the importance of the interface. In this work we explore thin film superconductivity in a new direction by engineering superconductor/normal metal heterostructures with atomically flat interface. Using in-situ scanning tunneling microscopy/spectroscopy, we explore the superconductivity of the Pb/Ag heterostructure by independently tuning the thicknesses of the atomically flat Ag films and superconducting Pb films respectively. The intriguing role of the Ag thin films on the superconductivity of Pb thin films will be reported.

[1]NSF grant DMR-0906025, CMMI-0928664, Welch Foundation F-1672, and Texas Advanced Research Program 003658-0037-2007

10:12AM Y23.00012 Tunneling Measurements of the Exchange Field in Superconducting Al-EuS Bilayers[1] , PHILIP ADAMS, YIMIN XIONG, SHANE STADLER, Louisiana State U., GIANLUIGI CATELANI, Yale University — We present tunneling density of states measurements of the proximity-induced exchange field in superconducting Al-EuS bilayers. By depositing thin Al films onto an insulating EuS layer we demonstrate that one can induce an exchange field of several tesla in the superconducting Al. Contrary to expectations, this exchange field is a strong function of the applied field below 2 T. This applied-field dependence is not associated with the alignment of domains in the EuS, but instead appears to be an intrinsic effect. In addition, we show that the exchange field decreases significantly with increasing temperature below 1 K.

[1]Supported by DOE under grant DE-FG02-07ER46420

10:24AM Y23.00013 Exploring the Parameter Space of the Anti-Proximity Effect[1] , MEENAKSHI SINGH, JIAN WANG, MINGLIANG TIAN, Physics Department, Penn State University, THOMAS MALLOUK, Chemistry Department, Penn State University, MOSES CHAN, Physics Department, Penn State University — The anti-proximity effect, in which the superconductivity of a nanowire is weakened by the superconductivity of measuring bulk electrodes, has been reported in Zn nanowires (Tian et. al., PRL 95, 076802 (2005), Chen et. al., PRL 103, 127002 (2009)). The mechanism of this effect is not completely understood. We have studied the anti-proximity effect in Al nanowires in a variety of configurations. The effect is found to manifest only when the critical temperature (T_c) of the nanowire is greater than the T_c of its bulk form. The range of the effect is found to be $\sim 1\mu$m. The effect is seen in single nanowires in the absence of a magnetic field establishing that the effect depends on the nature of the measuring electrodes and is not caused by an external magnetic field. The anti-proximity effect has also been seen with the bulk superconductor not connected to the measurement circuitry.

[1]This work was funded by NSF grant number DMR-0820404.

Friday, March 25, 2011 8:00AM - 11:00AM –
Session Y24 DCOMP: Density Functional Theory II D167

8:00AM Y24.00001 Exact Exchange calculations for periodic systems: a real space approach , AMIR NATAN, NOA MAROM, ADI MAKMAL, LEEOR KRONIK, Weizmann Institute of Science, Israel, STEPHAN KUEMMEL, Bayreuth University, Germany — We present a real-space method for exact-exchange Kohn-Sham calculations of periodic systems. The method is based on self-consistent solutions of the optimized effective potential (OEP) equation on a three-dimensional non-orthogonal grid, using norm conserving pseudopotentials. These solutions can be either exact, using the S-iteration approach, or approximate, using the Krieger, Li, and Iafrate (KLI) approach. We demonstrate, using a variety of systems, the importance of singularity corrections and use of appropriate pseudopotentials.

8:12AM Y24.00002 Dissociation of diatomic molecules and the exact-exchange Kohn-Sham potential: the case of LiF , ADI MAKMAL, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel, STEPHAN KUEMMEL, Physikalisches Institut, Universitat Bayreuth, D-95440 Bayreuth, Germany, LEEOR KRONIK, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel — The incorrect fractional-charge dissociation of stretched diatomic molecules, predicted by semi-local exchange-correlation functionals, is revisited. This difficulty can be overcome with asymptotically correct non-local potential operators, but should also be absent in exact Kohn-Sham theory, where the potential is local. Here, we show, for the illustrative case of the LiF dimer, that the exact-exchange local Kohn-Sham potential, constructed within the Krieger, Li, and Iafrate (KLI) approximation, can lead to binding energy and charge dissociation curves that are qualitatively correct. This correct behavior is traced back to a characteristic "step" structure in the local exchange potential and its relation to the Kohn-Sham eigenvalues is analyzed.

8:24AM Y24.00003 A Projector Augmented Wave Treatment of Fock Exchange in Hartree-Fock and Optimized Effective Potential Calculations[1] , XIAO XU, N.A.W. HOLZWARTH, Wake Forest University — The use of orbital-dependent exchange-correlation functionals within electronic structure calculations has recently received renewed attention as a means of improving accuracy. In particular, the Fock exchange functional exactly cancels the electron self-interaction error which can be particularly significant in transition metals and other materials with localized orbitals. Since the Projector Augmented Wave (PAW) formalism[2] accurately evaluates the interaction integrals including all multiple moments, it is a natural choice for representing the Fock exchange functional within an efficient pseudopotential-like scheme. We have adapted the PAW formalism for use both in Hartree-Fock (HF) theory and in the KLI approximation to Optimized Effective Potential theory.[3] We show that the effects of core electrons are significant and can be accurately treated within a frozen core orbital approximation.[4] PAW-HF and PAW-KLI basis, projector, and pseudopotential functions are presented for several elements throughout the periodic table.

[1]Supported by NSF Grant DMR-0705239.
[2]P. E. Blöchl, *Phys. Rev. B* **50**, 17953 (1994).
[3]J. B. Krieger, Y. Li and G. J. Iafrate *Phys. Rev. A* **45** 101 (1992).
[4]Xiao Xu and N. A. W. Holzwarth, *Phys. Rev. B* **81** 245105 (2010).

8:36AM Y24.00004 Localized resolution of identity for efficient Hartree-Fock exchange, based on numeric atom-centered orbitals , JUERGEN WIEFERINK, VOLKER BLUM, XINGUO REN, PATRICK RINKE, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — Methods based on an exact exchange operator (EX) are increasingly popular, but are still restricted to analytical basis functions (e. g. Gaussians) for medium system sizes. We here introduce a localized resolution-of-identity approach for the two-electron Coulomb operator, based on expanding single-particle basis function products separately into auxiliary atom-centered basis sets that are restricted to two centers. Our approach produces accurate results for all-electron EX, can be applied both to analytical and numeric basis functions, requires only $\mathcal{O}(N^2)$ intermediate storage and retains a path towards $\mathcal{O}(N)$ EX for large systems. We demonstrate a total-energy accuracy of < 1 meV/atom for systems including Alanine chains and the S22 benchmark molecule set [1], using the numeric atom-centered orbital based all-electron electronic structure code FHI-aims [2].

[1] P. Jurečka *et al.*, Phys. Chem. Chem. Phys. **8**, 1985 (2006).
[2] V. Blum *et al.*, Comput. Phys. Comm. **180**, 2175 (2009).

8:48AM Y24.00005 Analytic Treatment of the Pair Density in Kohn-Sham Density Functional Theory[1] , MARKUS DAENE, Oak Ridge National Laboratory, ANTONIOS GONIS, Lawrence Livermore National Laboratory, DON M. NICHOLSON, G. MALCOLM STOCKS, Oak Ridge National Laboratory — We have developed a new treatment of the LDA functional in Kohn-Sham density functional theory which is expressed in terms of the pair density of a non-interacting system of particles, thus avoiding from the outset self-interaction effects. The pair density is expressed explicitly in terms of the density using a orthonormal and complete basis expressed as a functional of the density. This allows its functional differentiation with respect to the density by analytic means. The method is illustrated with numerical results for the potential in the case of one and three dimensional systems and is compared to the potentials obtained from the Hartree term.

[1]This material is based upon work supported as part of the Center for Defect Physics, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

9:00AM Y24.00006 Wave Function Functionals for the Density , MARLINA SLAMET, Sacred Heart University, XIAOYIN PAN, Ningbo University, VIRAHT SAHNI, Brooklyn College, CUNY — In recent work we have developed[1] a constrained-search variational method for the construction of wave functions that are functionals of a function $\chi : \Psi = \Psi[\chi]$. These wave function functionals are *simultaneously* normalized, reproduce the *exact* expectation of either single- or two-particle operators, and lead to rigorous upper bounds to the energy. In this paper we extend this method to the construction of wave function functionals $\Psi[\chi]$ that are simultaneously normalized, reproduce the density *exactly*, and lead to rigorous upper bounds to the energy. We apply the method to the ground state of the He atom to obtain wave function functionals that reproduce the density of an accurate correlated wave function. The wave function functionals as expected give rise to the exact expectation of non-differential single particle operators, and lead to accurate two-particle expectations and highly accurate energies.

[1]Pan, Slamet, and Sahni, Phys. Rev. A **81**, 042524 (2010).

9:12AM Y24.00007 Koopmans' condition for density-functional theory , ISMAILA DABO, CERMICS, University Paris-Est, ANDREA FERRETTI[1], NICOLAS POILVERT, Department of Materials Science and Engineering, Massachusetts Institute of Technology, YANLI LI, Department of Physics, Xiamen University, NICOLA MARZARI[2], Department of Materials Science and Engineering, Massachusetts Institute of Technology, MATTEO COCOCCIONI, Department of Chemical Engineering and Materials Science, University of Minnesota — In approximate Kohn-Sham density-functional theory, self-interaction manifests itself as the dependence of the energy of an orbital on its fractional occupation. Here, we first examine self-interaction in terms of the discrepancy between total and partial electron removal energies, and then highlight the importance of imposing the generalized Koopmans' condition to resolve this discrepancy. In the process, we derive a correction to approximate functionals that, in the frozen-orbital approximation, eliminates the unphysical occupation dependence of orbital energies up to the third order in the single-particle densities. This non-Koopmans correction brings physical meaning to single-particle energies; when applied to common local or semilocal density functionals it provides results that are in excellent agreement with experimental data while providing an explicit total energy functional that preserves or improves on the description of established structural properties.

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9:24AM Y24.00008 Density Functional Theory for Open Systems[1] , ANTONIOS GONIS, Lawrence Livermore National Laboratory, DON NICHOLSON, MALCOLM STOCKS, XIAOGUANG ZHANG, Oak Ridge National Laboratory — We provide a formal proof of the convexity relation, $2E[N] \leq E[N-1] + E[N+1]$, characterizing the total energy of interacting N-electron systems under the action of a given external potential, hitherto assumed to be true only on experimental grounds. This is used to prove the inequality, $I(N) - A(N) \geq 0$, where $I(N)$ and $A(N)$ are, respectively, the ionization potential and electron affinity of a N-electron system.

[1]Sponsored by Divisions of MSE and SUF, Office of BES, and by CDP, an EFRC, US DOE. We also thank Mel Levy for discussion.

9:36AM Y24.00009 Volume effects in band gap predictions for solids , ANUBHAV JAIN, Massachusetts Institute of Technology, MARIA K. CHAN, Argonne National Laboratory, RICKARD ARMIENTO, GERBRAND CEDER, Massachusetts Institute of Technology — The *ab initio* prediction of band gaps for solids is important for fundamental and practical reasons. Many approaches exist to remedy the "band gap problem" in Density Functional Theory (DFT) in which band gaps are severely underestimated. We recently proposed the Δ-sol method [1], an adaptation of the ΔSCF method towards solids, in which the fundamental gap is evaluated using total energies from DFT. Using Δ-sol, we obtained band gaps for over 100 crystalline semiconductors at accuracies similar to those of hybrid functionals such as HSE, but at significantly smaller computational costs. However, the accuracy of band gap predictions from first principles remains dependent on accurate determination of lattice parameters and cell volumes. In this talk, we discuss the effects of the accuracy in lattice parameters on predicted band gaps. We present results on the accuracy of cell volumes determined using several exchange-correlation functionals: LDA, PBE, HSE and AM05, and compare the dependence of Kohn-Sham gaps and band gaps predicted using Δ-sol on cell volumes. Finally we discuss optimal approaches for predicting band gaps for compounds with unknown lattice parameters.

[1] M. K. Y. Chan and G. Ceder, Phys. Rev. Lett. 105, 196403 (2010)

9:48AM Y24.00010 Fundamental gaps in finite systems from the eigenvalues of generalized kohn-sham method , TAMAR STEIN, HELEN EISENBERG, Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, Hebrew University, Jerusalem, LEEOR KRONIK, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth, ROI BAER, Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, Hebrew University, Jerusalem — We present a broadly-applicable, physically-motivated first-principles approach to determining the fundamental gap of finite systems. The approach is based on using a range-separated hybrid functional within the generalized Kohn-Sham approach to density functional theory. Its key element is the choice of a range-separation parameter such that Koopmans' theorem for both neutral and anion is obeyed as closely as possible. We demonstrated the validity, accuracy, and advantages of this approach on first, second and third row atoms, the oligoacene family of molecules, and a set of hydrogen-passivated silicon nanocrystals. This extends the quantitative usage of density functional theory to an area long believed to be outside its reach.

10:00AM Y24.00011 Self-optimizing Kohn-Sham hybrid functional , ISAAC TAMBLYN, Molecular Foundry, LBNL, ROI BAER, Hebrew University, Jerusalem, LEEOR KRONIK, Weizmann Institute of Science, Israel, JEFFREY NEATON, Molecular Foundry, LBNL — Recent work using range-separated hybrid functionals has confirmed the importance of including long-range exchange in treatments of phenomena such as charge transfer reactions. Using a self-optimizing [1,2] form of the BNL [3] functional, we present results for structural, electronic, and thermochemical properties of a large set of molecules (including the G2 and G3 test sets). The success of this approach, as well as its ability to describe reaction barriers, will be discussed.

[1] T. Stein, L. Kronik, and R. Baer, JACS, 131 (8), 2818, 2009
[2] T. Stein, H. Eisenberg, L. Kronik, and R. Baer, "Fundamental gaps of finite systems from the eigenvalues of a generalized Kohn-Sham method", Phys. Rev. Lett., in press.
[3] E. Livshits and R. Baer, PCCP, 9, 2932 , 2007

10:12AM Y24.00012 TDDFT and qualitative properties of excited states: three illustrative applications using DMol^3 , BERNARD DELLEY, Paul Scherrer Institut, CMT — Three applications of DMol^3 TDDFT [1] are presented to show possible new frontiers in each case. First, excitations involving multiplet structure for the example of the Ti^{4+} ion are discussed, showing that atomic multiplet splitting is fully exhibited within TDDFT. This approach to multiplets exhibits notable similarities and also notable differences with a first principles based Condon-Shortley-Cowan multiplet theory. Second, UV-VIS spectra of benzene and derivative molecules are discussed by comparing experimental log plots of molar extinction with a TDDFT results completed by the Gaussian envelope model for the vibrational progression. The envelope model provides a natural scale for comparing TDDFT excitations with measured absorption spectra. In the third example, excited states of $(Fe(CN)_5NO)^{-2}$ are studied along the reaction coordinate connecting the long lived metastable states that can be produced by optical excitation.

[1] B. Delley, J. Phys. Cond. Mat. 22, 384208, 2010.

10:24AM Y24.00013 Exact Time-Dependent Kohn-Sham Potential for an Interacting Few-Body System , RUDOLPH J. MAGYAR, Sandia National Laboratories — Time-dependent density functional theory enables practical simulations of the dynamic many-electron systems, but one of the biggest obstacles to reliable application is the quality of the approximate potential. It is often difficult to determine whether ever-more sophisticated approximations properly include new physics, as there exist few benchmark exact potentials. Towards this ends, we have developed and tested a scheme to extract the exact (non-adiabatic) time-dependent Kohn-Sham potential for few body systems. We will present some examples on 1D model systems. The approach is general and can be used to back engineer high-level quantum mechanical simulations to gain insight into TDDFT on a broad scale. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of the Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

10:36AM Y24.00014 TDDFT approach to study nonlinear excitonic effects in Four-Wave Mixing processes[1] , VOLODYMYR TURKOWSKI, Physics Department and NSTC, University of Central Florida, Orlando, FL 32816, MICHAEL N. LEUENBERGER, Physics Department and NSTC, University of Central Florida, Orlando FL 32816 — We develop a time-dependent density-functional theory (TDDFT) formalism to study nonlinear effects in the processes in Four-Wave Mixing experiments. Namely, we generalize our recently proposed approach to calculate excitonic and biexcitonic eigen-energies within TDDFT on the dynamical case, which includes nonlinear effects, the like exciton-exciton interaction. In particular, we derive the TDDFT version of the nonlinear time-dependent equation for excitonic polarization with terms which correspond to exciton-exciton correlations through the memory functions. We have obtained the formula which relates the memory functions with the TDDFT exchange- correlation (XC) kernel. To test the formalism, we calculate the 2D Fourier spectra of a GaAs multi-quantum well system and compare them with experimenatal results in the case of several XC kernels. In addition, we compare the results with the ones obtained within a many-body method for non-linear effects in semiconductors. It is shown that the results obtained within the TDDFT approach may reproduce semi-quantively the 2D Fourier spectra, including the nonlinear effects, in the case of several phenomenological potentials.

[1]Work supported in part by NSF Grant No. ECCS-0901784 and AFOSR Grant No. FA9550-09-1-0450.

10:48AM Y24.00015 Long-range corrected time-dependent density functional theory with spin-orbit couplings , AYAKO NAKATA, TAKAO TSUNEDA, KIMIHIKO HIRAO, RIKEN, JST-CREST — Relativistic time-dependent density functional theory (TDDFT) is a powerful tool to include both of relativistic and correlation effects with low computational cost. However, TDDFT with conventional exchange functionals have severe problems in e.g. the reproducibility of charge transfer (CT) and Rydberg excitation energies and oscillator strengths. These problems are due to the lack of long-range exchange interactions in conventional exchange functionals. We have proposed long-range corrected (LC) DFT and have overcome these problems. Especially, LC-TDDFT succeeds in describing CT excitations with remarkable accuracy. CT excitations often play a major role in spin-forbidden transitions, because the spin-orbit couplings are significant for excitations inducing the changes in electron distributions. In this study, LC-DFT has been applied to a spin-orbit TDDFT to describe spin-forbidden transitions appropriately by TDDFT. Our results have demonstrated that LC-DFT accurately reproduces the splitting of ionization energies of heavy atoms and spin-forbidden excitation energies for which electrons are moved to widely-distributed orbitals.

Friday, March 25, 2011 8:00AM - 11:00AM –
Session Y25 DCMP: Superconductivity: Mainly HTSC Theory D166

8:00AM Y25.00001 The underdoped cuprates as fractionalized Fermi liquids , EUN GOOK MOON, SUBIR SACHDEV, Harvard University — We model the underdoped cuprates using fermions moving in a background with local antiferromagnetic order. The antiferromagnetic order fluctuates in orientation, but not in magnitude, so that there is no long-range antiferromagnetism, but a 'topological' order survives. The normal state is described as a fractionalized Fermi liquid (FL*), with electron-like quasiparticles coupled to the fractionalized excitations of the fluctuating antiferromagnet. The FL* and its mother state, algebraic charge liquid, reveal interesting features in the underdoped cuprates such as shift of the Fermi pocket center from the magnetic Brillouin zone boundary . Also, with transition to superconductivity, the normal states can explain puzzling experiment data such as a nodal-anti-nodal 'dichotomy' identifying characteristics of the two gaps. Implication of our model and extensions are discussed.

8:12AM Y25.00002 Collective Modes in the Loop Ordered Phase of Cuprates , YAN HE, UC Riverside — We show that the two branches of collective modes discovered recently in under-doped Cuprates with huge spectral weight are a necessary consequence of the loop-current state. Such a state has been shown in earlier experiments to be consistent with the symmetry of the order parameter competing with superconductivity in four families of Cuprates. We also predict a third branch of excitations and suggest techniques to discover it. Using parameters to fit the observed modes, we show that the direction of the effective moments in the ground state lies in a cone at an angle to the c-axis as observed in experiments.

8:24AM Y25.00003 Unconventional superconductivity in honeycomb lattice , YANG QI, Tsinghua University, KAI SUN, University of Maryland, ZHENGCHENG GU, Kavli Institute for Theoretical Physics, LIANG FU, Harvard University — Motivated by results of DMRG and tensor network simulations on doped t-J model on honeycomb lattice, we study superconductivity of singlet and triplet pairing in this model. We show that a coexistence of singlet and triplet pairing superconductivity is induced by antiferromagnetic order near half-filling. The superconducting state we obtain is a topological superconductor.

8:36AM Y25.00004 Superconductivity as a Condensate of Collective Cooper Pairs , CARLOS RAMIREZ, CHUMIN WANG, Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico — Along the last century, the fascinating phenomenon of superconductivity has recurrently been considered as a Bose-Einstein condensation (BEC) of Cooper pairs. However, creation and annihilation operators of the Cooper pairs do not satisfy the bosonic commutation relations [1] and then, the superconductivity theories based on the BEC have a weakness in their foundation. In this work, for the dilute limit we prove the bosonic nature of collective Cooper pairs (CCP), defined as linear combinations of Cooper pairs [2]. This bosonic nature is given rise from their diffuse character on the Cooper pairs, which allows the accumulation of many collective pairs at a single quantum state. Moreover, the superconducting ground state proposed by Bardeen, Cooper and Schrieffer (BCS) can be written in terms of these CCP, leading to a possible BEC theory of superconductivity. Finally, the energy spectra of CCP are calculated for a mixture of bosons and fermions, which permit to determine the condensation critical temperature as well as other thermodynamic properties of the CCP condensate.

[1] J. Bardeen, L.N. Cooper and J.R. Schrieffer, Phys. Rev. 108, 1175 (1957).
[2] C. Ramirez and C. Wang, Phys. Lett. A 373, 269 (2009).

8:48AM Y25.00005 Self-consistent Eliashberg theory, T_c, and the gap function in electron-doped cuprates , DHANANJAY DHOKARH, ANDREY CHUBUKOV, University of Wisconsin, Madison — We consider normal state properties, the pairing instability temperature, and the structure of the pairing gap in electron-doped cuprates. We assume that the pairing is mediated by collective spin excitations, with antiferromagnetism emerging with the appearance of hot spots. We use a low-energy spin-fermion model and Eliashberg theory up to two-loop order. We justify ignoring vertex corrections by extending the model to $N >> 1$ fermionic flavors, with $1/N$ playing the role of a small Eliashberg parameter. We argue, however, that it is still necessary to solve coupled integral equations for the frequency dependent fermionic and bosonic self-energies, both in the normal and superconducting state. Using the solution of the coupled equations, we find an onset of $d-$wave pairing at $T_c \sim 30$ K. To obtain the momentum and frequency dependent d-wave superconducting gap, $\Delta(\vec{k}_F, \omega_n)$, we derive and solve the non-linear gap equation. We find that $\Delta(\vec{k}_F, \omega_n)$ is a non-monotonic function of momentum along the Fermi surface, with its node along the zone diagonal and its maximum some distance away from it. We obtain $2\Delta_{\max}(T \to 0)/T_c \sim 4$. We argue that the value of T_c, the non-monotonicity of the gap, and $2\Delta_{\max}/T_c$ ratio are all in good agreement with the experimental data on electron-doped cuprates.

9:00AM Y25.00006 Spin-space entangled orbitals in a Hartree-Fock scheme predicting the AF and insulator properties of La2CuO4 , ALEJANDRO CABO MONTES DE OCA, Departamento de Fisica Teorica, Instituto de Cibernetica, Matematica y Fisica, La Habana, Cuba, ALEJANDRO CABO-BIZET, Centro de Estudios Aplicados al Desarrollo Nuclear, La Habana, Cuba — Its is argued that spin-orbit entangled single particle states in a Hartree-Fock scheme can describe the insulator and antiferromagnetic nature of La2CuO4, as independent particle properties. Therefore, a currently considered as a Mott insulator material, is represented as a Slater one. This curious outcome is not strange if we consider that, strictly speaking, correlation quantities should be defined by the differences between the exact result and the "best" Hartree-Fock one. The discussion opens a road for understanding the connections between the successful phenomenological Mott picture and the First Principle (Slater) schemes of calculations. The results also furnish a simple framework for further studying the normal state properties of HTc superconductors. In particular, the microscopic structure of the antiferromagnetic order and the isolator size of the gap in La2CuO4 are both explained as coherent effects coming from the entangled "spin-orbit" structure of the single particle Hartree-Fock states. The possibility of the stability of the isolator gap when temperature rises up to the experimental Neel value is argued to be allowed by the same entanglement effect.

9:12AM Y25.00007 Anomalous Isotope Effect in Low and High Tc Superconductors: the contribution of the electronic structure , G.L. ZHAO, Southern University and A&M College — Some of the low and high Tc superconductors exhibit an anomalous isotope effect, where the exponent (α) for the isotope effect is much smaller than $1/2$. We present first-principles calculations of the electronic structures of the selected superconductors, including Zirconium (Zr) and $YBa_2Cu_3O_7$(YBCO). The characteristically narrow electron bands around the Fermi levels (E_f) in these materials suggest that the rapid variations of the densities of states around E_f, within the range of phonon energy, can have a noticeable effect on the total coupling matrix elements. Such effect may explain the anomalous isotope effect on Tc in these superconductors. The work is funded in part by NSF and the Air Force Office of Scientific Research.

9:24AM Y25.00008 Electronic Specific Heat and Dissipative Viscosity of Hole-Doped Cuprates , PARTHA GOSWAMI, D.B. College, University of Delhi — We investigate a d-density wave (DDW) mean field model Hamiltonian in the momentum space suitable for the hole-doped cuprates, such as YBCO, in the pseudo-gap phase to obtain the Fermi surface(FS)topologies, including the elastic scattering by disorder potential ($|v_0|$). For the chemical potential $\mu = -$ 0.27 eV (at 10% doping level), and $|v_0| \geq |t|$ (where $|t| = 0.25$ eV is the first neighbor hopping), at zero/non-zero magnetic field (B) the FS on the first Brillouin zone is found to correspond to electron pockets around anti-nodal regions and barely visible patches around nodal regions. We next relate our findings regarding FS to the entropy per particle(S), the electronic specific heat C_{el} and the dissipative viscosity (η). The magneto-quantum oscillations in C_{el} are shown to take place in the moderate disorder regime ($|v_0| \sim$0.2 eV) only for B $\sim$ 40 T. For the density of viscosity $\eta(\mathbf{k})$ on the first Brillouin zone, we find that whereas the negative contribution arises from the electron pockets in the anti-nodal region, the positive contributions are from the hole-pockets in the nodal region. The KSS bound ($\eta/S \geq h/4\pi k_B$)is easily satisfied for the moderately strong disorder potential. The viscosity is found to be proportional to the magnetic field up to B $\sim$ 50 T.

9:36AM Y25.00009 The stripe-like collective excitation in cuprates: A variational Monte-Carlo study , CHUNG-PIN CHOU, TING-KUO LEE, Institute of Physics, Academia Sinica — In this study we report variational Monte-Carlo calculations of collective excitations for the extended $t-J$ model. We found a particular collective excitation involving modulation of charge, spin and pair field have a fairly small stiffness constant. These very easily excitable excitations are the same as the stripe-like states observed in our previous results for the $t-J$ model. This anomalous low rigidity from these low-lying collective excitations may provide a better understanding of the ubiquitous nature of the stripe states in cuprates.

9:48AM Y25.00010 Pairing theory of striped superconductivity[1] , SIEGFRIED GRASER, ARNO KAMPF, THILO KOPP, FLORIAN LODER, University of Augsburg — Starting from a pairing Hamiltonian with an attractive interaction for electrons on nearest-neighbor sites on a square lattice we present a Hartree-Fock scheme which allows for spin and charge density order simultaneously with d-wave superconductivity. Specifically for filling 7/8 the stable groundstate solution is a striped superconductor with a stripe wavelength of eight lattice constants and π-shifted order parameters for d-wave pairing and antiferromagnetism. The superconducting state contains Cooper pairs with finite center of mass momenta $\mathbf{q}$ and $-\mathbf{q}$ corresponding to half the wavelength for the stripe pattern of the charge density. Despite the d-wave symmetry of the local pairing amplitude the striped superconductor is fully gapped. We characterize the striped superconducting state in real-space and in momentum space and discuss its possible relevance to $La_{1.875}Ba_{0.125}CuO_4$.

[1]This work was supported by the DFG through TRR 80.

10:00AM Y25.00011 Pair Density Wave correlations in the Kondo-Heisenberg Model[1] , EDUARDO FRADKIN, Department of Physics, University of Illinois, EREZ BERG, Department of Physics, Harvard University, STEVEN KIVELSON, Department of Physics, Stanford University — We show, using density matrix renormalization group calculations complemented by field theoretic arguments, that the spin gapped phase of the one dimensional Kondo-Heisenberg model exhibits quasi-long range superconducting correlations *only* at a non-zero momentum. The local correlations in this phase resemble those of the pair density wave state which was recently proposed to describe the phenomenology of the striped ordered high temperature superconductor $La_{2-x}Ba_xCuO_4$, in which the spin, charge, and superconducting orders are strongly intertwined.

[1]Supported in part by the NSF, under grants DMR- 0758462, DMR-0531196, and DMR-0757145, and by the DOE under Contracts DE-FG02-07ER46453 and DE-FG02-06ER46287

10:12AM Y25.00012 Uniform and pair-Density-Wave SC states in asymmetric ladders[1] , AKBAR JAEFARI, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign — We consider the problem of the superconducting state in ladder fermionic systems and focus on two possible types of condensates: a uniform ("d-wave") state and a pair-density wave state (PDW). The uniform SC state is known to occur generically in symmetric hole-doped ladders. Recently it was shown that the PDW state occurs in the Kondo-Heisenberg chain on a broad range of parameters. The Kondo-Heisenberg chain is an extreme version of an asymmetric two-leg ladder. These facts suggest that there must be a quantum phase transition between these two states as a function of the relative doping of the two legs of a ladder. We investigate the nature of this quantum phase transition in the weak coupling limit, by taking advantage of bosonization methods available for 1D systems, and investigate the mechanism of this phase transition. We speculate on the relevance of these results to 2D systems. References: S. R. White, R. M. Noack and D. J. Scalapino: Phys. Rev. Lett 73 (1994) A.E. Sikkema, I. Affleck, and S.R. White, Phys. Rev. Lett. 79, 929 (1997) E. Berg, E. Fradkin, S. A. Kivelson, Phys. Rev. Lett. 105, 146403 (2010) O. Zachar and A. M. Tsvelik, Phys. Rev. B 64, 033103 (2001)

[1]This work was supported in part by the NSF grant DMR 0758462 and by the DOE grant DE-FG02-07ER46453.

10:24AM Y25.00013 Unconventional superconductivity nearby antiferromagnetism in quasi-1D conductors:the role of electron-phonon interaction , CLAUDE BOURBONNAIS, Departement de physique, Universite de Sherbrooke, Sherbrooke, QC, Canada, J1K-2R1 and Canadian Institute for Advanced Research, Toronto, Canada, HASSAN BAKRIM, Departement de physique, Universite de Sherbrooke, Sherbrooke, QC, Canada, J1K-2R1 — The stabilization of unconventional superconductivity (SCd) close to a spin-density-wave state (SDW) under pressure in organic conductors like the Bechgaard salts points out the primary importance of the repulsive Coulomb term in the origin of these phases. However, the electron-(acoustic) phonon interaction is known to be finite in practice, as borne out for example by diffuse X-ray scattering experiments. The question then arises about the role of this coupling, if any, in the mechanism of interaction between SDW and SCd orders in such materials. In this work, we address this issue using the renormalization group method. This is done in the framework of the quasi-1D electron gas model with repulsive direct Coulomb terms and weak retarded electron-phonon interaction, which are treated on equal footing. The impact of electron-phonon interaction on the SDW and SCd instability lines of the phase diagram and on the strength of spin correlations in the normal phase are analyzed at arbitrary phonon frequency, and discussed in connection with experiments in organic superconductors like the Bechgaard salts.

10:36AM Y25.00014 Resonant alteration of supercurrent in guiding structures with complex de Gennes distance and its magnetic-field-induced restoration , OLEG OLENDSKI, King Abdullah Institute for Nanotechnology — Properties of the superconducting 2D disk and 3D wire are calculated within the framework of linearized Ginzburg-Landau theory with the complex de Gennes distance Λ in the boundary condition. As a result, the self-adjointness of the Hamiltonian is lost, its eigenvalues E become complex too and the discrete bound states of the disk turn into the quasibound states with their lifetime defined by the eigeneneries imaginary parts E_i. Accordingly, the longitudinal supercurrent undergoes alteration with its attenuation/amplification being E_i-dependent too. It is shown that E_i as a function of the de Gennes imaginary part Λ_i exhibits a pronounced sharp extremum with its magnitude being the largest for the zero real part Λ_r of the de Gennes distance. Increasing magnitude of Λ_r quenches the $E_i - \Lambda_i$ resonance and at large Λ_r the eigenenergies E approach the asymptotic real values independent of the de Gennes length imaginary component. The extremum is also wiped out by the applied longitudinal uniform magnetic field. The finite lifetime of the disk quasibound states stems from the Λ_i-induced currents flowing through the superconductor boundary. The effect can be observed in the superconductors by applying to them the external electric field.

10:48AM Y25.00015 A real space study of the effect of disorder on superconductivity , SHREEMOYEE GANGULY, Department of Materials Science, S.N.Bose National Centre for Basic Sciences, JD-III Salt Lake City, Kolkata 700098, India, A.VENKATASUBRAMANIAN TEAM, KARTICK TARAFDER TEAM, INDRA DASGUPTA TEAM, ABHIJIT MOOKERJEE TEAM — Our method of studying the effect of disorder on superconductivity is based on the augmented space formalism that goes beyond mean-field approximations for configuration averaging and effectively deals with the influence of configuration fluctuations of the neighbourood of an atom. In the regime of validity of Anderson's theorem our results for s- and d-wave dirty superconductors has excellent agreement with existing results. The formalism is extended and tested for random negative **U** Hubbard model. Having verified the reliability of our method we use it to study environment dependent, inhomogeneous randomness in disordered superconducting systems. Our model can be easily extended to study multi-band systems which takes us a step closer to studying real materials.

Friday, March 25, 2011 8:00AM - 10:48AM –

Session Y26 DMP DCOMP: Focus Session: Iron Based Superconductors – Orbital Order D162/164

8:00AM Y26.00001 Effect of doping on the crystalline structure and superconductivity properties in $Ca_{1-x}Na_xFe_2As_2$ single crystals[1] , LEONARDO CIVALE, NESTOR HABERKORN, BORIS MAIOROV, MARCELO JAIME, Los Alamos National Laboratory, Los Alamos, NM, USA, G. CHEN, W. YU, Renmin University of China, Beijing, China — We have studied the crystalline structure and the superconducting properties of $Ca_{1-x}Na_xFe_2As_2$ single crystals for various levels of the chemical doping (x). We performed a comparative analysis of the angular dependent $H_{c2}(\Theta)$ (where Θ is the angle between the magnetic field and the c axis) for x$\sim$0.5 and x $\sim$ 0.75, corresponding to $T_c \sim$ 19 K and 33 K, respectively. We found that in both cases $H_{c2}(\Theta)$ near T_c exhibits a single band character with the same anisotropy $\gamma \sim 1.8$. In the crystal with $T_c \sim 33$ K we detected the presence of a narrow vortex-liquid phase, in agreement with the expectation from estimates based on the Lindemann criterion and the Ginzburg number. We also found large and anisotropic flux creep rates, with temperature dependences that indicate glassy relaxation. We analyzed those results in terms of single vortex and collective pinning regimes associated with random and correlated disorder.

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

8:12AM Y26.00002 First-principles study of orbital-selective magnetism in FeAs-based superconductors , HYUNGJU OH, DONGHAN SHIN, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University — $LaFeAsO_{1-x}F_x$ and related compounds show unconventional superconductivity (SC) in the vicinity of the antiferromagnetism (AFM). These compounds are featured with multiple Fermi surfaces with strong orbital characters. We perform first-principles calculations of the electronic and magnetic properties in LnFeAsO (Ln=La, Ce, Pr, Nd, Sm, and Gd) as a function of Fe magnetic moment to study material-dependent interplay between orbitals and magnetic moments. With this approach, we show orbital-selective magnetic phases in small-Fe-moment regime: d_{xy} magnetic phase, which is itinerantly driven by orbital selection of Fermi-surface nesting, and d_{yz} magnetic phase, which is driven by local interactions. The Fe magnetic moments in the two phases show different coupling strengths to Fermi-surface electrons orbital-selectively, suggesting different roles in SC and in AFM, and making orbital characters of the Fe magnetic moment resolvable by measuring the electronic structures. This work was supported by the NRF of Korea (Grant No. 2009-0081204). Computational resources have been provided by KISTI Supercomputing Center (Project No. KSC-2008-S02-0004)

8:24AM Y26.00003 Orbital characters of the iron-pnictides[1] , DONGLAI FENG, Fudan University — The orbital degree of freedom plays an important role in the physics of iron-based high-temperature superconductors and their parent compounds. For example, possible orbital ordering has been associated with the spin density wave, and we recently found that the superconducting gap sizes are different at the same Fermi momentum for two bands with different spatial symmetries. We studied the orbital characters of the electronic structure in optimally electron-doped $BaFe_{1.85}Co_{0.15}As_2$ by exploiting the polarization-sensitivity of the orbitals in angle resolved photoemission spectroscopy. The orbital characters of the low energy electronic structure and Fermi surface in three dimensional momentum space are determined. Our results indicate that the previous orbital assignments of band structure calculations are just partially correct. Particularly, the contributions of the d_{xy} and d_{x2-y2} orbitals were not right. Our results lay the foundation for constructing realistic microscopic models of iron-based superconductors. Furthermore, we studied the transport properties and electronic structure of magnetically detwinned NaFeAs, and $AEFe_2As_2$. We identify the roles of various orbitals in the spin density wave formation.

[1]This work supported by the NSFC, MOST and STCSM of China.

8:36AM Y26.00004 Dichotomy between Large Local and Small Ordered Magnetic Moments in Iron-Based Superconductors , PHILIPP HANSMANN, Vienna University of Technology, RYOTARO ARITA, Department of Applied Physics, University of Tokyo, ALESSANDRO TOSCHI, SHIRO SAKAI, GIORGIO SANGIOVANNI, KARSTEN HELD, Institut for Solid State Physics, Vienna University of Technology — We study a four-band model for iron-based superconductors within the local density approximation combined with dynamical mean-field theory (LDA+DMFT). This successfully reproduces the results of models which take As p degrees of freedom explicitly into account and has several physical advantages over the standard five d-band model. Our findings reveal that the new superconductors are more strongly correlated than their single-particle properties suggest. Two-particle correlation functions unveil the dichotomy between local and ordered magnetic moments in these systems, calling for further experiments to better resolve the short time scale spin dynamics.

8:48AM Y26.00005 High-energy x-ray diffraction studies of $AEFe_2As_2$ compounds[1] , D.K. PRATT, A. KREYSSIG, M.G. KIM, S. RAN, A. THALER, S.L. BUD'KO, R.J. MCQUEENEY, P.C. CANFIELD, A.I. GOLDMAN, Ames Laboratory, USDOE and Iowa State University — The relationship between structure, magnetism and superconductivity has become a major theme in studies of the iron arsenide family of superconductors. We have used high-energy x-ray diffraction, together with two-dimensional area detectors, to image large regions of reciprocal space in order to gain further insight into the structural transitions in the $AEFe_2As_2$ (AE = Ca, Sr, Ba) compounds. Here we present results of our study of the impact of annealing and temperature on the structure of these materials.

[1]We thank D. Robinson for his excellent support of the measurements. This work was supported by the Office of Basic Energy Sciences, U.S. Department of Energy.

9:00AM Y26.00006 High Resolution X-ray Scattering Studies of Structural Phase Transitions in $BaFe_{2-x}Cr_xAs_2$, B.D. GAULIN, J.P. CLANCY, J.J. WAGMAN, McMaster University, A.S. SEFAT, Oak Ridge National Laboratory — While the effects of electron-doping on the parent compounds of the 122 family of Fe-based superconductors have been extremely well-studied in recent years, far less is known about the influence of hole-doping in compounds such as $BaFe_{2-x}Cr_xAs_2$. In contrast to the electron-doped 122 systems, the hole-doped compounds do not become superconducting. Furthermore, while the hole-doped compounds exhibit similar structural and magnetic phase transitions, they appear to be much less sensitive to dopant concentration. We have performed high resolution x-ray scattering and magnetic susceptibility measurements on single crystal samples of $BaFe_{2-x}Cr_xAs_2$ for Cr concentrations ranging from $0 \leq x \leq 0.67$. These measurements allow us to determine the magnetic and structural phase transitions for this series and map out the low temperature phase diagram as a function of doping. In particular, we have carried out detailed measurements of the tetragonal (I4/mmm) to orthorhombic (Fmmm) structural phase transition which reveal how the orthorhombicity of the system evolves with increasing Cr concentration and how this correlates with the values of T_s and T_m.

9:12AM Y26.00007 Orbital Order and Spontaneous Orthorombicity in Iron Pnictides[1] , RAJIV SINGH, University of California, Davis — Phase diagram of the Iron Pnictide families of superconductors show a tetragonal to orthorhombic transition, sometimes coincident with the antiferromagnetic phase transition and sometimes at temperatures clearly above the antiferromagnetic phase transition. Inelastic neutron scattering spectra show exchange constants with strong spatial anisotropy. Recent photoemission measurements in mechanically detwinned samples show clear evidence of unequal orbital occupation and strikingly different spectra for dxz and dyz iron orbitals. Scanning Tunneling Microscopy and transport measurements have also shown substantial orthorhombicity in these materials. We discuss a simple microscopic picture for coupled spin and orbital degrees of freedom as the root cause for such an anisotropy and discuss the extent to which this picture can be distinguished from spin-frustration induced Ising nematic fluctuations as being the dominant driver for this phenomena.

[1]Supported by NSF-DMR1004231, Work in collaboration with C.-C. Chen, J. Maciejko, A.P. Sorini, B. Moritz and T.P. Devereaux.

9:48AM Y26.00008 Commensurate antiferromagnetic ordering in $Ba(Fe_{1-x}Co_x)_2As_2$ determined by x-ray resonant magnetic scattering at the Fe K edge[1] , M.G. KIM, A. KREYSSIG, Y.B. LEE, Ames Laboratory and Dep. of Physics and Astronomy, Iowa State University, Ames, J.W. KIM, Advanced Photon Source, Argonne National Laboratory, D.K. PRATT, A. THALER, S.L. BUD'KO, P.C. CANFIELD, B.N. HARMON, R.J. MCQUEENEY, A.I. GOLDMAN, Ames Laboratory and Dep. of Physics and Astronomy, Iowa State University, Ames — We describe x-ray resonant magnetic diffraction measurements at the Fe K edge of both the parent $BaFe_2As_2$ and superconducting $Ba(Fe_{0.953}Co_{0.047})_2As_2$ compounds. From these high-resolution measurements we conclude that the magnetic structure is commensurate for both compositions. The energy spectrum of the resonant scattering is in reasonable agreement with theoretical calculation using the full-potential linear augmented plane-wave method with a local density functional. The calculation suggests that the resonant scattering at the Fe K edge in the σ-to-π scattering channel arises from dipole allowed transitions from the core $1s$ states to the unoccupied $4p$ states that are spin polarized due to hybridization with the $3d$ states close to the Fermi energy.

[1]The work at the Ames Laboratory was supported by the DMSE, Office of Basic Energy Science, the US DOE, under contract No. DE-AC02-07CH11358.

10:00AM Y26.00009 Antiferromagnetic ordering in the absence of a structural distortion in $Ba(Fe_{1-x}Mn_x)_2As_2$[1] , A.I. GOLDMAN, M.G. KIM, A. KREYSSIG, A. THALER, D.K. PRATT, W. TIAN, J.L. ZARESTKY, Ames Laboratory, USDOE and Iowa State University, M.A. GREEN, NIST Center for Neutron Research, S.L. BUD'KO, P.C. CANFIELD, R.J. MCQUEENEY, Ames Laboratory, USDOE and Iowa State University — Neutron and x-ray diffraction studies of $Ba(Fe_{1-x}Mn_x)_2As_2$ for low doping concentrations ($x \leq 0.176$) reveal that at a critical concentration, $0.102 < x < 0.118$, the tetragonal-to-orthorhombic transition abruptly disappears whereas magnetic ordering with a propagation vector of ($1/2$ $1/2$ 1) persists. Among all of the iron arsenides this observation is unique to Mn doping, and unexpected because all models for stripe-like antiferromagnetic order anticipate an attendant orthorhombic distortion due to magnetoelastic effects. We discuss these observations and their consequences in terms of previous studies of $Ba(Fe_{1-x}TM_x)_2As_2$ compounds (TM = transition metal), and models for magnetic ordering in the iron arsenide compounds.

[1]Thiw work was supported by the Office of Basic Energy Sciences, U.S. Department of Energy

10:12AM Y26.00010 An empirical method to account for spin-fluctuation suppression of magnetism in Fe pnictides , PETER BLAHA, TU Wien, IGOR MAZIN, MICHELLE JOHANNES, Naval Research Laboratory — Parent materials of Fe-based superconductors, such as $BaFe_2As_2$, are itinerant antiferromagnets, and as such should be better described by LDA calculations than are strongly-correlated cuprates. To an extent, this is true, but LDA, being a mean-field approximation, underestimates the suppression of the long-range magnetism due to spin fluctuations. These can be accounted for within Moria's self-consistent renormalization theory, which, however, includes unknown parameters such as the mean amplitude of the spin-fluctuations. We propose to include Moria's renormalization empirically, through a scaling of the LDA exchange-correlation magnetic field by a uniform constant factor, tuned so as to reproduce the observed phase diagram. This is a much more physical method to produce electronic bands with a proper exchange splitting, than adding an artificial "negative-U" term within an LDA+U formalism, a technique used now. We will report the results of such renormalized calculations for $BaFe_2As_2$ and, for comparison, for a prototypical itinerant magnet, $ZrZn_2$.

10:24AM Y26.00011 In-plane resistivity anisotropy in underdoped $Ba(Fe_{1-x}Ni_x)_2As_2$ and $Ba(Fe_{1-x}Cu_x)_2As_2$[1] , HSUEH-HUI KUO, JIUN-HAW CHU, JAMES ANALYTIS, LEO YU, KRISTIAAN DE GREVE, PETER MCMAHON, YOSHIHISA YAMAMOTO, IAN FISHER, Stanford University — Underdoped Fe arsenide superconductors suffer a structural transition that is either coincident with, or precedes the onset of long range antiferromagnetic order. Crystals tend to form a dense array of twins upon cooling through the structural transition, but uniaxial pressure can be used to almost completely detwin samples, enabling measurement of the associated in-plane electronic anisotropy. Initial experiments on detwinned samples of $Ba(Fe_{1-x}Co_x)_2As_2$ revealed a large in-plane resistivity anisotropy which varied non-monotonically with cobalt concentration. Here we present data extending the initial study to include detwinned samples of $Ba(Fe_{1-x}Ni_x)_2As_2$ and $Ba(Fe_{1-x}Cu_x)_2As_2$. The composition-dependence of the resistivity anisotropy ρ_b/ρ_a reveals a striking correlation with that of the Hall coefficient for all three substitution series.

[1]This work is supported by the DOE, Office of Basic Energy Sciences, under Contract No. DE-AC02-76SF00515.

10:36AM Y26.00012 Quasiparticle interference of C_2-symmetric surface states in LaOFeAs parent compound , XIAODONG ZHOU, CUN YE, PENG CAI, Department of Physics, Tsinghua University, Haidian, Beijing 100084, P.R. China, XIANGFENG WANG, XIANHUI CHEN, National Laboratory for Physical Science at Microscale and Dept of Physics, University of Science and Technology of China, Hefei, 230026, P.R. China, YAYU WANG, Department of Physics, Tsinghua University, Haidian, Beijing 100084, P.R. China — We present scanning tunneling microscopy studies on the LaOFeAs parent compound of iron pnictide superconductors [1]. High resolution spectroscopic imaging reveals strong standing wave patterns induced by quasiparticle interference of two-dimensional surface states. Fourier analysis shows that the distribution of scattering wavevectors exhibits pronounced two-fold (C_2) symmetry, strongly reminiscent of the nematic electronic state found in $CaFe_{1.94}Co_{0.06}As_2$ [2]. The implications of these results to the electronic structure of the pnictide parent states will be discussed.

[1] X.Zhou *et al.* arXiv:1008.2642
[2] T.M.Chuang *et al.* Science **327**, 181 (2010)

Friday, March 25, 2011 8:00AM - 11:00AM –
Session Y27 GQI: Focus Session: Semiconductor Qubits- In Search of Majorana C155

8:00AM Y27.00001 Non-Abelian statistics and topological quantum information processing in 1D wire networks , JASON ALICEA, YUVAL OREG, GIL REFAEL, FELIX VON OPPEN, MATTHEW P.A. FISHER — Topological quantum computation provides an elegant way around decoherence, as one encodes quantum information in a non-local fashion that the environment finds difficult to corrupt. Here we establish that one of the key operations—braiding of non-Abelian anyons—can be implemented in one-dimensional semiconductor wire networks. Previous work [Lutchyn et al., arXiv:1002.4033 and Oreg et al., arXiv:1003.1145] provided a recipe for driving semiconducting wires into a topological phase supporting long-sought particles known as Majorana fermions that can store topologically protected quantum information. Majorana fermions in this setting can be transported, created, and fused by applying locally tunable gates to the wire. More importantly, we show that networks of such wires allow braiding of Majorana fermions and that they exhibit non-Abelian statistics like vortices in a p+ip superconductor. We propose experimental setups that enable the Majorana fusion rules to be probed, along with networks that allow for efficient exchange of arbitrary numbers of Majorana fermions. This work paves a new path forward in topological quantum computation that benefits from physical transparency and experimental realism.

8:12AM Y27.00002 Majorana fermions in nanowires without gating superconductors[1] , CHIEN-HUNG LIN, HOI YIN HUI, JAY SAU, SANKAR DAS SARMA, Condensed Matter Theory Center and Joint Quantum Institute, Department of Physics, University of Maryland, College Park, Maryland 20742-4111, USA — Majorana fermions have been proposed to be realizable at the end of the semiconductor nanowire on top of an s-wave superconductor [1,2]. These proposals require gating the nanowire directly in contact with a superconductor which may be difficult in experiments. We analyze [1,2] in configurations where the wire is only gated away from the superconductor. We show that some signatures of the Majorana mode remain but the Majorana mode is not localized and hence not suitable for quantum computation. Therefore we propose an 1D periodic heterostructure which can support localized Majorana modes at the end of the wire without gating on the superconductor.

[1] Jay D. Sau et al., arXiv:1006.2829, Phys Rev B (in press)
[2] Roman M. Lutchyn et al., Phys. Rev. Lett. 105, 077001 (2010)

[1]This work is supported by DARPA-QuEST, JQI-NSF-PFC, and LPS-NSA.

8:24AM Y27.00003 Effects of Interactions on a Topological Phase Exhibiting Majorana Fermions in Quantum Wires , MILES STOUDENMIRE, JASON ALICEA, UC Irvine — The ability to create and manipulate Majorana fermions in condensed matter systems is not only of fundamental interest for understanding topological phases but also provides a realistic route toward quantum computation. Recently, a series of devices have been proposed that could realize exotic Majorana physics in relatively conventional settings; among the most promising is a superconducting wire system with strong spin-orbit coupling. Because superconducitivity is induced in this system by proximity effect, the system remains superconducting even with net repulsive interactions. The effects of such interactions on this system have until now remained unexplored. Using the Density Matrix Renormalization Group method, we explore the fate of the topological phase in the presence of interactions. Obtaining a matrix product state representation of the degenerate ground states is especially helpful as it allows us to determine detailed properties of the Majorana edge states. Furthermore, we find that interactions significantly expand the topological region of the phase diagram, a result which strengthens proposals to realize Majorana fermions in such wire systems experimentally.

8:36AM Y27.00004 The exchange statistics of Majorana fermions in quasi-one-dimensional networks , DAVID J. CLARKE, University of California, Riverside, JAY D. SAU, University of Maryland, College Park, SUMANTA TEWARI, Clemson University — Under appropriate external conditions a semiconductor with strong spin-orbit coupling in proximity to an s-wave superconductor can be in a topological superconducting (TS) phase. In the topological phase, various defects of the order parameter trap zero energy excitations called Majorana bound states. In a wire geometry the relevant defects are the two ends of the topological region, and each traps a localized zero energy excitation. A network of such wires allows the pairwise exchange of the Majorana bound states. Alicea et al. have shown that these bound states obey non- Abelian exchange statistics, and have proposed [1] such a system as a platform for topological quantum computation (TQC). Here we show that the particular realization of non- Abelian statistics produced in a Majorana wire network is highly dependent on the local properties of individual wire junctions. For a simply connected network, the possible realizations can be characterized by the chirality of individual junctions. We demonstrate how this chirality may be calculated for a particular junction. There is in general no requirement for junction chiralities to remain consistent across a wire network. Careful control of the junction chirality is required for TQC applications of Majorana wire networks. [1] J. Alicea et al., arXiv:1006.4395.

8:48AM Y27.00005 Interferometry and topological quantum computation using Majorana Fermions at semiconductor/superconductor interfaces[1] , JAY SAU, CMTC, Dept of Physics, University of Maryland, College Park, SUMANTA TEWARI, Dept of Physics, Clemson Unversity, South Carolina, SANKAR DAS SARMA, CMTC, Dept of Physics, University of Maryland, College Park — Majorana Fermions are hitherto unobserved exotic Fermionic excitations, which are their own anti-particles. Recently, a lot of excitement has been generated by proposals to realize Majorana fermions in topological superconductors in a rather general class of topological superconductors, some of which may be as simple as the interface 1D or 2D InAs and Al in the appropriate parameter regime might have exotic topological properties and Majorana Fermions [1]. In my talk, I will discuss recent proposals for performing interferometry in 2D and 1D versions of such systems [2] together with ideas for performing Quantum Computation [3] using such robust Majorana fermion based qubits.

[1] J. Sau, S. Tewari, R. Lutchyn, T. Stanescu, S. Das Sarma, arxiv:1006.2829 PRB (in press). [2] J. Sau, S. Tewari, S. Das Sarma, arxiv:arXiv:1004.4702. [3] J. Sau, S. Tewari, S. Das Sarma, arxiv:arXiv:1007.4204 PRA(in press)

[1]This work is supported by DARPA-QuEST, JQI-NSF- PFC, and LPS-NSA.

9:00AM Y27.00006 Topological Phases in Dissipative Quantum Transport , MARK RUDNER, Harvard, MICHAEL LEVIN, Maryland, LEONID LEVITOV, MIT — Recently, a new type of topological quantization was discovered in dissipative quantum transport on a one dimensional bipartite lattice with decay [1]. The transition between distinct topological phases is accompanied by a discontinuous change in the expected displacement covered by a particle before it decays. Here we show that this behavior extends to a much wider family of models, and provide a prescription for computing the topological invariant which distinguishes all of the phases which arise in the general case. When the underlying hopping problem without decay possesses time reversal symmetry, we show that the expected displacement, averaged with respect to all initial states, is quantized. The topological nature of this phenomenon, which is unique to systems with decay, places it on a similar footing as other robust topological phenomena such as the quantization of the Hall conductance [2], or of the adiabatically-pumped charge in periodically-driven 1D systems [3]. Correspondingly, here we find that quantization is robust against a range of perturbations and certain types of decoherence. Similarities and differences with the phases of one-dimensional topological insulators will be discussed. [1] M. S. Rudner and L. S. Levitov, Phys. Rev. Lett. 102, 065703 (2009). [2] D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. 49, 405 (1982). [3] D. J. Thouless, Phys. Rev. B 27, 6083 (1983).

9:12AM Y27.00007 Counting Majorana zero modes in superconductors , LUIZ SANTOS, Harvard University, YUSUKE NISHIDA, MIT, CLAUDIO CHAMON, Boston University, CHRISTOPHER MUDRY, PSI, Switzerland — We present a counting formula for computing the number of (Majorana) zero modes bound to topological point defects. The counting formula is evaluated in a gradient expansion for systems with charge-conjugation symmetry. We will consider examples that include Dirac fermions and the chiral p-wave superconductor in two-dimensional space. In all cases, we explicitly relate the counting of zero modes to Chern numbers.

9:24AM Y27.00008 Non-Abelian order in s-wave superconductors: Phases and quantum transitions[1] , SUMANTA TEWARI, Physics & Astronomy, Clemson University, Clemson, SC, TUDOR STANESCU, Department of Physics, West Virginia University, Morgantown, WV, JAY SAU, Condensed Matter Theory Center, Dept. of Physics, University of Maryland, College Park, MD, PARAG GHOSH, Dept. of Physics and Astronomy, George Mason University, Fairfax, VA, SANKAR DAS SARMA, Condensed Matter Theory Center, Dept. of Physics, University of Maryland, College Park, MD — Non-Abelian topological superconductivity has been predicted to occur in s-wave superconductors with a sizable spin-orbit (SO) coupling. As is now well known, such a system can be used for topological quantum computation. When an external Zeeman splitting crosses a critical value, the system passes from a regular, non-topological, superconducting phase to a topological one. On the other hand, in the absence of SO coupling this critical value corresponds to the Zeeman splitting above which the system loses its s-wave superconductivity. We are thus led to the paradoxical conclusion that the topological superconducting phase appears in a parameter regime at which the system actually is non- superconducting in the absence of SO coupling. In this work we resolve this paradox.

[1]Work supported by DARPA-MTO Grant No: FA 9550-10-1-0497, DARPA QuEST, and JQI-NSF-PFC.

9:36AM Y27.00009 Induced Chiral f-wave Superconducting Pairing and Majorana Fermions in a Hole-doped Semiconductor[1] , CHUANWEI ZHANG, LI MAO, Department of Physics and Astronomy, Washington State University, Pullman, Washington, 99164 USA, JUNREN SHI, International Center for Quantum Materials, Peking University, Beijing 100871, China, QIAN NIU, Department of Physics, The University of Texas, Austin, Texas 78712 USA — We show that a chiral f + if-wave superconducting pairing may be induced in the lowest heavy hole band of a hole-doped semiconductor thin film through proximity contact with an s-wave superconductor. The chirality of the pairing originates from the 3π Berry phase accumulated for a heavy hole moving along a close path on the Fermi surface. There exist three chiral gapless Majorana edge states, in consistence with the chiral f + if-wave pairing. We show the existence of zero energy Majorana fermions in vortices in the semiconductor-superconductor heterostructure by solving the Bogoliubov-de-Gennes equations numerically as well as analytically in the strong confinement limit. The proposed semiconductor/superconductor heterostructure can be used as a platform for observing non-Abelian statistics and performing TQC.

[1]This work is supported by DARPA-YFA, DARPA-MTO, ARO, 973 program, NSFC, DoE, and the Welch Foundation.

9:48AM Y27.00010 Anyonic entanglement renormalization , ROBERT KOENIG, ERSEN BILGIN, Institute for Quantum Information, Caltech — We introduce a family of variational ansatz states for chains of anyons which optimally exploits the structure of the anyonic Hilbert space. This ansatz is the natural analog of the multi-scale entanglement renormalization ansatz for spin chains. In particular, it has the same interpretation as a coarse-graining procedure and is expected to accurately describe critical systems with algebraically decaying correlations. We numerically investigate the validity of this ansatz using the anyonic golden chain and its relatives as a testbed. This demonstrates the power of entanglement renormalization in a setting with non-abelian exchange statistics, extending previous work on qudits, bosons and fermions in two dimensions.

10:00AM Y27.00011 Protected phase gates for superconducting qubits , PETER BROOKS, JOHN PRESKILL, California Institute of Technology — Quantum systems with inherent error-correcting properties offer a powerful tool for building quantum computers to be insensitive to the effects of errors. Kitaev [arXiv:cond-mat/0609441] has proposed an intrinsically fault-tolerant qubit design based on superconducting systems. The phase gate $\Lambda(i)$ in this system is performed by coupling the qubit to a quantum LC oscillator for a period of time. The evolution of the oscillator can be understood as being protected by a family of continuous variable quantum codes at every point in its evolution, providing natural robustness against random variations in the duration and strength of the coupling. We present the results of numerical simulations of this system which investigate the fidelity of the phase gate operation as a function of the duration mistiming. We discuss the robustness of the gate under the effect of anharmonic perturbations to the oscillator and oscillator coupling, and adiabaticity requirements for this scheme to properly function.

10:12AM Y27.00012 Resilience of Topological Codes to Depolarization , RUBEN S. ANDRIST, Department of Physics, ETH Zurich, HECTOR BOMBIN, Perimeter Institute for Theoretical Physics, MIGUEL ANGEL MARTIN-DELGADO, Departamento de Fisica, Universidad Complutense, HELMUT G. KATZGRABER, Department of Physics, Texas A&M University & ETH Zurich — Standard error correction is based on redundant storage of quantum information. However, in topological quantum error correction decoherence effects are prevented by encoding logical qubits in nonlocal degrees of freedom, while actively correcting for errors that occur locally in the system. Previous studies have shown that the two hallmark topological codes—the toric code and color codes—are stable against bit-flip/phase-flip and measurement errors. In this work we study the effects of the depolarizing channel to both the toric code and topological color codes. By mapping the quantum problem onto a disordered statistical-mechanical 8-vertex model we compute the error tolerance of these systems using large-scale Monte Carlo simulations. Our results show that the error threshold increases significantly for both the toric code and color codes.

10:24AM Y27.00013 Local equivalence of topological order: Kitaev's code and color codes , GUILLAUME DUCLOS-CIANCI, Universite de Sherbrooke, HECTOR BOMBIN, Perimeter Institute for Theoretical Physics, DAVID POULIN, Universite de Sherbrooke — We demonstrate that distinct topological codes can be mapped onto each other by local transformations. The existence of such a local mapping can be interpreted as saying that these codes belong to the same topological phase. When used as quantum error correcting codes, the local mapping also enables us to use any decoding algorithm suitable for one of these codes to decode other codes in the same topological phase. We illustrate this idea with the topological color code and the topological subsystem color code that are found to be locally equivalent to two copies of Kitaev's toric code. We are therefore able to decode these two codes that had no previously known efficient decoding algorithm, and find error thresholds comparable to previously estimated optimal values. These local mappings could have additional use for fault-tolerant quantum computation. In particular, one could in principle take advantage of the features (transversal gates, topological gates, etc.) of all the codes that are locally equivalent by switching between them during the computation in a fault-tolerant fashion.

10:36AM Y27.00014 Exactly solvable 3D quantum model with finite temperature topological order , ISAAC KIM, Institute of Quantum Information — We present a family of exactly solvable spin-$\frac{1}{2}$ quantum hamiltonians on a 3D lattice. The degenerate ground state of the system is characterized by a quantum error correcting code whose number of encoded qubits are equal to the second Betti number of the manifold. These models 1) have solely local interactions 2) admit a strong-weak duality relation with an Ising model on a dual lattice 3) have topological order in the ground state, some of which survive at finite temperature. The associated quantum error correcting codes are all non-CSS stabilizer codes.

10:48AM Y27.00015 Universal Behavior of Entanglement in 2D Quantum Critical Dimer Models , BENJAMIN HSU, EDUARDO FRADKIN, UIUC — We examine the scaling behavior of the entanglement entropy for the 2D quantum dimer model (QDM) at criticality and derive the universal finite sub-leading correction γ_{QCP}. We compute the value of γ_{QCP} without approximation working directly with the wave function of a generalized 2D QDM at the Rokhsar-Kivelson QCP in the continuum limit. Using the replica approach, we construct the conformal boundary state corresponding to the cyclic identification of n-copies along the boundary of the observed region. We find that the universal finite term is $\gamma_{QCP} = \ln R - 1/2$ where R is the compactification radius of the bose field theory quantum Lifshitz model, the effective field theory of the 2D QDM at quantum criticality. We also demonstrated that the entanglement spectrum of the critical wave function on a large but finite region is described by the characters of the underlying conformal field theory. It is shown that this is formally related to the problems of quantum Brownian motion on n-dimensional lattices or equivalently a system of strings interacting with a brane containing a background electromagnetic field and can be written as an expectation value of a vertex operator.

Friday, March 25, 2011 8:00AM - 11:00AM –

Session Y29 GQI: Focus Session: Superconducting Qubits - Coherence and Materials II C148

8:00AM Y29.00001 Investigating decoherence in the transmon qubit using a 3D resonator[1] , HANHEE PAIK, D.I. SCHUSTER[2], L. BISHOP[3], A.P. SEARS, G. KIRCHMAIR, L. FRUNZIO, M.H. DEVORET, R.J. SCHOELKOPF, Yale University — We studied the coherence times of transmon qubits using three-dimensional resonators. The three-dimensional (3D) superconducting resonant cavity is machined with aluminum alloy, whose quality factor is higher than 5 million at 10 mK inside a magnetic shield. The transmons are fabricated on sapphire substrates whose internal Q was not lower than 2 million when evaluated in the 3D resonator. We measured the relaxation and dephasing times of the qubits and were able to draw a lower bound on these numbers.

[1]This work is funded by IARPA.
[2]current affiliation : Univ. of Chicago
[3]current affiliation: JQI, Univ. of Maryland

8:12AM Y29.00002 Decoherence in Improved Transmon Qubits , ADAM SEARS, HANHEE PAIK, DAVID SCHUSTER, LEV BISHOP, GERHARD KIRCHMAIR, LUIGI FRUNZIO, MICHEL DEVORET, ROB SCHOELKOPF, Yale University — The transmon is a simple superconducting qubit which has less dependence on the usual sources of 1/f noise, and has coherence which is mostly limited by a source of anomalous dissipation. The quality factors of transmon qubits on sapphire are observed to be $\sim$ 50,000, similar to that of transmission line resonators made with the same geometry. It is likely that both these devices may be limited by surface dielectric losses. We will report on the design and characterization of transmon qubits which are fabricated with reduced dielectric losses to possibly increase coherence times.

8:24AM Y29.00003 Measurements of quasiparticle tunneling rate in a superconducting transmon qubit , LUYAN SUN, Departments of Physics and Applied Physics, Yale University, LEONARDO DICARLO, MATTHEW REED, LEV BISHOP, TERRI YU, GIANLUIGI CATELANI, LEONID GLAZMAN, LUIGI FRUNZIO, MICHEL DEVORET, ROBERT SCHOELKOPF, Departments of Physics and Applied Physics, Yale University — A practical quantum computer requires qubits with long coherence times in order to perform many quantum gates. For a superconducting qubit, non-equilibrium quasiparticle tunneling is one possible source of decoherence. Spectroscopy measurements of a superconducting transmon qubit can be used to set a bound on the quasiparticle tunneling rate. When operated in the low E_J/E_C regime, the transmon qubit transition frequency switches between two well-resolved branches due to quasiparticle tunneling. A selective π pulse applied to one of these two branches can excite the qubit only if the qubit is at that frequency. Thus by repeatedly applying π pulses to interrogate the qubit state, the quasiparticle dynamics can be studied. We will present our results on the quasiparticle tunneling rate in a transmon qubit.

8:36AM Y29.00004 Dynamical decoupling and noise spectroscopy with a superconducting flux qubit , JONAS BYLANDER, SIMON GUSTAVSSON, FEI YAN, Massachusetts Institute of Technology, FUMIKI YOSHIHARA, KHALIL HARRABI, Institute of Physical and Chemical Research RIKEN, DAVID CORY, MIT and University of Waterloo, YASUNOBU NAKAMURA, JAW-SHEN TSAI, RIKEN and NEC Corporation, WILLIAM D. OLIVER, MIT Lincoln Laboratory — We demonstrate dynamical decoupling in a superconducting flux qubit with a long energy-relaxation time, $T_1 = 12\,\mu$s. Low-frequency noise acts to dephase the qubit, reducing its transverse coherence time T_2. At the noise-optimal bias point we observe a free-induction decay time $T_2^* = 2.5\,\mu$s and T_1-limited spin-echo decay, $T_{2E} = 2\,T_1$. Biased away from this point, the increased sensitivity to flux noise leads to increased echo and free-induction decay rates. We moderate the dephasing effects of this noise by applying dynamical-decoupling sequences with up to 200 π-pulses. Using the CPMG sequence, we achieve a more than 50-fold enhanced decay time over T_2^*, and Gaussian pure-dephasing times $T_\varphi > 100\,\mu$s. We use the filtering property of this pulse sequence to facilitate spectroscopy of the environmental noise and reconstruct its $1/f$ power spectral density, which we independently confirm by a Rabi-spectroscopy approach. We characterize the noise sources coupling to the energy-bias and tunnel-coupling terms of the Hamiltonian.

8:48AM Y29.00005 Multi-mode circuit quantum electrodynamics , JEROME BOURASSA, Universite de Sherbrooke, JAY M. GAMBETTA, IQC and University of Waterloo, ALEXANDRE BLAIS, Universite de Sherbrooke — In circuit QED experiments with low anharmonicity superconducting qubits, like the transmon, it has been shown how the many-level structure of the qubits can give rise to non-trivial effects. Examples are the straddling regime [1] and high-power qubit readout induced by qubit nonlinearities [2]. In the same spirit, there are also clear experimental evidences to the effect that higher resonator modes play an important role in setting the size of the qubit-qubit flip-flop interaction mediated by virtual resonator photons [3] and the qubit decay rate due to the Purcell effect [4]. In this talk we explore how these higher modes can be taken into account in a theoretical description of the system, and how they affect the flip-flop and Purcell decay rates.

[1] Houck et al., Phys Rev. A 76, 042319 (2007); Srinivasan et al, V26.00006, 2010 March Meeting.
[2] Reed et al, Phys. Rev. Lett. 105, 173601 (2010), Bishop et al, Phys. Rev. Lett. 105, 100505 (2010), Boissonneault et al, Phys. Rev. Lett. 105, 100504 (2010).
[3] Filipp et al, arXiv:1011.3732v1
[4] Houck et al, PRL 101, 080502 (2008)

9:00AM Y29.00006 Dissipation in the ultra-strong coupling regime , FELIX BEAUDOIN, Universite de Sherbrooke, JAY GAMBETTA, Institute for Quantum Computing, University of Waterloo, ALEXANDRE BLAIS, Universite de Sherbrooke — It has recently been shown that the ultra-strong coupling regime, in which the rotating-wave approximation breaks down, can be obtained using a flux qubit coupled to a transmission line [1]. This regime has been observed experimentally in [2, 3]. We will show the usual quantum optics master equation fails in this context and give a more accurate one. We will also explain how non-trivial properties of the ground state could be experimentally studied.

[1] J. Bourassa et al, Phys. Rev. A 80, 32109 (2009)
[2] T. Niemczyk et al, Nature Physics 6, 772-776 (2010)
[3] P. Forn-Díaz et al., arXiv:1005.1559v1 (2010)

9:12AM Y29.00007 Strong frequency dependence of coupling of a Cooper- pair box qubit to Quantum Noise , B. SURI, Dept.of Phys., Univ.of MD., Z. KIM, Dept.of Phys., Univ. of MD., V. ZARETSKEY, S. NOVIKOV, Dept. of Phys., Univ. of MD., K.D. OSBORN, A. MIZEL, Lab. for Physical Sciences, B.S. PALMER, Lab.for Physical Sciences, F.C. WELLSTOOD, Dept. of Phys., Univ. of MD., JQI, CNAM — Our system consists of an Al/AlO_x/Al Cooper-pair box (CPB) charge qubit coupled to a lumped element resonator, which in turn is coupled to a transmission line. From the measured Rabi frequency, for a given microwave frequency f and amplitude in the transmission line, we can extract the coupling of qubit to the transmission line. We observe an order of magnitude variation in this coupling over the range of $f = 4$ to 8GHz which is in agreement with the variation of our measured lifetimes. Assuming that our qubit is coupled directly to a 50Ω impedance with the measured coupling, we find that for $f = 6$ to 7 GHz the lifetime of 30μs measured at the charge sweet spot can be well explained by quantum noise. At $f = 4$GHz, we observe an order of magnitude weaker coupling and a T_1 of 200μs .

9:24AM Y29.00008 Dephasing Measurements of a Cooper-pair box , VITALEY ZARETSKEY, Dept. of Physics, Univ. of Maryland, S. NOVIKOV, B. SURI, Z. KIM, Dept. Of Physics, Univ. Of Maryland, F. C. WELLSTOOD, JQI, CNAM, Dept. of Physics, Univ. of Maryland, B. S. PALMER, Lab. For Physical Sciences — We present data on the dephasing properties of our Al/AlO_X/Al Cooper-pair box (CPB) qubit. The CPB had a charging energy E_C/h = 6.25 GHz and a maximum E_J/h = 19 GHz which was decreased by an external magnetic field to an effective E_J/h of 6.1 GHz. The qubit was capacitively coupled to a lumped element microwave resonator ($f_0 = 5.446$ GHz, $Q_L = 1.8 \times 10^4$) which was in turn coupled to a transmission line. To manipulate the qubit, a microwave pulse at 6.1 GHz was sent to the transmission line. The state of the qubit was then measured by sending a second microwave pulse at f_0 and measuring the amplitude and phase of the transmitted power. We observed Rabi oscillations with Rabi frequencies from 1.94 to 5.32 MHz decay with time constants in the range T' = 0.6 to 1.6 μs. We measured an inhomogeneous dephasing time (T_2*) of 322 ns by performing a Ramsey fringe experiment. Assuming $1/f$ charge noise is the dominant dephasing mechanism we extracted a $1/f$ charge noise amplitude of $1.6\times10^{-3}e/\sqrt{Hz}$ at 1 Hz.

9:36AM Y29.00009 Improved T2 in Josephson Phase Qubits , DANIEL SANK, RAMI BARENDS, RADOSLAW BIALCZAK, YU CHEN, JULIAN KELLY, MICHAEL LENANDER, ERIK LUCERO, MATTEO MARIANTONI, MATTHEW NEELEY, AARON O'CONNELL, PETER O'MALLEY, AMIT VAINSENCHER, HOAHUA WANG, MARTIN WEIDES, JAMES WENNER, THEODORE WHITE, YI YIN, JIAN ZHAO, ANDREW CLELAND, JOHN MARTINIS, UCSB — Phase qubit gate fidelities are limited by individual device dephasing times (T2). Reduction of dephasing is therefore an important immediate goal for phase qubit experiments. A simple way to reduce dephasing is to increase the device loop inductance in order to lower the noise currents driven by magnetic flux noise; T2 should scale linearly with loop inductance. Surface spin models for flux noise also predict that wider loop traces should reduce the noise. We present data on T2 for phase qubits with varied loop inductance and trace width. We present data from experiments in which we find that doubling the loop inductance increases T2 by 25%.

9:48AM Y29.00010 Evidence for coherent quantum phase slips from dephasing of fluxonium qubit[1] , ARCHANA KAMAL, NICHOLAS MASLUK, Yale University, VLADIMIR MANUCHARYAN, Harvard University, JENS KOCH, Northwestern University, LEONID GLAZMAN, MICHEL DEVORET, Yale University — Phase slips are events in which the phase across a superconducting wire changes by 2π. The thermally activated phase slips at high temperatures are well understood but the coherent phase slips caused by quantum fluctuations well below the critical temperature have, so far, eluded observation. We report new decoherence data for the fluxonium qubit [1] that provide evidence for coherent quantum phase slips across the qubit inductance, implemented with a long array of Josephson tunnel junctions. Coherent quantum phase slips result in broadening of the qubit transition frequency due to Aharonov-Casher interference of multiple phase slip paths (or flux tunneling through different junctions) encircling random offset charges on array islands [2].

[1] V.E. Manucharyan et al., Science 326, 113 (2009).
[2] D. Ivanov et al., Phys. Rev. B 65, 024509 (2002).

[1]Work supported by IARPA, ARO and NSF.

10:00AM Y29.00011 Relaxation mechanisms of the fluxonium qubit[1] , NICHOLAS MASLUK, ARCHANA KAMAL, Yale University, VLADIMIR MANUCHARYAN, Yale University, Harvard University, JENS KOCH, Northwestern University, LEONID GLAZMAN, MICHEL DEVORET, Yale University — Fluxonium is a highly anharmonic artificial atom, which utilizes an inductance formed by an array of large Josephson junctions to shunt the junction of a Cooper-pair box. The first excited state transition frequency is widely tunable with flux, yet can be read out over the entire five octave range due to interactions of the 2nd excited state with the readout cavity, enabling a dispersive readout. We present T1 times of several fluxonium samples over the full range of flux dependent transition energies. By mapping out the qubit lifetimes we are able to distinguish between the contributions due to the Purcell effect and quantify dissipation internal to the qubit. With this understanding, we can design a qubit with minimized contribution from internal losses, which should push lifetimes further into the tens of microseconds. [1] V. E. Manucharyan et al., Science 326, 113 (2009).

[1]Work supported by IARPA, ARO and NSF.

10:12AM Y29.00012 1/f noise and susceptibility-magnetization correlation in disordered ferromagnets[1] , KOSTYANTYN KECHEDZHI, Rutgers, The State University of New Jersey — We consider a strongly disordered ferromagnet modeled by Ising spins placed at random in 2D with ferromagnetic interactions decaying exponentially with inter-site distance. Ferromagnetic phase in this model arises due to formation of infinite percolation cluster of strongly interacting spins. Fractal nature of the percolation cluster manifests itself in the dynamics of the system in the vicinity of the percolation transition. Simulating the dynamics with single spin flip Monte Carlo algorithm we observe 1/f power spectra of magnetization noise in a wide temperature range near the transition. Subjected to external AC magnetic field the system shows significant cross-correlation between susceptibility and magnetization in the ferromagnetic phase. This results suggest a possible explanation of the inductance-flux cross-correlation recently observed in SQUIDs [1].

[1] S. Sendelbach, D. Hover, M. Muck, and R. McDermott, Phys. Rev. Lett. 103, 117001 (2009)

[1]This work is done in collaboration with Lara Faoro and Lev B. Ioffe

10:24AM Y29.00013 Are "pinholes" the cause of excess current in superconducting tunnel junctions? A study of Andreev current in highly resistive junctions[1] , MARKKU STENBERG, TINE GREIBE, CHRISTOPHER WILSON, THILO BAUCH, VITALY SHUMEIKO, PER DELSING, Chalmers University of Technology — In highly resistive superconductor—insulator—superconductor (SIS) and superconductor—insulator—normal-metal (SIN) junctions, "excess" subgap current is usually observed. We have studied subgap conductance in Al/AlO_x/Al and Al/AlO_x/Cu tunnel junctions. In the former, we observed a huge (two orders of magnitude) decrease in subgap conductance upon the transition from the SIS to the SIN regime. In the latter, we observed several signatures of coherent diffusive two-particle transport. We use the quasiclassical Keldysh-Green function theory to quantify the contributions of the single- and two-particle processes on subgap conductance. Our observations indicate insignificance of highly transparent microscopic defects ("pinholes") in the tunneling barrier, and we therefore argue that the common "pinhole" scenario is not the explanation for the observed excess subgap current in SIS tunnel junctions.

[1]This research was partly funded by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), through the Army Research Office.

10:36AM Y29.00014 Critical current noise and junction resonators in Josephson junction from interacting trap states , MOHAMMAD H. ANSARI, Institute for Quantum Computing, IQC and University of Waterloo, FRANK K. WILHELM-MAUCH, Institute for Quantum Computing, IQC and University of Waterloo — We analyze the impact of trap states in the oxide layer of superconducting tunnel junctions on the fluctuation of the Josephson current. These are known to inhibit the coherent operation of superconducting qubits. These have a twofold effect: Occupying trap states blocks out parts of the critical current of the Josephson junction. Electrons can also cross the junction via hopping across a trap. We are extending previous studies of noninteracting traps to the case where the traps have on-site electron repulsion. We use second order perturbation theory which allows to obtain analytical results but limited to small and intermediate repulsion. Remarkably, it still reproduces the main features of the model as identified from the Numerical Renormalization group. We present analytical formulations for the subgap bound state energies, the singlet-doublet phase boundary, and the spectral weights, which are in agreement with recent Numerical Renormalization Group analysis. We show that interactions can reverse the supercurrent across the trap. We finally work out the resonance noise spectrum in the presence of on-site repulsive electrons and suggest a criteria for the fabrication of parameters that may help to suppress low frequency noise from superconducting quantum computation devices.

10:48AM Y29.00015 Energy relaxation mechanisms in capacitively shunted flux qubits , ANTONIO CORCOLES, JIM ROZEN, MARY BETH ROTHWELL, GEORGE KEEFE, DAVID DI VINCENZO, MARK KETCHEN, JERRY CHOW, CHAD RIGETTI, JACK ROHRS, MARK BORSTELMANN, MATTHIAS STEFFEN, IBM, IBM QUANTUM COMPUTING GROUP TEAM — Energy losses in superconducting qubits remain a major object of study in the road towards scalable, highly coherent qubit devices. The current understanding of the loss mechanisms in these devices is far from being complete and it is sometimes difficult to experimentally separate the different contributions to decoherence. Here we compare a traditional three Josephson-junction flux qubit to the recently implemented capacitively shunted flux qubit [1], whose energy decay is thought to be limited by dielectric losses arising from native oxides in the shunting capacitor. Keeping all parameters identical except for the shunting capacitance, we obtain energy relaxation times that are comparable for both types of qubit. This suggests that the energy relaxation time is not limited by junction losses in capacitively shunted flux qubits. We discuss some other possible loss mechanisms present in these devices.

[1] M. Steffen *et al.* Phys. Rev. Lett. **105**, 100502 (2010)

Friday, March 25, 2011 8:00AM - 10:00AM –

Session Y30 DCMP: Nanowires and Nanotubes: Fundamentals and Applications C147/154

8:00AM Y30.00001 Apparent Power-Law Behavior of Conductance in Disordered Quasi-One-Dimensional Systems[1] , ALEKSANDR RODIN, MICHAEL FOGLER, UCSD — Observation of power-law dependence of conductance on temperature and voltage has been reported for a wide variety of low-dimensional systems(nano-wires, nano-tubes, and conducting polymers). This behavior has been attributed to the Luttinger liquid effects expected in a pure one-dimensional wire. However, the systems studied were neither one-dimensional nor defect-free. Using numerical simulations we show that the power-law behavior can arise from variable-range hopping in an ensemble of non-interacting disordered wires connected in parallel. This power-law behavior holds in restricted ranges of voltage and temperature, typical of experimental situations. Physically, it comes from rare, but highly conducting hopping paths that appear by chance in some members of the ensemble. The power-law exponents and their dependence on system parameters are consistent with the great majority of available empirical data.

[1]Supported by Grant NSF DMR-0706654

8:12AM Y30.00002 Equilibration of a One-Dimensional Wigner Crystal , K.A. MATVEEV, Argonne National Laboratory, A.V. ANDREEV, University of Washington, M. PUSTILNIK, Georgia Institute of Technology — Equilibration of a one-dimensional system of interacting electrons requires processes that change the numbers of left- and right-moving particles. At low temperatures such processes are strongly suppressed, resulting in slow relaxation towards equilibrium. We study this phenomenon in the case of spinless electrons with strong long-range repulsion, when the electrons form a one-dimensional Wigner crystal. We find the relaxation rate by accounting for the umklapp scattering of phonons in the crystal. For the integrable model of particles with inverse-square repulsion, the relaxation rate vanishes. We apply our results to calculation of the correction to the conductance of a long quantum wire due to the equilibration processes.

8:24AM Y30.00003 STM images of carbon-nanotube quantum dots: Seeing a Wigner molecule of correlated electrons , ANDREA SECCHI, MASSIMO RONTANI, CNR-NANO S3 and University of Modena, Italy — The paradigm of few-electron complexes in quantum dots (QDs) relies on the idea that the lowest quantized levels are filled according to Pauli's exclusion principle. If Coulomb repulsion is sufficiently strong to overcome the kinetic energy cost of localization, a different scenario is predicted: a "Wigner" molecule (WM) forms, made of electrons frozen in space according to a geometrical pattern. Despite considerable experimental effort, evidence of the WM in semiconductor QDs has been elusive so far. Here we demonstrate theoretically that WMs occur in gate-defined QDs embedded in typical semiconducting carbon nanotubes (CNTs). The unambiguous signatures of the WM state must be searched in the scanning tunneling microscopy (STM) images of the electrons. Through exact diagonalisation (ED) calculations, we unveil the inherent features of the electron molecular states. We show that, like nuclei in a usual molecule, electrons have localized wave functions and hence negligible exchange interactions. ED results for single and double QDs provide a simple interpretation for transport experiments in ultraclean CNTs.

8:36AM Y30.00004 All-Semiconducting nanotube networks Thin Film Transistors: An insight towards High Performance Printed Nanoelectronics , DHEERAJ JAIN, NIMA ROUHI, KATAYOUN ZAND, PETER BURKE, University of California, Irvine — In this work, we present our progress towards devices fabrication using all semiconducting nanotubes as the starting material. A critical issue is the ink formulation and dependence of electronic properties on the nanotube density after deposition. These are some of the first spin-on, all semiconducting nanotube devices ever made and initial results are quite promising for printed RF electronics. Semiconducting single-walled nanotube (99%) ink was used to deposit nanotube network on APTES modified Si/SiO_2 substrate. Following the nanotube deposition, source and drain electrodes (Pd/Au) were deposited using standard photolithography and E-beam evaporation. The Si wafer was used for back gating and SiO_2 as the gate dielectric. The impact of density of nanotube was studied for 3 random densities. We also studied the effect of gate length on mobility, and on/off ratio, for devices with different gate lengths ($10\sim100$ μm). DC characterization of devices shows a high mobility, up to 40 cm^2/V-s, and good on/off ratio up to the order of 10^4 in some cases. Since we are using 99% semiconducting ink, a high on/off ratio is expected, which is true in our devices. The on/off ratio of more than 1000 and mobilities up to $\sim$40 cm^2/V-s were observed in almost all devices.

8:48AM Y30.00005 Spin-valley blockade and electron valley resonance in carbon-based quantum dots , GUIDO BURKARD, ANDRAS PALYI[1], University of Konstanz, Germany — The spin blockade effect in the electric conduction through two semiconductor quantum dots connected in series has allowed the monitoring of spin-breaking effects, notably single-spin rotations induced via external fields in electron spin resonance (ESR) and spin decoherence due to the hyperfine coupling to the nuclear spin environment. Electrons in double quantum dots in carbon nanotubes and graphene comprise a valley isospin in addition to their spin. We show that this can lead to a spin-valley blockade which is sensitive to both spin and valley breaking effects. The hyperfine interaction due to residual ^{13}C nuclear spins turns out to be both spin- and valley-breaking, while non-magnetic atomic impurities can lead to pure valley-breaking. We study the magnetic-field dependent leakage current in the spin-valley blockade, also taking into account the spin-orbit interaction in carbon nanotubes. In analogy to ESR, we propose a resonance effect for the valley isospin (electron valley resonance) driven by an oscillatory electric field in a graphene or carbon nanotube quantum dot. References: A. Palyi and G. Burkard, Phys. Rev. B 80, 201404 (2009); Phys. Rev. B 82, 155424 (2010); arXiv: 1010.4338 (2010).

[1]present address: Eötvös University, Budapest, Hungary

9:00AM Y30.00006 Single tube electric transport properties of synthesized Titania nanotubes , MOHAMED ABDELMOULA, LATIKA MENON, Northeastern University — Titania nanotube arrays fabricated by means of electrochemical anodization is currently the main interest of several research groups due to its promising applications. The high aspect ratio, durability, cheap and scalable fabrication technique make it highly attractive material for efficient solar cell. In this regard extensive research work is being carried out to investigate its properties. In our previous work we were able to find a mechanism for separating a single titania nanotube from the titania nanotube arrays and to measure its electric transport properties using e-beam lithography technique, In this work we investigated the effect of thermal annealing on the transport properties, we studied the effect of different annealing temperatures, heating and cooling rates, and in different gases. As a result, we were able to find the optimal annealing conditions to enhance the transport properties in blank titania nanotube. Under these optimal conditions, we were able to study the effect of coating TNTs with N719 dye and gold nanoparticles on the transport properties. As a result of our work we were able to optimize the treatments for more efficient solar cell fabrication.

9:12AM Y30.00007 Computer Simulated Cold Welding of Gold Nanowires[1] , EDISON DA SILVA, ZENNER PEREIRA, Institute of Physics "Gleb Wataghin," UNICAMP, 13083-970, Campinas - SP, Brazil — Recently cold welding was achieved in gold and silver nanowires (NWs) with diameters in the range of 4 to 10 nm [1]. Since metallic contacts are of great importance in electronic devices, the ability of welding them without temperature change is quite remarkable and of interest. In the present work we use computer simulations to produce cold welding in gold NWs at room temperature. We used molecular dynamics with many body effective potentials based on the embedded-atom method EAM using the LAMMPS code to simulate first the braking of gold NWs, the two produced NWs are then cold welded and similarly as the experiments, the newly welded NWs showed fcc structures as the pristine samples. The structural analysis is done with two independent methods [2] and strain stress curves of the breaking and welding are present. Our computer simulation compare very well with the experiments.

[1] Y. Lu, *et al.* Nature Nanotechnology 5, 218 - 224 (2010)
[2] E. Z. da Silva and Z.S. Pereira, Phys. Rev. B **81**, 195417 (2010).

[1]Work is supported by CNPq, CAPES, FAPESP and FAEPEX. CENAPAD-SP and IFGW are acknowledged for computer time.

9:24AM Y30.00008 Nanowire FET as a measurement tool: A method for distiguishing molecular configurations using Debye Screening effect[1] , ALEKSANDAR VACIC, JASON CRISCIONE, NITIN RAJAN, TAREK FAHMY, MARK REED, Yale University — Silicon nanowires/nanoribbons configured as field effect transistors (FETs) with receptor modified surface can be utilized for sensing of charged biomolecular species due to surface potential modulation upon receptor-ligand binding. However, charged ionic species of the sensing buffers interfere with a sensing process by lowering the effective charge of the bound molecules sensed by an FET. In this work, we exploit the Debye screening effect on the device signal by modulating the ionic strength of the sensing buffer i.e. the Debye length, to distinguish between the different configurations of the receptor-ligand complex. We compare our experimental data with a theoretical model and are able to extract characteristic length parameters of the receptor-ligand system. We will discuss the use of the suggested method for the sensing of conformational changes of biomolecules. References Sorensen M. H., Mortensen N. A., Brandbyge M., Appl. Phys. Lett. 91, 102105 (2007) Stern E., Vacic A., Rajan N. K., et al. Nature Nanotechnology 5, 138 (2010)

[1]This work was partially supported by the National Institutes of Health (NIH R01EB008260), DTRA (HDTRA1-10-1-0037), ARO (W911NF-08-1-0365), the Canadian Institute for Advanced Research (CIfAR).

9:36AM Y30.00009 Silicene Nano-Ribbons: Strong Resistance Towards Oxidation due to sp^2 Hybridization of the Si Valence Orbitals , GUY LE LAY, CINaM-CNRS, PAOLA DE PADOVA, CLAUDIO QUARESIMA, CNR-ISM, BRUNO OLIVIERI, CNR-ISAC, PAOLO PERFETTI, CNR-ISM — We have synthesized for the first time silicene, that is, a new silicon allotrope analogous to graphene recently theoretically predicted [1], in the form of a massively parallel array of quantized zigzag nano-ribbons with a common "magic" width of 1.6 nm. They display characteristic linear band dispersions similar to the Dirac cones of graphene, in correspondence with their hexagonal arrangement seen in STM imaging [2]. Here we show, through the angle-dependence of REEL spectra taken at the Si $L_{2,3}$ edge, the typical signatures of 2p $\rightarrow$ π^* and 2p $\rightarrow$ σ^* transitions associated with sp^2 hybridization of the Si valence orbitals. We further show through high-resolution synchrotron radiation Si 2p core-level spectroscopy measurements that the afore mentioned silicene grating is very resistant toward oxidation. Typically, the oxygen uptake starts at about 10^4 higher doses than on the clean Si(111)7x7 surface. Indeed, this striking behavior is directly related to the sp^2 bonding, an additional confirmation of the silicene (i.e., graphene-like) nature of the nano-ribbons.

[1] S. Cahangorov et al., Phys. Rev. Lett., **102**, 236804 (2009).
[2] P. De Padova et al., Appl. Phys. Lett. **96**, 261905 (2010).

9:48AM Y30.00010 Low- Temperature Magneto-conductance In Carbon Nano-tubes , YUICHI OCHIAI, ATSURO SEINO, MICHIO KIDA, NOBUYUKI AOKI, Chiba University, TAKESHI NAKANISHI, AIST, JONATHAN BIRD, SUNY Buffalo, G-COE COLLABORATION, CHIBA UNIV VBL COLLABORATION — Angular dependent magneto-resistance (MR) has been studied in Multi- walled carbon nano-tubes (MWNTs). In case of thin MWNTs, the flux cancelation has been observed in the low temperature MR. Based on the theoretical studies on the scattering behaviors in the carbon nano-tube (CNT) and flux cancelation in one dimensional transport in CNT, we can analyze an intrinsic carrier scattering based on our MR result of the angular dependence between the angle of thin MWNT axis in parallel and perpendicular directions to the magnetic fields. Also, we can discuss on the positive MR appeared in the perpendicular field direction into the thin MWNT axis.

Friday, March 25, 2011 8:00AM - 10:24AM –
Session Y31 DCMP: Amorphous Solids, Glasses & Liquids II C145

8:00AM Y31.00001 Synthesis, Homogenization and Molecular Structure of Chalcogenide glasses[1]

, SIDDHESH BHOSLE, KAPILA GUNASEKERA, PUNIT BOOLCHAND, University of Cincinnati, PING CHEN, Boise State University — Over the years, bulk glasses have been synthesized by reacting starting materials in evacuated (10^{-5} Torr to 10^{-7}Torr) quartz tubings for various periods at suitable elevated temperatures. The lack of a non-invasive structural probe to track spatial heterogeneity of samples during synthesis has been an impediment to tune synthesis conditions, and obtain a homogeneous product. We have developed a Raman profiling technique to understand the homogenization kinetics of Ge_xSe_{100-x} melts, and find dry samples (2 gram size) take 7 days of reaction at 950°C to homogenize on a scale of 50 microns, while wet ones homogenize quicker (∼3 days), but possess physical properties measurably different from their dry counterparts. Rotating sample tubes during synthesis assists in homogenization of samples incrementally but not dramatically. A score of compositions were homogenized across the 10% < x < 33.3% range, and calorimetric, Raman scattering, and molar volume data accumulated. These data provide clear evidence for three distinct regimes of behavior as a function of Ge content, which are identified with the three elastic phases discussed earlier.[2]

[1]Supported by NSF grant DMR 08-53957.
[2]P.Boolchand et al. J.Non-Cryst. Solids 293, 348 (2001).

8:12AM Y31.00002 Elastic phases in $Ge_xSb_xSe_{100-2x}$ ternary glasses[1]

, K. GUNASEKERA, P. BOOLCHAND, University of Cincinnati, M. MICOULAUT, University of Paris VI — The rigidity and stress phase transitions in titled ternary glasses are examined in Raman scattering, modulated DSC and molar volume measurements, and found to occur at $x_c(1) = 14.9\%$ (rigidity) and $x_c(2) = 17.5\%$ (stress). Raman scattering provides evidence of the structural motifs populated in these networks. Using Size Increasing Cluster Agglomeration, Rigidity theory and the decoded structural motifs, we have calculated the rigidity and stress transitions in the first step of agglomeration to occur at $x_c(1)^t = 15.2\%$ and $x_c(2)^t = 17.5\%$ respectively, in reasonable accord with experiments. Theory predicts and experiments confirm that these transitions will coalesce if edge-sharing Ge- tetrahedral motifs were absent in the structure, a circumstance that prevails in the Ge-deficient $Ge_7Sb_xSe_{93-x}$ ternary, where a narrow IP is reported.[2] These results underscore the central role played by topology in determining the elastic phases of network glasses.

[1]Supported by NSF grant DMR 08-53957.
[2]B.J. Madhu et al. Eur. Phys. J. B 71,21 (2009).

8:24AM Y31.00003 Short Range Order Signature in Crystalline and Amorphous GeSbTe Xanes Spectra[1]

, JEAN-YVES RATY, CÉLINE OTJACQUES, RENGIN PEKOZ, University of Liège, CHRISTOPHE BICHARA, CNRS- University Aix-Marseille, VINCE LORDI, Lawrence Livermore National Laboratory — A new implementation of XANES spectra calculations within DFT and PAW potentials is used to compute the XANES spectra of various amorphous and crystalline GeSbTe structures. A clear correlation between the local order, either tetrahedral or distorted octahedral, and the shape of the XANES signal is observed. These calculations provide a new interpretation of past XANES measurements, relating essentially the phase change mechanism to a moderate modification of the local environment of the Ge atoms.

[1]This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. This work was supported by the Belgian PAI 3/42 program and the FNRS-FRFC.

8:36AM Y31.00004 ABSTRACT WITHDRAWN –

8:48AM Y31.00005 Photocrystallization in a-Se films with and without As-Se buffer layers

, B.A. WEINSTEIN, R.E. TALLMAN, G.P. LINDBERG, Dep. of Physics, Univ. at Buffalo, Buffalo, NY, USA, J.A. ROWLANDS, A. REZNIK, Thunder Bay Regional Resch. Inst., Ontario, Canada, M. KUBOTA, K. TANIOKA, NHK Research Labs, Tokyo, Japan — Photo-induced crystallization is studied for temperatures of 250 - 435 K in amorphous Se (a-Se) HARP* imaging targets using Raman spectroscopy to detect the appearance and growth-rate of trigonal Se in these thin-film structures. We observe striking differences between HARP films in which a thin buffer layer of As-Se alloy is, or is not, deposited prior to growth of the principal a-Se photoconductive layer. Films containing an As-Se buffer appear to be much more stable; no photocrystallization is found within the temperature range studied, even after 3.5 hours of laser exposure (0.17W/mm^2 at 647nm). Whereas for films with no As-Se buffer, photocrystallization readily occurs in two temperature regimes below and above the a-Se glass transition (Tg ∼310K), and there is a regime in the neighborhood of Tg where photocrystallization is absent. We discuss these results in terms of a polymerization model under the competing effects of shear-strain at the substrate and As-cross-linking in the buffer layer, which, respectively, tend to promote and inhibit crystallization in the thick Se over-layer. **High-gain Avalanche Rushing Photodetector*.

9:00AM Y31.00006 Diffraction studies of short- and intermediate-range order of phosphorus-selenium glasses

, DAVID PRICE, ALEKSEI BYTCHKOV, MARIANA MILOSHOVA, EUGENE BYCHKOV, SHINJI KOHARA, LOUIS HENNET — We present state-of-the-art neutron and X-ray diffraction data that provide a definitive picture of the short- and intermediate-range structure of P-Se glasses spanning both glass regions. Specific goals were (1) to obtain detailed information about the development with increasing of intermediate-range order on the length scale around 10 Å, based on the behavior of the first sharp diffraction peak; and (2) to obtain a reliable statistical picture of the short-range order, using the information about types and concentrations of local structural units provided by recent NMR measurements to interpret the trends observed as the P concentration is varied. Particular attention is given to the fine structure of the first peak in the pair distribution function and to a feature in the structure factor at 7.5 Å^{-1}, highlighted by Sergi et al. as a signature of molecular units.

9:12AM Y31.00007 Structure investigation of ultra-small CdSe nanoparticles using the atomic PDF

, AHMAD S. MASADEH, Dept of Phys, University of Jordan, Amman 11942, Jordan, SIMON J.L. BILLINGE, EMIL S. BOZIN, Dept of Applied Phys and Applied Math., Columbia University, NY, 10027, and Condensed Matr. Dept., BNL., Upton, NY, 11973 USA, JAMES R. MCBRIDE, SANDRA J. ROSENTHAL, Dept of Chem, Vanderbilt University, Nashville, TN 37235, USA — The size-dependent structure of CdSe nanoparticles, with diameter ranging from 1.5 to 3.6 nm, has been studied using the atomic pair distribution function (PDF) method. The samples are prepared by the methods of Peng *et al* [1], with modifications. The structure of the smallest stable size, (∼1.5 nm), have been found to posses locally distorted wurtzite structure, with no clear evidence of a heavily disordered surface region [2]. The PDF data of the smallest particle show an extra structural peak appears around r = 3.5 A indicates there is structure modification happened in this sample. This peak start appearing the nanoparticles PDF data gradually as nanoparticle size decreases. The structural parameters are reported quantitatively. We measure a size-dependent strain on the Cd-Se bond which reaches 1.0% at the smallest particle size [3]. The size of the well-ordered core extracted directly from the data agrees with the size determined from other methods.
[1] Peng, et al, *JACS.*, 120, 5343-5344 (1998). [2] Gilbert et al, *Science*, 305, 651-654 (2004). [3] Masadeh et al. *PRB* **76**, 115413 (2007).

9:24AM Y31.00008 Evidence of an Intermediate Phase in bulk alloy oxide glass sysem[1] , S. CHAKRABORTY, P. BOOLCHAND, University of Cincinnati — Reversibility windows have been observed in modified oxides (alkali-silicates and -germanates) and identified with Intermediate Phases(IPs).[2] Here we find preliminary evidence of an IP in a ternary oxide glass, $(B_2O3)_5(TeO_2)_{95-x}(V2O5)_x$, which is composed of network formers. Bulk glasses are synthesized across the 18% $<$ x $<$ 35% composition range, and examined in Raman scattering, modulated DSC and molar volume experiments. Glass transition temperatures T_g(x) steadily decrease with V_2O_5 content x, and reveal the enthalpy of relaxation at T_g to show a global minimum in the 24% $<$ x $<$ 27% range, the reversibility window (IP). Molar volumes reveal a minimum in this window. Raman scattering reveals a Boson mode, and at least six other vibrational bands in the 100 cm^{-1} $< \nu <$ 1700 cm^{-1} range. Compositional trends in vibrational mode strengths and frequency are established. These results will be presented in relation to glass structure evolution with vanadia content and the underlying elastic phases.

[1]Supported by NSF grant DMR 08-53957.

[2]V. Rompicharla J. Phys.: Condens. Matter 20, 202101 (2008).

9:36AM Y31.00009 Glasses, Stress, Attenuation and Thermal Conductivity[1] , JIANSHENG WU, CLARE YU, University of California, Irvine — A wide variety of amorphous materials exhibit similar behavior in their thermal properties. Examples include universal features in the specific heat,thermal conductivity, and ultrasonic attenuation. Recent experiments from the Parpia group at Cornell find that high stress silicon nitride thin film resonators exhibit a remarkably high Q factor, exceeding that of amorphous SiO_2 by 2 to 3 orders of magnitude over a broad range of temperatures, and even exceeding that of single crystal silicon at room temperature. We present a model of why the stress reduces the attenuation. The basic assumption is that high stress increases the potential barriers of the excitations of defects that produce the loss, thus reducing the effective density of lossy fluctuators. We predict that high stress could lead to high thermal conductivity and low dielectric loss, making high stress SiN an excellent candidate as a substrate for integrated circuits.

[1]This work was supported by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), through the Army Research Office.

9:48AM Y31.00010 Highly stable glasses as a general phenomenon: Physical vapor depositions of four different trisnaphthylbenzene isomers , KEVIN DAWSON, University of Wisconsin-Madison, LEI ZHU, LAURA KOPFF, ROBERT J. MCMAHON, LIAN YU, M.D. EDIGER — Glasses of each of the trisnaphthylbenzene (TNB) isomers, a low molecular weight glass forming family of four isomers, were created by physical vapor deposition. These glasses were analyzed using differential scanning calorimetry and wide angle x-ray scattering, and then compared to glasses prepared by quenching each melt. All four isomers produced stable glasses (increased onset temperature, large enthalpy overshoot, and excess x-ray scattering) when vapor-deposited at 0.85 T_g and at low deposition rates. This result is surprising as one of the TNB isomers readily crystallizes when cooled as a liquid. When coupled with previous experiments, these results show that stable glasses are not just produced by a small set of good glass forming molecules but seem to be a general phenomenon. Thus physical vapor deposition can be used as a general route to create unusual glasses for future scientific exploration and technological uses.

10:00AM Y31.00011 In-situ characterization of vapor-deposited glasses of toluene by differential AC chip nanocalorimetry , MATHIAS AHRENBERG, University of Rostock, KATIE WHITAKER, University of Wisconsin-Madison, HEIKO HUTH, University of Rostock, MARK D. EDIGER, University of Wisconsin-Madison, CHRISTOPH SCHICK, University of Rostock, UNIVERSITY OF ROSTOCK TEAM, UNIVERSITY OF WISCONSIN-MADISON TEAM — We use ac nanocalorimetry to investigate extraordinarily stable glasses of toluene prepared by vapor deposition. For that purpose we've built a vapor deposition chamber that allows in-situ characterization of vapor-deposited organic glasses down to liquid nitrogen temperature. With highly sensitive nanocalorimeters in a differential setup, we are able to measure ng-samples over a frequency range from 0.1 Hz up to 8 kHz. The device was used to investigate the transformation of as-deposited stable toluene glasses into ordinary glasses. For films about 100 nm thick, the transformation was studied as a function of time at constant temperature above the common glass transition and as function of temperature at constant heating rate. The stability of the thin films was investigated as a function of substrate temperature and deposition rate.

10:12AM Y31.00012 Thermal Evolution of Defects and Hydrogenated Surfaces in nc-Si:H[1] , KRISTIN KIRILUK, DON WILLIAMSON, Colorado School of Mines, DAVID BOBELA, National Renewable Energy Lab, ARUN MADAN, FENG ZHU, MV Systems, Inc., P. CRAIG TAYLOR, Colorado School of Mines — Photovoltaics research has created a push for new materials and nanotechnology is a primary focus. The most familiar of the nanomaterials is hydrogenated nanocrystalline silicon (nc-Si:H). nc-Si:H has less light-induced degradation than a-Si:H and is cheaper to make than crystalline silicon. X-ray diffraction (XRD), small angle X-ray scattering (SAXS), and electron spin resonance (ESR) experiments explored the crystallite size, orientation and defect density on nc-Si:H samples with varying crystalline volume fraction (CVF). Samples with CVF $\sim$ 50% show preferential [220] crystallite orientation, whose microstructure changes with thermal annealing. Modeling of SAXS data for as-grown material shows that the crystallite surfaces are 20% to 40% hydrogenated. After high temperature annealing, hydrogen leaves these surfaces and the ESR signal increases by about 10 times. We discuss these results and then speculate on the relationship between hydrogen, defects, and microstructure.

[1]This work has been supported by the NSF under grants DMR-0702351, and by the NSF REMRSEC under grant DMR-08-20518.

Friday, March 25, 2011 8:00AM - 10:00AM –
Session Y33 DCMP: Cold Fusion C143/149

8:00AM Y33.00001 Justifying Condensed Matter Nuclear Phenomena Using Hot Fusion Data , XING ZHONG LI, Tsinghua University, Beijing 10084, China — The selective resonant tunneling model [1] has been successful in describing 6 major fusion cross-section data (d+T, d+D, d+He3, t+T, t+He3, p+D). The new formula needs only 3 parameters; however, it gives much better results than what were given by the 5-parameter formula in NRL Plasma Formulary. It provides an opportunity to find the resonance energy level which is necessary to explain the Condensed Matter Nuclear Phenomena in metal-hydrides. The proton-lithium fusion data, the astrophysical S-factor data, the K-electron capture data of beryllium, and the anomalous ratio of the isotope abundance of lithium in palladium-hydride (7Li/6Li) will be presented as an example for this justification. Thus, selective resonant tunneling model explains not only the 3 puzzles in Condensed Matter Nuclear Science (i.e. tunneling the Coulomb barrier, excess heat without commensurate neutron radiation, and the missing gamma radiation), but also 7 sets of hot fusion data. It predicts that there must be neutrino radiation accompanied with Condensed Matter Nuclear Phenomena in metal-hydrides.

[1] Xing Z. Li, et al., Nucl. Fusion 48 125003 (2008).

8:12AM Y33.00002 -dimensional Symmetry Catalysts for A-Z Gas Loading Fusion , TALBOT CHUBB, Greenwich Corp., Arlington, VA 22207 — An epitaxial mating of a metal layer to a chemically stable ionic crystal minimizes system energy for cold fusion based on Bloch function symmetry and using gas loading and nm-Pd at a favored interface.[1] To achieve epitaxy second and third metal layers need to have imperfections. One thinks of the stable ionic crystal as a template and the nano-Pd solid as a malleable lattice. The interior volume of the nano-Pd solid has a face-centered cubic structure. ZrO2 was the template ionic crystal used in A-Z gas loading studies at elevated T in (2005). A template crystal using the sapphire crystal equivalent of a double-layer graphene crystal is suggested. Impurity Rh and Ru are suggested as impurity atoms in the nano-metal (as in gem-quality Zircon) and a amall amount of interstitial H in addition to dominant D as involved in diffusion. Ref. [1] "Interface Modeling of Cold Fusion," Talbot A. Chubb, Proc. ICCF14, Book 2, pp 534-539 (2008).

8:24AM Y33.00003 Comparison of Calorimetry: MIT and Fleischmann-Pons Systems , MELVIN H. MILES, University of La Verne, La Verne, CA 91750, PETER HAGELSTEIN, Masschusetts Institute of Technology — The history of cold fusion shows that the MIT heat conduction calorimetry in 1990 reported a sensitivity of 40 mW while the Fleischmann-Pons Dewar calorimetry achieved a sensitivity of 0.1 mW. Additional information about the MIT calorimetry allows a more detailed analysis. The major finding is that the MIT calorimetric cell was so well insulated with glass wool (2.5 cm in thickness) that the major heat transport pathway was out of the cell top rather than from the cell into the constant temperature water bath. It can be shown for the MIT calorimeter that 58% of the heat transport was through the cell top and 42% was from the cell into the water bath. Analysis of the Fleischmann-Pons Dewar cell shows that under conditions similar to the MIT experiments, almost all of the heat flow would be from the Dewar calorimetric cell to the constant temperature water bath. Furthermore, the sensitivity of the Fleischmann- Pons temperature measurements was 0.001 K versus 0.1 K for the MIT calorimetric cell. Evaluations of the calorimetric equations and data analysis methods leads to the conclusion that the Fleischmann-Pons calorimetry was far superior to that of MIT.

8:36AM Y33.00004 Can LENR Energy Gains Exceed 1000? , DAVID J. NAGEL, The George Washington University — Energy gain is defined as the energy realized from reactions divided by the energy required to produce those reactions. Low Energy Nuclear Reactions (LENR) have already been measured to significantly exceed the energy gain of 10 projected from ITER,possibly 15 years from now. Electrochemical experiments using the Pd-D system have shown energy gains exceeding 10. Gas phase experiments with the Ni-H system were reported to yield energy gains of over 100. Neither of these reports has been adequately verified or reproduced. However, the question in the title still deserves consideration. If, as thought by many, it is possible to trigger nuclear reactions that yield MeV energies with chemical energies of the order of eV, then the most optimistic expectation is that LENR gains could approach one million. Hence, the very tentative answer to the question above is yes. However, if LENR could be initiated with some energy cost, and then continue to "burn," very high energy gains might be realized. Consider a match and a pile of dry logs. The phenomenon termed "heat after death" will be examined to see if it might be the initial evidence for nuclear "burning."

8:48AM Y33.00005 Lattice Assisted Nuclear Reactions From Nanostructured Metamaterials Electrically Driven at Their Optimal Operating Point , MITCHELL R. SWARTZ, JET Energy, PO Box 81135, Wellesley Hills, MA 02481 — In lattice assisted nuclear reactions, hydrogen-loaded alloys enable near room temperature deuterium fusion and other nuclear reactions (1). The structural metamaterial shape of some D-loaded Pd nanostructures and deuterium flux (2) through them, driven by an applied electric field, appear to play decisive roles. The spiral Phusor®-type cathode with open helical cylindrical geometry in a high electrical resistance solution is a LANR metamaterial design creating intrapalladial deuteron flow. Optimal operating point technology allows improved and more reproducible operation (3). LANR power gain can be considerable. In situ imaging has revealed that the excess power gain is linked to non-thermal near-IR emission when the LANR devices are operated at their OOP. LANR devices have shown power gains more than 200%, and short term power gains to $\sim$8000%. 1. Swartz, M, J. Sci. Exploration, 23, 4, 419-436 (2009). 2. Swartz, M, Fusion Technology, 22, 2, 296-300 (1992); 26, 4T, 74-77 (1994); 32, 126-130 (1997). 3. Swartz. M, Fusion Technology, 31, 63-74 (1997).

9:00AM Y33.00006 The Use of SSNTD's in the Pd-D Co-deposition Experiment , FRANCIS TANZELLA, Materials Research Laboratory, SRI International, Menlo Park, CA, 94025, USA. , MICHAEL M.C.H. MCKUBRE, SRI International, Menlo Park, CA, 94025, USA. — An early derivative experiment of the original Fleischman-Pons electrochemical experiment [1-3] was that of Szpak et al [4-5]. Szpak et al. chose to electro- deposit bulk metal palladium on a conductive metal substrate from a deuterium oxide (D2O) solution of a Pd salt, as opposed to electrolytically loading a bulk Pd cathode in a D2O solution. Recent work, by Boss et al [6] has concentrated on using solid state nuclear track detectors (SSNTD, specifically CR-39) to search for evidence of nuclear particles. In most of these experiments the CR-39 was immersed in the electrolyte, which makes the interpretation of the tracks potentially ambiguous because of the possibility of chemical damage. However, different interpretations of results presented have concluded that the data argue for the generation of alpha particles, protons, and/or neutrons. We have chosen to reproduce one version of these recent experiments using CR-39 immersed and separated from the electrolyte with a 6 μm thick piece of Mylar® film. A 60 μm thick piece of polyethylene, used as a protective cover during handling, was occasionally allowed to remain on the film to facilitate thermalization of possible product neutrons. 1. Fleischmann, M., S. Pons, and M. Hawkins, "Electrochemically induced nuclear fusion of deuterium". J. Electroanal. Chem., 1989. 261, 301

9:12AM Y33.00007 LENR BEC Clusters on and below Wires through Cavitation and Related Techniques , ROGER STRINGHAM, Firstgate Energies, PO Box 1230 Kilauea, HI 96754, Phone: 808 828 2859, JULIE STRINGHAM, Firstgate Energies, PO Box 1230 Kilauea, HI 96754 — During the last two years I have been working on BEC cluster densities deposited just under the surface of wires, using cavitation, and other techniques. If I get the concentration high enough before the clusters dissipate, in addition to cold fusion related excess heat (and other effects, including helium-4 formation) I anticipate that it may be possible to initiate transient forms of superconductivity at room temperature.

9:24AM Y33.00008 Use of Helium Production to Screen Glow Discharges for Low Energy Nuclear Reactions (LENR) , THOMAS O. PASSELL, TOP Consulting, P.O. Box 336, Palo Alto, CA 94302-0336 — My working hypothesis of the conditions required to observe low energy nuclear reactions (LENR) follows: 1) High fluxes of deuterium atoms through interfaces of grains of metals that readily accommodate movement of hydrogen atoms interstitially is the driving variable that produces the widely observed episodes of excess heat above the total of all input energy. 2) This deuterium atom flux has been most often achieved at high electrochemical current densities on highly deuterium-loaded palladium cathodes but is clearly possible in other experimental arrangements in which the metal is interfacing gaseous deuterium, as in an electrical glow discharge. 3) Since the excess heat episodes must be producing the product(s) of some nuclear fusion reaction(s) screening of options may be easier with measurement of those "ashes" than the observance of the excess heat. 4) All but a few of the exothermic fusion reactions known among the first 5 elements produce He-4. Hence helium-4 appearance in an experiment may be the most efficient indicator of some fusion reaction without commitment on which reaction is occurring. This set of hypotheses led me to produce a series of sealed tubes of wire electrodes of metals known to absorb hydrogen and operate them for $>$100 days at the $<$1 watt power level using deuterium gas pressures of $\sim$100 torr powered by 40 Khz AC power supplies. Observation of helium will be by measurement of helium optical emission lines through the glass envelope surrounding the discharge. The results of the first 18 months of this effort will be described.

9:36AM Y33.00009 Conventional Physics can Explain Excess Heat in the Fleischmann-Pons Cold Fusion Effect , SCOTT CHUBB, Infinite Energy Magazine — In 1989, when Fleischmann and Pons (FP) claimed they had created room temperature, nuclear fusion in a solid, a firestorm of controversy erupted. Beginning in 1991, the Office of Naval Research began a decade-long study of the FP excess heat effect. This effort documented the fact that the excess heat that FP observed is the result of a form of nuclear fusion that can occur in solids at reduced temperature, dynamically, through a deuteron (d)+d?helium-4 reaction, without high-energy particles or ? rays. This fact has been confirmed at SRI and at a number of other laboratories (most notably in the laboratory of Y. Arata, located at Osaka University, Japan). A key reason this fact has not been accepted is the lack of a cogent argument, based on fundamental physical ideas, justifying it. In the paper, this question is re-examined, based on a generalization of conventional energy band theory that applies to finite, periodic solids, in which d's are allowed to occupy wave-like, ion band states, similar to the kinds of states that electrons occupy in ordinary metals. Prior to being experimentally observed, the Ion Band State Theory of cold fusion predicted a potential d+d?helium-4 reaction, without high energy particles, would explain the excess heat, the helium-4 would be found in an unexpected place (outside heat- producing electrodes), and high-loading, x?1, in PdDx, would be required.

9:48AM Y33.00010 Electrochemical and Electron Probe Microanalysis Measurements on Nanostructured Palladium , JAN MARWAN, BAM Federal Institute for Research and Testing, Division VI.4 Surface technologies,12200 Berlin, Germany, VANESSA RACKWITZ, Forschung & Entwicklung, Rudower Chaussee 29, D-12489 Berlin, Germany — The hydrogen region of nanostructured Pd in the cyclic voltammetry in 1 M H2SO4 was more resolved than that of plain Pd because of the thin walls of the nanostructure and the high surface area. We could distinguish the hydrogen adsorption and absorption processes. The permeation of hydrogen into the Pd metal lattice occurs with fast kinetics when the Pd surface is blocked by either crystal violet or Pt. We believe that the hydrogen absorption process takes place without passing through the adsorbed state so that hydrogen diffuses directly into the Pd bulk. This process speeds up when the formation of adsorbed hydrogen is suppressed by the coverage of poisons. These results were compared to those obtained in a heavy water solution to which the Pd electrode was exposed. Adsorption characteristics of deuterium on the Pd metal surface are slightly different to those obtained for hydrogen in previous studies. Diffusion of deuterium into the Pd metal lattice works with fast kinetics under appropriate surface modification. We are also interested in studying the Pd structure before and after long term electrolysis in light and heavy water using electron probe micronanalysis (EPMA) with a energy dispersive spectrometer (EDS)

Friday, March 25, 2011 8:00AM - 11:00AM –
Session Y35 DCMP: Topological Insulators: Applications C140

8:00AM Y35.00001 Physical Vapor Deposition Growth of Topological Insulator Nanostructures[1] , LOREN ALEGRIA, ANASUA CHATTERJEE, ZHONG ZHANG, MICHAEL PRETKO, JAMES TING, SHIVANG PATEL, JASON PETTA, Princeton University — Nanostructures consisting of strong topological insulators are of interest for the fabrication of devices in which surface state transport is dominant. We report Bi_2Se_3 nanoribbon and nanoplatelet growth using a multi-zone furnace.[2] Nanoribbons are grown by the vapor-liquid-solid method, using Au nanoparticles or Au thin films ($\sim$5 nm) as catalysts, while nanoplatelets are grown on bare silicon. We systematically vary the growth parameters, including the temperatures of the powdered Bi_2Se_3 precursor and growth substrate, the growth pressure and duration, the rate of the Argon carrier gas flow, size of the gold catalyst, and the quantity of Bi_2Se_3 source material. Typical nanoribbon growth occurs at 450°C and 350 Torr, with the precursor held at 530°C in an Argon carrier gas flow rate rate of 140 sccm. Typical platelet growth occurs at lower pressures and temperatures. High resolution transmission electron microscopy, diffraction, and energy dispersive x-ray analysis are used to characterize the synthesized structures.

[1]Funded by the Sloan and Packard Foundations, and the NSF supported Princeton Center for Complex Materials.

[2]D. Kong *et al.*, Nano Lett. **10**, 329 (2010).

8:12AM Y35.00002 Topological insulators for high performance terahertz to infrared applications , XIAO ZHANG, Stanford University, JING WANG, Tsinghua University, SHOU-CHENG ZHANG, Stanford University — Topological insulators in the Bi2Se3 family have an energy gap in the bulk and a gapless surface state consisting of a single Dirac cone. Low frequency optical absorption due to the surface state is universally determined by the fine structure constant. When the thickness of these three dimensional topological insulators is reduced, they become quasi-two dimensional insulators with enhanced absorbance. The two dimensional insulators can be topologically trivial or non-trivial depending on the thickness, and we predict that the optical absorption is larger for topological non-trivial case compared with the trivial case. Since the three dimensional topological insulator surface state is intrinsically gapless, we propose its potential application in wide bandwidth, high performance photo-detection covering a broad spectrum ranging from terahertz to infrared. The performance of photodetection can be dramatically enhanced when the thickness is reduced to several quintuple layers, with a widely tunable band gap depending on the thickness.

8:24AM Y35.00003 Two Dimensional Transport Induced Linear Magneto-resistance in Topological Insulator Bi_2Se_3 Nanoribbons[1] , DONG LIANG, HAO TANG, RICHARD QIU, XUAN GAO, Dept of Physics, Case Western Reserve University, Cleveland, OH 44106 — Bulk Bi_2Se_3 has been proposed and confirmed as a type of three-dimensional (3D) topological insulators (TI's) with a single Dirac cone for the surface state. Although the existence of topological surface state in Bi_2Se_3 has been established by surface sensitive techniques (ARPES, STM), the transport properties of two dimensional (2D) surface state in 3D TI's has been plagued by the dominating conductivity from bulk carriers. Here, we report the study of a novel linear magneto-resistance (MR) under perpendicular magnetic fields in Bi_2Se_3 nanoribbons, and show that this linear MR is purely due to 2D transport by angular dependence experiments. The 2D magneto-transport induced linear MR in Bi_2Se_3 nanoribbons is in agreement with the recently discovered linear MR from topological surface state in bulk Bi_2Te_3, and the MR of other gapless semiconductors and graphene. We further show that the linear MR of Bi_2Se_3 nanoribbons persists up to room temperature, underscoring the potential of exploiting TI's for room temperature magneto-electronic applications.

[1]The authors thank ACS PRF grant #48800-DNI10 for partial funding support.

8:36AM Y35.00004 Quantum impurity spin in Majorana edge modes , RYUICHI SHINDOU[1], Department of Physics, Tokyo Institute of Technology, AKIRA FURUSAKI, Condensed Matter Theory Laboratory, RIKEN, Japan, NAOTO NAGAOSA, Department of Applied Physics, University of Tokyo and CERG and CMRG, RIKEN, Japan — We show that Majorana edge modes of two-dimensional spin-triplet topological superconductors (superfluids) have Ising-like spin density whose direction is determined by the d-vector characterizing the spin-triplet pairing symmetry in the bulk. Thus, when a quantum impurity spin is introduced at the edge of the spin-triplet topological superconductors (superfluids), the exchange coupling between this impurity spin and the Majorana modes becomes Ising-type. Observing this, we argue that, under the external magnetic fields, this quantum impurity spin exhibits anisotropic dissipative quantum dynamics due to the 'background' massless Majorana edge modes. We also discuss how the magnetic response of this impurity spin can serve as a local probe for spin-triplet superconducting order parameter in the bulk.

[1]This work was done when the first author was affiliated to Condensed Matter Theory Laboratory in RIKEN.

8:48AM Y35.00005 Surface state transport in Bi2Se3 nanodevices , HADAR STEINBERG, VALLA FATEMI, PABLO JARILLO-HERRERO, MIT — We report on electronic transport measurements on thin (<100 nm) Bi2Se3 devices and show that the density of the surface states can be modulated via the electric field effect by using a top-gate with a high-k dielectric insulator. The conductance dependence on geometry, gate voltage, and temperature all indicate that transport is governed by parallel surface and bulk contributions.

9:00AM Y35.00006 Thermoelectric transport of edge/surface states of topological insulators , SHUICHI MURAKAMI, Department of Physics, Tokyo Institute of Technology and PRESTO-JST, RYUJI TAKAHASHI, Department of Physics, Tokyo Institute of Technology — In my talk we theoretically study thermoelectric properties of topological insulators (TI) [1], where novel properties of edge/surface states are expected to appear. As compared to the number of bulk states, the edge/surface states are very few; we therefore consider a narrow ribbon for 2D and a thin slab for 3D TI to make the edge/surface-state transport larger. By considering edge/surface and bulk transport together, we calculate the charge and heat conductivity, and Seebeck coefficient. We find that in 2D TI the bulk and edge transport compete each other in the thermoelectric transport. By lowering temperature, the thermoelectric figure of merit ZT has a minimum, corresponding to the bulk-to-edge crossover, and then increases again at low temperature where the edge state dominates. The crossover is estimated to be at around 5K-10K for 10nm-width ribbon. We also discuss surface state transport for 3D TI as well.

[1] R. Takahashi and S. Murakami, Phys. Rev. B81, 161302 (R) (2010).
[2] S. Murakami, R. Takahashi, O. A. Tretiakov, Ar. Abanov, J. Sinova, arXiv:1010.2304.

9:12AM Y35.00007 Mobility and thermopower of surface and bulklike charges in Bi and Sb nanowires[1] , T.E. HUBER, Howard University, Washington, DC 20059, A. ADEYEYE, Howard University, Washington DC 20059, A. NIKOLAEVA, L. KONOPKO, Academy of Sciences of Moldova and International Laboratory of High Magnetic Fields and Low Temperature Physics, R.C. JOHNSON, M.J. GRAF, Boston College, Chestnut Hill, MA 02467 — Topological insulators (TI) surface charges are predicted to have high mobilities and other properties. Bi and Sb, that are classified as TI trivial and true, respectively, are interesting candidates but are not very good bulk insulators. However, in very thin nanowires, quantum confinement opens a gap for the bulk states that is not expected to change the material's TI character. We studied the electronic transport of 18-nm to and 200-nm diameter nanowires in arrays, fabricated by Bi injection in porous alumina, via coupled measurements of resistance and thermopower (4-300 K). Surface carriers and holes Landau level spectra were analyzed to extract densities. The nanowires low temperature thermopower (T<100 K) is -1 T microvolt/(K^2) consistent in sign and magnitude with surface electrons. Coexistence of bulklike holes with surface electrons, consistent with the carrier's hybridization that is expected in Bi, is observed. Results for Sb will be presented also.

[1]Support by Army Research Office, Materials and National Science Foundation (PREM) is acknowledged.

9:24AM Y35.00008 Raman spectroscopy of exfoliated Bi2Se3 , LUKE SANDILANDS, FRANK ZHAO, CHRISTIANNE BEEKMAN, JOHN BASHUCKY, University of Toronto, DANIEL KWOK, Rutgers University, NARA LEE, SANG-WOOK CHEONG, Rutgers University, KENNETH BURCH, University of Toronto — The study of topological insulators is often frustrated by the presence of a residual bulk conductivity arising from defects which makes isolating the surface contribution to a given measurement difficult. Nanoscale topological insulators are therefore an appealing alternative to bulk crystals, as a small volume should emphasize surface contributions and allow the suppression of the residual bulk carriers by gating. To this end we have produced, via mechanical exfoliation, nanocrystals as thin as a 2 nm of the topological insulator Bi2Se3 on Mica substrates. Exfoliated crystals of a variety of thicknesses have been characterized by optical, Raman, and atomic force microscopies. We observe an emergent mode at 158 cm-1 which is attributed to the breaking of inversion symmetry at the Bi2Se3 surfaces. The utility of this emergent mode for determining nanocrystal thickness is discussed.

9:36AM Y35.00009 Mechanical Exfoliation and Electron Transport of Topological Insulator Nanoribbons , SEUNG SAE HONG, WORASOM KUNDHIKANJANA, Department of Applied Physics, Stanford University, JUDY CHA, Department of Materials Science and Engineering, Stanford University, KEJI LAI, Department of Applied Physics, Stanford University, DESHENG KONG, Department of Materials Science and Engineering, Stanford University, ZHI-XUN SHEN, Department of Applied Physics, Stanford University, YI CUI, Department of Materials Science and Engineering, Stanford University — Bismuth selenide (Bi_2Se_3), a stoichiometric material of a single Dirac-cone band structure, is one of the most promising candidates to realize the topologically non-trivial surface state protected by time reversal symmetry. Especially, many exotic physical phenomena are predicted to emerge in low dimensional nanostructures of Bi_2Se_3, such as the crossover between 3D to 2D topological insulator. Due to the weak Van der Waals interaction between adjacent quintuple layers (QLs), Bi_2Se_3 can be exfoliated down to a few QLs. We will present the mechanical exfoliation of topological insulator nanoribbons by an atomic force microscope (AFM) tip, which enables ultra-thin topological insulator down to a single QL. Electron transport measurement on low dimensional topological insulator will be also discussed, as well as the conductivity mapping experiment using a microwave scanning probe technique.

9:48AM Y35.00010 Topological surface states along antiwires , ALEXANDER PUNNOOSE, WEI LIU, City College of New York — Surface states along amorphous columnar defects in three-dimensional topological insulators are considered. The response of these states to a magnetic field and their contribution to thermoelectric transport will be discussed.

10:00AM Y35.00011 Bias dependence of h/e and h/2e Aharonov-Bohm oscillations in topological insulators[1] , PRAMEY UPADHYAYA, FAXIAN XIU, YABIN FAN, IGOR OVCHINNIKOV, KANG WANG, University of California Los Angeles, UNIVERSITY OF CALIFORNIA LOS ANGELES TEAM — Recently Aharonov-Bohm (AB) oscillations were observed in Bi_2Se_3 nanoribbons by Peng *et al.* [1] as a direct evidence for the existence of surface states in topological insulator. However, the resistance showed only h/e oscillations with a minimum in resistance at zero flux while the ballistic and diffusive theory predicts either h/e oscillations with a maximum in resistance at zero flux or h/2e oscillations with a minimum in resistance at zero flux respectively [2]. A possible explanation of the results of Peng *et al.* was given in the theory of disordered topological insulators proposed by Bardarson *et al* .[2] and Zhang *et al.* [3] where they attributed the results of Peng *et al.* to presence of weak disorder. Furthermore authors of [2] and [3] studied dependence of h/e and h/2e oscillations on disorder strength and doping using their proposed theory. In this work we look at the effect of doping by studying bias dependence of AB oscillations using a gated device and observe both h/e and h/2e oscillations whose relative strength depends on the applied bias and compare the proposed theory of ref. [2] and [3] with the experimental results. [1] H. Peng, *et al.* Nature Mater. 9, 225 (2010).[2] J. Bardarson, *et al*, Phys. Rev. Lett. 105, 156803 (2010).[3] Y. Zhang and A. Vishwanathan, Phys. Rev. Lett. 105, 206601 (2010).

[1]This work was in part supported by Marco Focus Center on FENA -Functional Engineered Nano Architectoncis.

10:12AM Y35.00012 Spin polarization and transport of surface states in the topological insulators Bi_2Se_3 and Bi_2Te_3 from first principles[1] , OLEG YAZYEV, JOEL MOORE, STEVEN LOUIE, UC Berkeley and LBNL — We investigate the band dispersion and the spin texture of topologically protected surface states in the reference bulk topological insulators Bi_2Se_3 and Bi_2Te_3 by using a first-principles approach. Exceptionally strong spin-orbit interaction in these materials entangles the electronic states across broad energy ranges thus reducing the spin-polarization of the topologically protected surface states to ∼50% in both cases. This reduction is absent in simple phenomenological models but of important implications to essentially any application of bulk topological insulators in spintronics and likely to some other phenomena. We further propose a way of controlling the magnitude of spin polarization associated with a charge current in thin films of topological insulators by means of an external electric field. The proposed dual-gate device configuration provides new possibilities for electrical control of spin.

[1]Support by NSF Grant Nos. DMR07-05941, DMR08-04413, US DOE Cont. No. DE-AC02-05CH1123 and Swiss NSF Fellowship PBELP2-123086. Computer resources provided by NICS.

10:24AM Y35.00013 Manipulating surface states in topological insulator nanostructures , FAXIAN XIU, LIANG HE, KANG L. WANG, University of California Los Angeles — Topological insulators show unique properties resulting from massless, Dirac-like surface states that are protected by time-reversal symmetry. Theory predicts that the surface states exhibit quantum spin Hall effect that allows for spins to transport without scattering. However, to date, the direct manipulation of these states with external means remains a significant challenge owing to the predominance of bulk carriers. Here we show the first experimental evidence of surface-state modulation through the observation of voltage-controlled quantum oscillations in Bi2Te3 nanostructures. The surface conduction can be dramatically enhanced with external gate bias. Up to 51 percent of the total conductance is attributed to the surface states. The ability to manipulate the surface states mark an important milestone in the development of TI materials and may further open up exciting and novel applications in nanoelectronics and spintronics.

10:36AM Y35.00014 Aharonov-Bohm oscillations in disordered topological insulator nanowires , JENS H. BARDARSON, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA, P.W. BROUWER, Dahlem Center for Complex Quantum Systems and Institut fur Theoretische Physik, Freie Universitat Berlin, Arnimallee 14, 14195 Berlin, Germany, J.E. MOORE, Department of Physics, University of California, Berkeley, Berkeley, California 94720, USA — A direct signature of electron transport at the metallic surface of a topological insulator is the Aharonov-Bohm oscillation observed in a recent study of Bi_2Se_3 nanowires [Peng *et al.*, Nature Mater. 2010] where conductance was found to oscillate as a function of magnetic flux ϕ through the wire, with a period of h/e and $maximum$ conductance at zero flux. This seemingly agrees neither with diffusive theory (period of $h/2e$) nor with ballistic theory, which in the simplest form predicts a period of h/e but a $minimum$ at zero flux due to a nontrivial Berry phase. We show how the magneto-conductance depends on doping and disorder strength, provide a possible explanation for the experiments, and discuss further experiments that could verify the theory.

10:48AM Y35.00015 Terahertz conductivity of Bi_2Se_3 topological insulator thin films[1] , ROLANDO VALDÉS AGUILAR, L.S. BILBRO, Department of Physics & Astronomy, Johns Hopkins University, Baltimore, MD 21218, N. BANSAL, Y-S. KIM, S. OH, Department of Physics & Astronomy, Rutgers University, Piscataway, NJ 08854, C. CHANG, Y. ZHANG, K. HE, X. MA, Institute of Physics, The Chinese Academy of Sciences, Beijing, 100190, P.R. China, X. ZHU, Q-K. XUE, Department of Physics, Tsinghua University, Beijing, 100084, P. R. China, N.P. ARMITAGE, Department of Physics & Astronomy, Johns Hopkins University, Baltimore, MD 21218 — We report a study of high quality MBE grown Bi_2Se_3 topological insulator thin films. We have measured the ac conductivity in the terahertz region using time domain terahertz spectroscopy. By measuring films with different thickness we can set limits on the value of the bulk and surface conductivites. We will also report on measurements of the Faraday rotation using polarized light at these frequencies.

[1]Work supported by The Institute of Quantum Matter under DOE grant DE-FG02-08ER46544 and by the Gordon and Betty Moore Foundation.

Friday, March 25, 2011 8:00AM - 10:36AM –

Session Y36 DCMP: Graphene: Optical Properties II C142

8:00AM Y36.00001 Raman spectroscopy of graphite in high magnetic fields , YOUNGHEE KIM, National High Magnetic Field Laboratory, ANTONIO LOMBARDO, Engineering Department, Cambridge University, NIKOLAI G. KALUGIN, Department of Materials and Metallurgical Engineering, New Mexico Tech, JUNICHIRO KONO, Department of Electrical & Computer Engineering, Rice University, ANDREA C. FERRARI, Engineering Department, Cambridge University, DMITRY SMIRNOV, National High Magnetic Field Laboratory — Recently, much attention has been paid to electron-phonon coupling in graphene. In particular, significant re-normalization and broadening of long-wavelength optical phonons are predicted to occur through resonant interaction with Landau-quantized Dirac fermions. We report here on a high-field magneto-Raman spectroscopy study of highly-oriented pyrolytic graphite (HOPG) and natural graphite at temperatures down to 5 K and in magnetic fields up to 45 T. The E_{2g} graphite phonon line exhibits anticrossing-like behavior at approximately 30 T, which we attribute to the magneto-phonon resonance (MPR) of graphite's massless holes at the H-point. Additionally, we observed features related to inter-Landau-level transitions at the K-point of graphite. We also observed weak graphene-like signatures of MPR, indicating the existence of graphene flakes on the graphite surface.

8:12AM Y36.00002 Raman measurements of graphene in magnetic fields , SEBASTIAN REMI, ANNA SWAN, BENNETT B. GOLDBERG, Boston University — Electron phonon interactions in graphene are effectively measured using Raman spectroscopy. For example the G-Band of graphene grown on SiC shows characteristic anticrossings when tuning an external magnetic field exactly at the resonances between the G-Band phonon and the electronic Landau Levels. We measure the micro Raman spectra of mechanically exfoliated graphene lithographically prepared as field effect devices. Unlike prior high magnetic field studies, this provides charge tunability and allows simultaneous Raman and transport measurements under variable B-field. Our initial results show a Landau Level dependent splitting of the G-band for magnetic fields B $>$ 10T. We present our latest results of studies of the Raman G and 2D Band and single and bilayer graphene at T=4.2K and fields to 12T.

8:24AM Y36.00003 Raman Maps of Carbon Nanoscrolls and their Bundles , GUANGJUN CHENG, IRENE CALIZO, XUELEI LIANG, BRENT SPERLING, JAMES MASLAR, CURT A. RICHTER, ANGELA R. HIGHT WALKER, National Institute of Standards and Technology (NIST), Gaithersburg, MD 20899 — Recent theoretical simulations and experimental data have shown that carbon nanoscrolls, formed by rolling a single layer of graphene, exhibit different electronic and optical properties from carbon nanotubes or the planar graphene sheet. They hold promise in a variety of applications areas such as energy storage and nanomechanics. Here, we present our investigation on the formation of carbon nanoscrolls and their bundles from large-area graphene originally grown on copper foil by chemical vapor deposition. When graphene is transferred from a copper foil onto a silicon wafer using wet chemistry, both filled and unfilled carbon nanoscrolls are produced upon the rupture of graphene. These nanoscrolls can further form bundles. The results from Raman mapping, optical microscopy, scanning electron microscopy, and atomic force microscopy measurements will be presented and the formation mechanism will be discussed.

8:36AM Y36.00004 Controlling Inelastic Light Scattering Quantum Pathways in Graphene , JASON HORNG, CHI-FAN CHEN, CHEOL-HWAN PARK, BRYAN W. BOUDOURIS, BAISONG GENG, CAGLAR GIRIT, ALEX ZETTL, MICHAEL CROMMIE, RACHEL SEGALMAN, STEVEN LOUIE, FENG WANG, UC Berkeley — Graphene exhibits unique tunable optical properties. Researchers have observed infrared absorptions in graphene interband transitions as well as intraband transitions can be modified substantially through electrostatic gating. At the same time, inelastic Raman scattering from few layer graphene is readily observable and widely used to characterize graphene quality, and to probe graphene electron-phonon interactions. In strongly gated graphene, Raman scattering from graphene can also be varied from electrical doping through direct change of electronic transitions. In this talk, I will describe how the Raman intensity of G-mode and 2D-mode Raman varies with the Fermi energy in doped graphene.

8:48AM Y36.00005 Ab initio calculation of double-resonant Raman spectra for bilayer graphene , PAOLA GAVA, LSI - Ecole Polytechnique, MATTEO CALANDRA, MICHELE LAZZERI, FRANCESCO MAURI, IMPMC - Universite Paris 6 — The discovery that the application of an external electric field induces a band gap opening in bilayer graphene attracted a lot of interest on this system, due to important applications in nanoelectronics [1]. Raman spectroscopy is one of the most important experimental techniques for the characterisation of carbon based materials, providing informations on carriers concentration [2], disorder [3], number of layers on multi-layers graphene systems [4], and phonon properties. Most of the theoretical studies on multi-layers graphene are performed using a Tight Binding (TB) model, and full calculation of Raman matrix elements to obtain frequencies, intensities and linewidths of Raman bands has not been performed up to now. The developpement of a fully ab initio theoretical tool to compute Raman spectra is therefore higly desirable and particularly relevant for systems where a simple TB parametrization of the electronic structure and of the electron-phonon interaction is not available. In this talk I will discuss a recently developped methodology to compute fully ab initio double-resonant Raman spectra and I will present results for bilayer graphene.

[1] Ohta et al, Science **313**, 951 (2006), [2] Malard et al, PRL **101**, 257410 (2008), [3] Lucchese et al, Carbon **48**, 1592 (2010), [4] Ferrari et al, PRL **97**, 187401 (2006)

9:00AM Y36.00006 Observation of out-of-plane vibrations in few-layer graphene using combination and overtone Raman modes , SUK HYUN KIM, CHUN HUNG LUI, LEANDRO MALARD, GABRIEL LANTZ, FRANÇOIS LAVERGE, Columbia University, RIICHIRO SAITO, Tohoku University, TONY HEINZ, Columbia University, HEINZ TEAM, SAITO TEAM — We have studied three distinct higher-order Raman features, appearing at $\sim$ 1660, 1730 and 1760 cm^{-1}, in graphene samples of 1-6 layers thickness and both Bernal and rhombohedral stacking. By detailed analysis of the measured dispersions of these lines using double-resonance theory, we have identified the features, respectively, as the LO+ZA, LO+ZO' combination modes and the 2ZO overtone mode. Here LO, ZA, and ZO, and ZO' denote, respectively, the in-plane longitudinal optical mode, the out-of-plane acoustic, optical and layer-breathing modes. All three of these Raman features are absent in single-layer graphene, which lacks the layer-breathing vibration and exhibits particularly high symmetry. The line shape of LOZO' mode shows a dramatic dependence on the stacking order of the layers and can serve as a means of identifying stacking order in few-layer graphene. In addition, the LOZO' mode allows us to access the properties of the low-energy layer-breathing (ZO') mode in few-layer graphene samples.

9:12AM Y36.00007 Infrared Kerr and Faraday Measurements in Gated, Multi-Layer SiC Graphene , C.T. ELLIS, A.V. STIER, A. STABILE, M.-H. KIM, G. SAMBANDAMURTHY, B.D. MCCOMBE, J. CERNE, Dept of Physics, University at Buffalo, SUNY, B.J. SCHULTZ, S. BANERJEE, Dept of Chemistry, University at Buffalo, SUNY, J.G. TISCHLER, Naval Research Laboratory — Magneto-optical Kerr and Faraday measurements are used to probe the Landau level structure of SiC graphene in the mid- and far-infrared regimes (100-1000 meV and 3-10 meV, respectively). Transmittance/reflectance spectroscopy probes the longitudinal conductivity (σ_{xx}), which is related to the sum of chiral response. In contrast, polarization sensitive techniques provide new insights into the electronic structure by probing the Hall conductivity (σ_{xy}), which reflects the difference in the chiral response. Samples, which are studied in applied fields (B) up to 7T and temperatures ranging from 10-300K, show robust features arising from two distinct sets of Landau level transitions. One set displays transition energies that are $\sqrt{B}$ dependent as expected of monolayer graphene. Interestingly, below a critical photon energy ($\sim$100 meV) these features become symmetric with B. The other set is consistent with expectations of bilayer graphene and graphite, showing a linear B dependence and the expected odd symmetry in B. Further investigation of Landau level behavior is accomplished by tuning the Fermi energy in samples with a gate. Work supported by NSF-DMR1006078.

9:24AM Y36.00008 Landau level-phonon resonances in graphene and their spectroscopic signatures in magneto-optical measurements , LIANG Z. TAN, Department of Physics, University of California at Berkeley, and Materials Sciences Division, Lawrence Berkeley National Lab, CHEOL-HWAN PARK, Department of Materials, University of Oxford, GERARD MARTINEZ, LNCMI, CNRS, Grenoble, France, STEVEN G. LOUIE, Department of Physics, University of California at Berkeley, and Materials Sciences Division, Lawrence Berkeley National Lab — The excited states and the optical spectra of a two-dimensional electronic system under a magnetic field are strongly influenced by the electron-phonon interaction when the energy spacing of the Landau levels is resonant with the frequency of an optical phonon. We have performed a theoretical study of these excited states in graphene, and have calculated the optical absorption spectra for a range of magnetic fields. Electron-electron interactions are found to redistribute the spectral weight of the coupled modes and have important consequences for the absorption spectra. Our results are in good agreement with recent magneto-optical transmission experiments on epitaxial graphene on SiC. This work was supported by NSF Grant No. DMR10-1006184 and U.S. DOE Contract No. DE- AC02-05CH11231.

9:36AM Y36.00009 Probing plasmons in graphene , LONG JU, BAISONG GENG, JASON HORNG, CAGLAR GIRIT, Dept of Physics, University of California at Berkeley, MICHAEL MARTIN, ZHAO HAO, HANS BECHTEL, Advanced Light Source Division, Lawrence Berkeley National Laboratory, XIAOGAN LIANG, Molecular Foundry, Lawrence Berkeley National Laboratory, ALEX ZETTL, FENG WANG, Dept of Physics, University of California at Berkeley — Plasmon behaviour in graphene is important for the understanding of many body interaction of 2D Dirac fermions. It also provides physical background for potential graphene applications in optoelectronics and ultrahigh speed THz electronics. In this talk, we will describe our study of plasmon behaviour in graphene using far-infrared spectroscopy and compare our experimental results to theoretical predictions.

9:48AM Y36.00010 Plasmon-Enhanced Photocurrent in a Graphene Nanoconstriction , SU-FEI SHI, Cornell University, XIAODONG XU, University of Washington, P.L. MCEUEN, D.C. RALPH, Cornell University — A plasmonic nanostructure can act like an optical antenna, concentrating light into a deep sub-wavelength volume and enabling manipulation of light-electron interactions at the nanometer scale. Achieving efficient coupling from such antennas to functional electrical devices has been challenging, because the region of field enhancement is so small. We report the use of a use a self- aligned fabrication process to couple a gold break junction acting as a plasmonic antenna with a sub-10-nm graphene constriction. The nonlinear electrical characteristics of the graphene device allow it to serve as a photodetector. We observe a photocurrent that is peaked at the plasmon frequency and strongly modulated by the polarization direction of the incident light. The enhancement of the local optical-frequency electric field induced by the plasmon is a factor of 1.5-10.

10:00AM Y36.00011 Thermal broadening effects on unstable plasmons in extrinsic graphene with injected carriers[1] , BEN YU-KUANG HU, The University of Akron, ANTTI-PEKKA JAUHO, Danmarks Tekniske Universitet and Aalto University — We study theoretically the charge density collective oscillations (plasmons) of an extrinsic (*i.e.*, doped) graphene system into which charge carriers (either electrons or holes) are injected. When the injected carriers are sharply peaked so that the distribution function of the injected carriers can be well approximated by $f_{\text{inject}}(\mathbf{p}) = n\delta(\mathbf{p} - \mathbf{p}_0)$, some of the plasmons in the system become unstable, in the sense that the amplitudes of these plasmons grow exponentially in time (at least initially, in the linear-response regime). This effect is analogous to the two-stream instability that is seen in classical plasma systems. As with the classical plasma system, thermal broadening of the injected carriers tends to suppress the instability. We report a theoretical study of the effect of the thermal broadening of the injected carriers on the plasmon instability in graphene, and we delineate the parameters where the thermal effects completely suppress the instability.

[1]Supported by the FiDiPro program at Aalto University and a Faculty Summer Fellowship at the University of Akron

10:12AM Y36.00012 Electromagnetic wave propagation through a graphene-based photonic crystal , OLEG BERMAN, VLADIMIR S. BOYKO, ROMAN YA. KEZERASHVILI, New York City College of Thechnology, City University of New York — A novel type of photonic crystal formed by embedding a periodic array of constituent stacks of alternating graphene and dielectric discs into a background dielectric medium is proposed [1]. The frequency band structure of a 2D photonic crystal with the square lattice of the metamaterial stacks of the alternating graphene and dielectric discs is obtained. The electromagnetic wave transmittance of such photonic crystal is calculated. The graphene-based photonic crystals have the following advantages that distinguish them from the other types of photonic crystals. They can be used as the frequency filters and waveguides for the far infrared region of spectrum at the wide range of the temperatures including the room temperatures. The photonic band structure of the graphene-based photonic crystals can be controlled by changing the thickness of the dielectric layers between the graphene discs and by the doping. The sizes of the graphene-based photonic crystals can be much larger than the sizes of metallic photonic crystals due to the small dissipation of the electromagnetic wave. The advantages of the graphene-based photonic crystal are discussed.

[1] O. L. Berman, V. S. Boyko, R. Ya. Kezerashvili, A. A. Kolesnikov, and Yu. E. Lozovik, Phys. Letts. A 374, 4784 (2010).

10:24AM Y36.00013 Effects of Layer Stacking on the Combination Raman Modes in Graphene , RAHUL RAO, Air force research laboratory, RAMAKRISHNA PODILA, Clemson University, RYUICHI TSUCHIKAWA, JYOTI KATOCH, DEREK TISHLER, University of Central Florida, APPARAO RAO, Clemson University, MASA ISHIGAMI, University of Central Florida — We have observed new combination modes in the range from 1650 – 2300 cm^{-1} in single-(SLG), bi-, few-layer and incommensurate bilayer graphene (IBLG) on silicon dioxide substrates. The M band at $\sim$1750 cm^{-1} is suppressed for both SLG and IBLG. A peak at $\sim$1860 cm^{-1} (iTALO$^-$) is observed due to a combination of the iTA and LO phonons. The intensity of this peak decreases with increasing number of layers and this peak is absent in bulk graphite. Two previously unidentified modes at $\sim$1880 cm^{-1} (iTALO$^+$) and $\sim$2220 cm^{-1} (iTOTA) in SLG are tentatively assigned as combination modes around the K point of the graphene Brillouin zone. The peak frequencies of the iTALO$^+$ (iTOTA) modes are observed to increase (decrease) linearly with increasing graphene layers.

Friday, March 25, 2011 8:00AM - 10:48AM –

Session Y38 DCP DBP: Focus Session: Non-Equilibrium Insights into Single Molecules and Cell Function II A130/131

8:00AM Y38.00001 Can Simple Biophysical Principles Yield Complicated Biological Functions? , JAN LIPHARDT, Physics Dept., UC Berkeley — About once a year, a new regulatory paradigm is discovered in cell biology. As of last count, eukaryotic cells have more than 40 distinct ways of regulating protein concentration and function. Regulatory possibilities include site-specific phosphorylation, epigenetics, alternative splicing, mRNA (re)localization, and modulation of nucleo-cytoplasmic transport. This raises a simple question. Do all the remarkable things cells do, require an intricately choreographed supporting cast of hundreds of molecular machines and associated signaling networks? Alternatively, are there a few simple biophysical principles that can generate apparently very complicated cellular behaviors and functions? I'll discuss two problems, spatial organization of the bacterial chemotaxis system and nucleo-cytoplasmic transport, where the latter might be true. In both cases, the ability to precisely quantify biological organization and function, at the single-molecule level, helped to find signatures of basic biological organizing principles.

8:36AM Y38.00002 Single-Molecule Analysis of Protein Large-Amplitude Conformational Transitions , HAW YANG, Princeton Uninversity — Proteins have evolved to harness thermal fluctuations, rather than frustrated by them, to carry out chemical transformations and mechanical work. What are, then, the operation and design principles of protein machines? To frame the problem in a tractable way, several basic questions have been formulated to guide the experimental design: (a) How many conformational states can a protein sample on the functionally important timescale? (b) What are the inter-conversion rates between states? (c) How do ligand binding or interactions with other proteins modulate the motions? (d) What are the structural basis of flexibility and its underlying molecular mechanics? Guided by this framework, we have studied protein tyrosine phosphatase B, PtpB, from M. tuberculosis (a virulence factor of tuberculosis and a potential drug target) and adenylate kinase, AK, from E. coli (a ubiquitous energy-balancing enzyme in cells). These domain movements have been followed in real time on their respective catalytic timescales using high-resolution single-molecule Förster resonance energy transfer (FRET) spectroscopy. It is shown quantitatively that both PtpB and AK are capable of dynamically sampling two distinct states that correlate well with those observed by x-ray crystallography. Integrating these microscopic dynamics into macroscopic kinetics allows us to place the experimentally measured free-energy landscape in the context of enzymatic turnovers.

9:12AM Y38.00003 Unfolding proteins with mechanical forces: From toy models to atomistic simulations[1] , DMITRII MAKAROV, University of Texas at Austin — The remarkable combination of strength and toughness, displayed by certain biological materials (e.g. spider silk) and often unmatched by artificial materials, is believed to originate from the mechanical response of individual load-bearing protein domains. Single-molecule pulling experiments carried out during the last decade showed that those proteins, when loaded, respond in a non-equilibrium fashion and can dissipate large amounts of energy though the breaking of sacrificial bonds. In my talk, I will discuss what structural properties correlate with mechanical strength and toughness at the single-molecule level, how thermodynamic stability is related to the mechanical stability, and why both atomistic simulations and simple models seem to fail to reconcile the mechanical responses of the same proteins measured under varied loading regimes. I will further discuss whether it is easier to unfold a protein mechanically by pulling at its ends or by threading it through a narrow pore. The latter process is believed to commonly occur in living organisms as an intermediate step in protein degradation.

[1]Supported by the NSF and the Robert A. Welch Foundation

9:48AM Y38.00004 Non-equilibrium microrheology of living cells , MING-TZO WEI, Bioengineering, Lehigh University, Bethlehem, PA, USA 18015, H. DANIEL OU-YANG, Physics and Bioengineering, Lehigh University, Bethlehem, PA, USA 18015 — Intracellular stresses generated by molecular motors can actively modify cytoskeletal network and change intracellular mechanical properties. We study the out-of-equilibrium microrheology in living cells using endogenous organelle particles as probes. This paper reports measurements of the intracellular mechanical properties using passive, particle-tracking and active, optical tweezers-based microrheology approaches. Using arguments based on the fluctuation-dissipation theorem, we compared the results from both approaches to distinguish thermal and non-thermal mechanical fluctuations in living cells.

10:00AM Y38.00005 Dissecting the heterogeneity of gene expressions in mouse embryonic stem cells[1] , LING-NAN ZOU, MATT THOMSON, S. JOHN LIU, FAS Center for Systems Biology, Harvard University, SHARAD RAMANATHAN, Department of Molecular and Cellular Biology, FAS Center for Systems Biology, Harvard University — A population of genetically identical cells, of the same nominal cell type, and cultured in the same petri dish, will nevertheless often exhibit varying patterns of gene expression. Taking mouse embryonic stem (ES) cells as a model system, we use immunofluorescence and flow cytometry to examine in detail the distribution of expression levels for various transcription factors key to the maintenance of the ES cell identity. We find the population-level distribution of many proteins, once rescaled by the average expression level, have very similar shapes. This suggest the largest component of observed heterogeneity comes from a single source. More subtly, we find the expression many of genes appears to modulate with the cell cycle. This may suggest that the program for maintaining ES cell identity is tightly coupled to the cell cycle machinery.

[1]This work is supported by the Harvard Stem Cell Institute and the Jane Coffin Childs Memorial Fund for Medical Research.

10:12AM Y38.00006 Synchronization of Cell Cycle Oscillator by Multi-pulse Chemical Perturbations , YIHAN LIN, YING LI, AARON DINNER, NORBERT SCHERER, University of Chicago — Oscillators underlie biological rhythms in various organisms and provide a timekeeping mechanism. Cell cycle oscillator, for example, controls the progression of cell cycle stage and drives cyclic reproduction in both prokaryotes and eukaryotes. The understanding of the underlying nonlinear regulatory network allows experimental design of external perturbations to interact and control cell cycle oscillation. We have previously demonstrated in experiment and in simulation that the cell cycle coherence of a model bacterium can be progressively tuned by the level of a histidine kinase. Here, we present our recent effort to synchronize the division of a population of bacterium cells by external pulsatile chemical perturbations. We were able to synchronize the cell population by phase-locking approach: the external oscillator (i.e. periodic perturbation) entrains the internal cell cycle oscillator which is in analogous to the phase-locking of circadian clock to external light/dark oscillator. We explored the ranges of frequencies for two external oscillators of different amplitudes where phase-locking occurred. To our surprise, non-periodic chemical perturbations could also cause synchronization of a cell population, suggesting a Markovian cell cycle oscillation dynamics.

10:24AM Y38.00007 Analysis of Cell Cycle Phase Response Captures the Synchronization Phenomena and Reveals a Novel Cell Cycle Network Topology , YING LI, YIHAN LIN, NORBERT SCHERER, AARON DINNER, University of Chicago — Cell cycle progression requires a succession of temporally-regulated sub-processes, including chromosome replication and cell division, which are each controlled by their own regulatory modules. The modular design of cell cycle regulatory network allows robust environmental responses and evolutionary adaptations. It is emerging that some of the cell cycle modules involve their own autonomous periodic dynamics. As a consequence, the realization of robust coordination among these modules becomes challenging since each module could potentially run out of sync. We believe that an insight into this puzzle resides in the coupling between the contributing regulatory modules. Here, we measured the phase response curve (PRC) of the cell cycle oscillator by driving the expression of a master regulator of the cell cycle in a pulsatile manner and measuring the single cell phase response. We constructed a return map that quantitatively explains the synchronization phenomena that were caused by periodic chemical perturbation. To capture the measured phase response, we derived a minimalist coupled oscillator model that generalizes the basic topology of the cell cycle network. This diode-like coupling suggests that the cell is engineered to ensure complete coordination of constituent events with the cell cycle.

10:36AM Y38.00008 Swimming Response of Individual Paramecia to Variable Forces[1] , ILYONG JUNG, MICHAEL WAGMAN, JAMES M. VALLES, JR., Brown University — Experiments demonstrate that swimming paramecia exhibit a negative force-kinetic response. In particular, upward swimming paramecia exert a stronger propulsive force as they fight their tendency to sediment. This response is remarkable because it suggests that paramecia can sense forces as small as their apparent weight, which is less than 100 pN. We are investigating the origins of this response by applying variable magnetic forces to individual swimming paramecia and measuring how their swimming trajectories change. We conduct the experiments at the National High Magnetic Field Laboratory where it is possible to achieve forces sufficient to stall the swimmers. We will present our latest data on how paramecia adjust the geometry of their helical trajectories under varying forces.

[1]This work is supported by the NSF through PHY0750360 and the NHMFL.

Friday, March 25, 2011 8:00AM - 10:48AM –

Session Y39 DCP: Focus Session: Imaging and Interfaces in Energy Science A124/127

8:00AM Y39.00001 Imaging Interfacial Structure and Reactivity with X-ray Reflectivity and Microscopy[1] , PAUL FENTER, Argonne National laboratory — A fundamental understanding of interfacial reactions is best achieved with ability to observe the systems of interest directly, ideally with molecular-scale resolution and/or sensitivities. X-ray-based approaches offer broad opportunities for probing complex interfaces in environments (e.g., liquids) that are normally inaccessible. I will describe two complimentary approaches for imaging interfaces. The first, X-ray reflection interface microscopy (XRIM), uses the weak interface-reflected X-ray beam to image laterally heterogeneous interfacial structures and processes using a full-field imaging approach. This approach incorporates all of the sensitivities of X-ray reflectivity (XR, including sensitivity to interfacial topography, structure and composition) as potential contrast mechanisms. Recent applications of XRIM will be described, including the abilities to observe: elementary surface topography (i.e., 6.5 Å-high steps) with ∼100 nm spatial resolution; interfacial reactivity; and liquid-solid interfaces, in-situ. A second, complementary, approach images the vertical distributions of element-specific sub-structures at an interface through the use of resonant dispersion at X-ray energies close to element's absorption edge (resonant anomalous X-ray reflectivity, RAXR). Recent applications of RAXR will be described including the ability to image element-specific distributions (i.e., ions near a charged liquid-solid interface) and its sensitivity for probing oxidation state specific structures at interfaces. The use of these techniques to observe charge transport at interfaces with respect to energy-related processes will be discussed.

[1]This work supported by the Geoscience Research Program of the US Department of Energy, Office of Basic Energy Sciences. This work is done in collaboration with M. J. Bedzyk, J. Catalano, S. S. Lee, C. Park, N. C. Sturchio, Z. Zhang, and P. Zschack.

8:36AM Y39.00002 Small-Pore Molecular Sieves SAPO-34 with Chabazite Structure: Theoretical Study of Silicon Incorporation and Interrelated Catalytic Activity , HONG WANG, JAMES LEWIS, West Virginia University, ZHONGMIN LIU, Dalian Institute of Chemical Physics — The catalytic conversion of methonal to olefin (MTO) has attracted attention both in industrial and academic fields. Strong evidence shows that small-pore molecular sieves with certain amount silicon incorporated (SAPO) present promising high catalytic activity in MTO conversion. Using DFT, we study the structural and electronic properties of chabazite SAPO-34. Although there are extensively experimental results show that silicon incorporation does not change the overall structure as the original AlPO structure, local structural changes are still created by silicon substitution, which probably accounted for the high catalytic activity. It is noted that the catalytic activity of SAPO-34 presents increasing trend along with the silicon incorporation amount increasing and maintain a flat peak even with more silicon incorporated. Hence, there is an optimal silicon incorporation amount which possibly yields the highest catalytic MTO conversion.

8:48AM Y39.00003 Nanosecond Scanning Tunneling Microscopy: resolving spin dynamics at the atomic scale , SEBASTIAN LOTH, IBM Research - Almaden — With the advent of nanoelectronics, functional electronic elements advance towards atomic dimensions and analysis techniques need to keep pace. Scanning tunneling microscopes (STM) have evolved into standard tools to measure the static electronic properties of nanostructures, molecules and atoms. Here we show how the STM can be used to access the equally important dynamical properties on time scales ranging from pico- to nanoseconds. We combine inelastic electron tunneling spectroscopy (IETS) with an all-electronic pump-probe measurement scheme and record the dynamical evolution of magnetic atoms on surfaces in the time domain [1]. We focus on the dynamics of electron spin relaxation in transition metal atoms placed onto a copper nitride decoupling layer on Cu(100). On this surface Fe atoms experience large magneto-crystalline anisotropy [2] that enables long spin lifetimes. At the same time the quantum mechanical nature of the discrete spin states allows for an additional path of spin relaxation: quantum tunneling of magnetization. We probe the dynamic behavior associated with this process and find that placing a Cu atom close to a Fe atom boosts the uniaxial anisotropy energy and creates a long-lived spin state with relaxation times in excess of 200 ns. The ability to probe individual nanostructures with atomic spatial and nanosecond temporal resolution opens a new avenue to explore spin dynamics and other dynamical phenomena on the intrinsic length scale of the underlying interactions.

[1] S. Loth, M. Etzkorn, C. P. Lutz, D. M. Eigler, A. J. Heinrich, Science 329 1628 (2010).
[2] C.F. Hirjibehedin, et al., Science 317, 1199 (2007).

9:24AM Y39.00004 Tracking Oxygen Vacancies in Thin Film SOFC Cathodes[1] , DONOVAN LEONARD, AMIT KUMAR, STEPHEN JESSE, SERGEI KALININ, Oak Ridge National Laboratory, YANG SHAO-HORN, ETHAN CRUMLIN, EVA MUTORO, Massachusetts Institute of Technology, MICHAEL BIEGALSKI, HANS CHRISTEN, STEPHEN PENNYCOOK, ALBINA BORISEVICH, Oak Ridge National Laboratory — Oxygen vacancies have been proposed to control the rate of the oxygen reduction reaction and ionic transport in complex oxides used as solid oxide fuel cell (SOFC) cathodes [1,2]. In this study oxygen vacancies were tracked, both dynamically and statically, with the combined use of scanned probe microscopy (SPM) and scanning transmission electron microscopy (STEM). Epitaxial films of $La_{0.8}Sr_{0.2}CoO_3$ (LSC_{113})and LSC_{113}/$LaSrCoO_4$(LSC_{214}) on a GDC/YSZ substrate were studied, where the latter showed increased electrocatalytic activity at moderate temperature. At atomic resolution, high angle annular dark field STEM micrographs revealed vacancy ordering in LSC_{113} as evidenced by lattice parameter modulation and EELS studies. The evolution of oxygen vacancy concentration and ordering with applied bias and the effects of bias cycling on the SOFC cathode performance will be discussed.

[1]Research is sponsored by the of Materials Sciences and Engineering Division, U.S. DOE.

9:36AM Y39.00005 First principles study of GaN(10$\underline{1}$0)/Water interface[1] , JUE WANG, MARIA VICTORIA FERNANDEZ-SERRA, XIAO SHEN, Stony Brook University — GaN/ZnO alloy semiconductors have been shown to be promising materials to serve as photo-anode in photocatalytical fuel cells. In recent study by Shen et al[2], the non polar GaN(10$\underline{1}$0) surface has been studied with atomistic modeling and a sequence of intermediate steps for the water oxidation process at the interface are proposed. Here we present a first principles molecular dynamics study of the GaN(10$\underline{1}$0)/Water interface. We found dissociation events happen within 1ps and we show a detailed analysis of the changes in structure and dynamics of water molecules interacting with a dissociating wet surface. The complex hydrogen bond network near the surface is also analyzed in detail, including a throughout study of the proton diffusion processes. We perform a detailed analysis of the dynamics of the hole localization. The link between water surface dissociation and quantum efficiency will be discussed.

[1]This work is supported by DOE grant DE-FG02-09ER16052
[2]X. Shen, Y.A. Small, J. Wang, P.B. Allen, M.V. Fernandez-Serra, M.S. Hybertsen and J.T. Muckerman *J. Phys. Chem. C* **114(32)**, 13695 (2010)

9:48AM Y39.00006 Ions at interfaces and their spectroscopic consequences , PHILLIP GEISSLER, U.C. Berkeley — The affinity of relatively small ions for air-water interfaces challenges our basic understanding of the basic driving forces for solvation. Here I will show that this adsorption is a general phenomenon for ions in polar solvents. Its physical origin lies in a precarious and unexpected balance of strong nonlinear contributions. The statistics of solvent electric fields suggests a key role for interfacial fluctuations. I will also present an intuitive perspective on surface-specific vibrational spectroscopy, and discuss observable signatures for ion adsorption at aqueous interfaces.

10:24AM Y39.00007 First-Principles Studies of Functionalized Si(111) in Air and in Water[1] , YAN LI, Brookhaven National Laboratory, GIULIA GALLI, University of California, Davis — We have investigated structural, electronic and vibrational properties of hydrogen and methyl-terminated Si(111) surfaces both in air and in contact with water, by combining density functional theory and many-body perturbation theory within the GW approximations. The computed surface dipole moments for both H-Si(111) and CH3-Si(111) surfaces were found to be consistent with measured electron affinities (EAs), and can be explain by simple electronegative trends. While GW self-energy corrections greatly improve the absolute values of EAs, the EA difference of the two surfaces remains overestimated by about 0.3 eV. The variations in CH3 frequencies, e.g. the umbrella mode and CH stretching mode, for the surface in air and water are also well reproduced by our calculations. The influence exerted by the adsorption of water molecules on the hydrophobic H-Si(111) and CH3-(111) surfaces, in particular, on the EAs and the surface vibrational frequencies will be discussed and compared with recent experiments.

[1] A. Aliano, Y. Li, G. Cicero and G. Galli, J. Phys. Chem. C 114, 11898 (2010).
[2] Y. Li and G. Galli, Phys. Rev. B 82, 045321 (2010).

[1]This work was funded by NSF under Grant No. CHE-0802907.

10:36AM Y39.00008 Interaction between surfaces with ionizable sites , STEPHEN BARR, ATHANASSIOS PANAGIOTOPOULOS, Chemical and Biological Engineering, Princeton University — A key factor controlling the interaction between surfaces in aqueous solutions is the surface charge density. Surfaces typically become charged though a titration process where surface groups can become ionized based on their dissociation constant and the pH of the solution. In this work we use a Monte Carlo method to treat this process explicity in a system with two planar surfaces in a salt solution. We find that the surface charge density changes as the surfaces come close to contact due to interactions between the ionizable groups on each surface. In addition, we observe an attraction between the surfaces above a threshold surface charge, in good agreement with previous theoretical predictions based on uniformly charged surfaces. However, close to contact we find the force is significantly different than the uniformly charged case. We also explore the role of salt concentration and the density of the ionizable sites.

Friday, March 25, 2011 8:00AM - 10:36AM –

Session Y40 DPOLY: Focus Session: Nanocomposite Physics II-Polymer Dynamics A122/123

8:00AM Y40.00001 Particles Bridge the Gap – Relevance of Polymer Graft Architecture on the Properties of Particle Brush Assemblies[1] , MICHAEL BOCKSTALLER, Carnegie Mellon University — Current interest in the assembly of ligand-coated nanoparticles into 2D and 3D array structures is driven by the opportunities for novel material technologies that derive from the interactions within nanoparticle superlattice structures. A common challenge in the solution-based assembly of particle superlattice structures is the propensity of hard-sphere type particle assemblies to crack formation and brittle fracture during solvent evaporation. Recent progress in controlled radical polymerization offers novel opportunities for polymer-stabilized particle systems (particle brushes) as building blocks of particle superlattice structures. This contribution will discuss synthetic strategies to realize particle brush systems with well defined polymer graft-architecture in the dense or semi-dilute brush regime and discuss the effect of polymer grafting on the structure formation and cohesive interactions in particle brush assemblies. In particular, it will be demonstrated chain entanglements between surface-grafted chains give rise to fracture through polymer-like crazing thus dramatically increasing the toughness and flexibility of the particle assembly. The modulus and toughness of polymer nanocomposites synthesized by self-assembly of particle brush systems will be shown to exceed those of "conventional" particle-filled polymer composites – a result that will be interpreted as a consequence of the particular conformational constraints of surface grafted chains.

[1]The author acknowledges financial support by AFOSR and DTRA.

8:36AM Y40.00002 How do Macromolecules Diffuse Through Pathways imposed by Nanoparticles? , RUSSELL COMPOSTO, KAREN WINEY, University of Pennsylvania, NIGEL CLARKE, Durham University, SANGAH GAM, University of Pennsylvania, JEFF METH, DuPont Co. — Macromolecular motion slows down in crowded biological and engineered systems. Polymer nanocomposites (PNC) containing nanotubes and nanospheres are ideal systems for probing the underlying mechanisms of diffusion in a crowded system. Here, we review the current experimental studies of tracer diffusion in PNC. For silica nanospheres (12nm and 28nm), the normalized diffusion coefficients fall on a master curve when plotted against the interparticle separation divided by the probe size. The entropic barrier model accounts for the reduced diffusion by the loss of chain entropy due to the constrictive bottlenecks between nanoparticles. A new flux-based model depicts confined chains as diffusing along narrow pathways arranged by the NPs. This model captures experimental results while accounting for the distribution of particle separations inherent to real PNC.

8:48AM Y40.00003 Macromolecular Diffusion in Polymer Nanocomposites , SANGAH GAM, University of Pennsylvania, JEFF METH, STEVE ZANE, DuPont Co., KAREN WINEY, University of Pennsylvania, NIGEL CLARKE, Durham University, RUSSELL COMPOSTO, University of Pennsylvania — Macromolecular diffusion in crowded systems is important in biological and engineered systems. We have studied macromolecular diffusion through a model polymer nanocomposite (PNC) containing phenyl grafted silica nanoparticles (NPs), randomly distributed in a polystyrene matrix. Over a wide range of NP loading and tracer molecular weight (M), the scaling of the diffusion coefficient with M is in excellent agreement with the entropic barrier model (EBM) previously used to describe diffusion of DNA through confined media (e.g., gels and nanopores). To investigate the effect of NP size, diffusion was measured in PNC's with silica NPs having diameters of 28 and 12 nm. The normalized diffusion coefficients (D/D_0) plotted against the interparticle separation relative to probe size (i.e., $ID/2R_g$) collapse on a master curve. Diffusion in a poly(methyl methacrylate):silica NP system was also investigated to understand how attractive interactions (i.e., enthalpy) perturb motion relative to the polystyrene and phenyl-silica NP system which is athermal. Finally, a flux-based model is proposed and compared with experimental results.

9:00AM Y40.00004 Role of Particle – Polymer Interactions on the Dynamics of Polymer Nanocomposites , GUGLIELMO CAPUANO, University of Naples, RAMAKRISHNA PONNAPATI, University of Houston, DOMENICO ACIERNO, University of Naples, RAMANAN KRISHNAMOORTI, University of Houston — Understanding the physics of polymers in the presence of nanoparticle fillers is of crucial importance, since it can lead to the formulation of truly engineered, functional nanocomposites with unique features and broad commercial utilization. The thermomechanical behavior of polymer nanocomposites qualitatively resembles those of polymer films confined to the nanoscale. It has been recently hypothesized that the suppression of physical aging in PMMA/silica nanocomposites is primarily due to hindered mobility of polymer molecules resulting from hydrogen bonding with hydroxyl units on the silica. Further, when solid nanoparticles are dispersed in polymer melts adsorption of polymer chains on the surface of nanoparticles alters the mobility of the chains far into the bulk, and several non-continuum effects are observed. We therefore investigate the effects of polymer-particle interactions on the relaxation dynamics and viscoelastic properties of a model nanocomposite based on a mixture of silica nanoparticles and poly(methyl acrylate). Narrow molecular weight distribution PMA was synthesized using ATRP and mixed with nanoparticles at different concentrations. Alterations in the viscoelastic behavior are attributed to filler structuring and interactions with the host polymer.

9:12AM Y40.00005 The relationship between the T_g depression and the speeding up of physical aging in polystyrene/gold nanocomposites , VIRGINIE M. BOUCHER, DIPC, DANIELE CANGIALOSI, ANGEL ALEGRIA, JUAN COLMENERO, CSIC — The effect of gold nanoparticles on the segmental dynamics, glass transition (T_g) and physical aging of polystyrene (PS) was studied in PS/Gold nanocomposites samples containing 5 and 15 wt.% of 60 nm spherical gold nanoparticles, surface-treated with thiolated-PS. While the segmental dynamics of PS, as assessed by broadband dielectric spectroscopy (BDS), was found to be unchanged in presence of gold nanoparticles, the calorimetric T_g of PS was shown to decrease with increasing the amount of nanoparticles in the samples. Furthermore, the physical aging of PS, monitored by measuring the enthalpy relaxation below T_g by means of DSC, was shown to speed up with increasing the nanoparticles weight fraction, i.e. the amount of PS/Gold interface in the hybrid material. Thus, the main conclusion of our work is that PS molecular mobility and out-of-equilibrium dynamics are decoupled in these nanocomposites. The significant effect of the amount of PS/Gold interface on both the physical aging rate of PS and the calorimetric T_g depression are quantitatively accounted for by a model based on the diffusion of free volume holes towards polymer interfaces, with a diffusion coefficient depending only on the molecular mobility.

9:24AM Y40.00006 Nanoparticle-directed self-assembly of amphiphilic block-copolymers[1] , SOJUNG PARK, University of Pennsylvania — The self-assembly of nanoparticles and amphiphilic polymers provides a powerful tool for the fabrication of functional composite materials for a range of applications spanning from nanofabrication to medicine. Here, we present how the incorporation of nanoparticles affects the self-assembly behavior of amphiphilic block-copolymers and how to control the morphology of nanoparticle-encapsulating polymer assemblies. Based on the approach, we have prepared various types of well-defined nanoparticle-encapsulating polymeric nanostructures, including polymersomes packed with magnetic nanoparticles and unique cavity-like quantum dot assembles. We found that the incorporation of nanoparticles drastically affects the self-assembly structure of block-copolymers by modifying the relative volume ratio between the hydrophobic block and the hydrophilic block. In addition, the nanoparticle-polymer and nanoparticle-solvent interactions impact the arrangement and the hybridization of nanoparticles in polymer matrix. These findings should form the basis for the design rules of the self-assembly of nanoparticles and polymer amphiphiles, which will allow one to create new hybrid structures with predesigned morphology and properties. Furthermore, we demonstrated that the morphology of nanoparticle-encapsulating polymer assemblies significantly affects their properties such as magnetic relaxation properties, underscoring the importance of the overall self-assembly structure and the nanoparticle arrangement in polymer matrixes.

[1]This work was supported by the NSF career award, the ARO young investigator award, and the MRSEC seed award (University of Pennsylvania).

10:00AM Y40.00007 Isothermal Crystallization of Poly(ethylene oxide) / Single Walled Carbon Nanotube Nanocomposites , ARNALDO LORENZO, TIRTHA CHATTERJEE, RAMANAN KRISHNAMOORTI, University of Houston — The isothermal crystallization behavior of poly(ethylene oxide)/single walled carbon nanotubes (PEO/SWNT) nanocomposites were studied with a focus on the *overall crystallization kinetics* and the *morphological* evolution of PEO using differential scanning calorimetry and in-situ small angle x-ray scattering measurements, respectively. The overall crystallization process of the PEO was strongly affected by lithium dodecyl sulfate (LDS) stabilized carbon nanotubes. Further, analysis of the overall crystallization kinetics showed that the PEO chains were topologically constrained by the presence of LDS with an increased energy barrier associated with nucleation and crystal growth, and the nanotubes further act as a barrier to chain transport or enhance the LDS action on the PEO chains. The energy penalty and diffusional barrier to chain transport in the nanocomposites disrupt the PEO crystal helical conformation. This destabilization leads to formation of thinner crystal lamellae and suggests that the crystallization kinetics is primarily controlled by the growth process. This study is particularly interesting considering the suppression of the PEO crystallinity in presence of small amounts of Lithium ion based surfactant and carbon nanotubes.

10:12AM Y40.00008 MD Simulations of DNA-Programmable Nanoparticle Self-Assembly[1] , CHRISTOPHER KNOROWSKI, ALEX TRAVESSET, Department of Physics and Astronomy and Ames Laboratory, Iowa State University, Ames, IA — Self-assembly through linker mediated hybridization is a powerful technique to control self-assembly at the nanoscale. Recent experiments with complementary ssDNA attached to Au nanoparticles have shown crystallization into BCC and FCC crystals. We give a brief overview of a coarse grained model and present molecular dynamics simulations of the model. We discuss its static and dynamical properties.

[1]This work has been supported by the DOE through Ames lab under Contract DE-AC02-07CH11358.

10:24AM Y40.00009 Hierarchical Superstructures from the Self-assembly of Giant Surfactants in Condensed State[1] , WEN-BIN ZHANG, XINFEI YU, XUEHUI DONG, YIWEN LI, KAN YUE, JINLIN HE, STEPHEN CHENG, Department of Polymer Science, College of Polymer Science and Polymer Engineering, The University of Akron — Giant surfactants are a class of tadpole-shaped hybrid nanomaterials with a functional nanoparticle as the head group and a polymer chain as the tail, such as perfluorochain-functionalized polyhedral oligomeric silsesquioxane end-capped poly(ε-caprolactone) (FPOSS-PCL). The self-assembly of FPOSS-PCL with different composition in bulk were studied using DSC, SAXS, WAXD, and TEM. The compact arranagement of the perfluorochains on the POSS nanoparticles clearly distinguishes them from the polymer chain, leading to the formation of nanophase-separated supramolecular structures such as spheres, cylinders, and bilayered lamellaes. This physical picture is rather unusual and quite reminescent to that observed in the aggregates of small-molecule surfactants. The striking similarity indicates the importance in tuning the interactions to control the hierarchical structure formation in hybrid nanomaterials.

[1]This work was supported by NSF (DMR-0906898).

Friday, March 25, 2011 8:00AM - 10:24AM –

Session Y41 DPOLY: Elastomers and Gels A115/117

8:00AM Y41.00001 Swelling Kinetics of a Microgel Shell , JOSHUA WAHRMUND, University of North Texas, JIN-WOONG KIM, LIANG-YIN CHU, Harvard University, CHANJIE WANG, Haynes and Boone, LLP, YONG LI, Kimberly-Clark Corporation, ALBERTO FERNANDEZ-NIEVES, Harvard University, DAVID A. WEITZ, Harveard University, ARKADII KROKHIN, ZHIBING HU, University of North Texas — Tanaka's approach to swelling kinetics of a solid gel sphere is extended to a spherical microgel shell. The boundary condition at the inner surface is obtained from the minimization of shear elastic energy. Temporal evolution of a shell is represented in a form of expansion over eigenfunctions of the corresponding diffusion equation. The swelling of Tanaka's solid spherical gel is recovered as a special case of our general solution if the inner radius approaches zero. To test our theoretical model, we prepared monodisperse poly-N-isopropylacrylamide (PNIPAM) hydrogel shells using a microfluidic device. The temporal dependence of the inner and outer radii of the shell was measured and the data was fitted to our theoretical model. As a result, we obtained the collective diffusion constants for shrinking and for swelling processes. The obtained values for microgel shells are in excellent agreement with the previous results obtained for sub-millimeter PNIPAM solid spheres in the same temperature interval. Our model shows that the characteristic swelling time of a gel shell should be proportional to the square of its outer radius—just as with Tanaka's model.

8:12AM Y41.00002 Indentation of polydimethylsiloxane submerged in organic solvents , YUHANG HU, Harvard University, XIN CHEN, GEORGE WHITESIDES, JOOST VLASSAK, ZHIGANG SUO — This study uses a method based on indentation to characterize a polydimethylsiloxane (PDMS) elastomer submerged in an organic solvent (decane, heptane, pentane, or cyclohexane). An indenter is pressed into a disk of a swollen elastomer to a fixed depth, and the force on the indenter is recorded as a function of time. By examining how the relaxation time scales with the radius of contact, one can differentiate the poroelastic behavior from the viscoelastic behavior. By matching the relaxation curve measured experimentally to that derived from the theory of poroelasticity, one can identify elastic constants and permeability. The measured elastic constants are interpreted within the Flory-Huggins theory. The measured permeabilities indicate that the solvents migrate in PDMS by diffusion, rather than by convection. This work confirms that indentation is a reliable and convenient method to characterize swollen elastomers.

8:24AM Y41.00003 Synthesis and mechanical properties of resilin-like hydrogels , JUN CUI, MELISSA LACKEY, University of Massachusetts Amherst, GREGORY TEW, University of Massachussets Amherst, ALFRED CROSBY, University of Massachusetts Amherst — Resilience measures a material's efficiency for mechanical energy storage. Many materials exhibit high resilience at low strains, but relatively few can maintain this performance at high strain levels. One of the most notable examples of a resilient material is resilin, a protein used strategically when Nature requires elasticity with minimal loss over large deformations. Similar to resilin in many aspects, we present a novel hydrogel network with well-defined architecture by introducing hydrophobic polydimethylsiloxane (PDMS) into hydrophilic polyethylene glycol (PEG)-based network. As a function of the PDMS to PEG ratio, we demonstrate that maximum water content can range from 97% to 80% and Young's modulus from 5kPa to 75kPa. Across this full range of network compositions and water content, the resiliency is nearly 100% for uniaxial strains exceeding 80%. This unique balance of properties is associated with two network attributes: uniformity in network connectivity and negligible secondary structures.

8:36AM Y41.00004 Pre-Stressed Double Network Elastomers And Hydrogels , NAVEEN SINGH, ALAN LESSER, Polymer Science and Engineering Dept., University of Massachusetts at Amherst — A new approach to prepare and characterize pre-stressed double network elastomers and hydrogel systems is investigated. In one example, a styrene-butadiene-styrene (SBS) tri-block copolymer system containing physical cross-links is used to achieve a pre-stressed double network by additional chemical crosslinking in a strained state using ultra-violet (UV) light. Unusual physical and mechanical properties that result from the interactions between each network are presented. These double network elastomers show a transition between competitive and collaborative behavior in their mechanical properties, as well as lower permanent set in both low and high strain regimes along with lower hysteresis. These networks exhibit lower modulus, along with lower coefficient of thermal expansion, still showing lower swelling ratios, which results from a competition of the networks. In another example, a new two-step curing schedule is utilized for Polyacrylamide based hydrogels, where a strain is induced in the middle of curing reaction. The final mechanical properties of these double network hydrogels are studied and compared to both first network and the single network formed without any step strain.

8:48AM Y41.00005 Topological effects on viscoelasticity of polyacrylamide hydrogels , JAN KALFUS, ALAN LESSER — Viscoelastic behavior of long linear chains in a concentrated solution is governed by the topology of the molecules and interchain excluded volume interaction. As a consequence, chain diffusive motion is significantly retarded and such an assembly of chains exhibits highly pronounced entropy elastic behavior. In this contribution, two types of additional chain confinements imposed on a concentrated solution of linear polyacrylamide (L-PAA) will be discussed. The confinement was realized either by adding silica nano-filler into the concentrated solution of L-PAA or by cross-linking of acrylamide in the concentrated solution of L-PAA. While in the first case the trapped entanglement interaction is caused by interaction of chains with large nano-filler surface, in the second case the L-PAA chains are trapped among the cross-links of the PAA network. Viscoelastic response of both types of composite systems exhibited generic characteristics. In both cases, the trapped entanglement interaction significantly changed the relaxation spectrum of the matrix polymer solution and considerably enhanced the linear elastic modulus.

9:00AM Y41.00006 Memory Effects in Strained Polymer Networks Caused By Multiple Stages of Crosslinking , JOANNE BUDZIEN, Frostburg State University — Polymer networks crosslinked in multiple strain states usually are analyzed with the independent network model. For networks that undergo scission in addition to crosslinking, however, the networks have been shown not to be completely independent. Even with complete removal of all crosslinks from a given network reacted in a particular strain state, the system still responds as though a portion of the original network remains. This talk will present simulation results of a coarse-grained model that has multiple networks with crosslinking and scission occurring in stages.

9:12AM Y41.00007 Viscoelastic Properties and Ionic Conductivity of Block Copolymer-Based Ion Gel Electrolytes[1] , SIPEI ZHANG, KEUN HYUNG LEE, C. DANIEL FRISBIE, TIMOTHY P. LODGE, University of Minnesota — The viscoelastic properties and ionic conductivity of block copolymer-based ion gels were investigated with polymer concentrations of 10 – 50 wt% over a temperature range of 25 – 200 °C. Ion gels were prepared through the self-assembly of poly(styrene-*b*-ethylene oxide-*b*-styrene) (SOS) and poly(styrene-*b*-methyl methacrylate-*b*-styrene) (SMS) triblock copolymers in a room-temperature ionic liquid, 1-ethyl-3-methylimidazolium bis(trifluoromethylsufonyl)imide ([EMI][TFSI]). The S end-blocks associate into micelles, whereas the O and M midblocks are well-solvated by this ionic liquid. Under oscillatory mechanical shear, two relaxation modes have been observed in the SMS ion gels. The faster mode corresponds to the relaxation of the M midblocks in the ionic liquid, while the slow mode reflects motion of the S end blocks within their micellar cores. Comparison of the solid gels and the liquid homopolymer solutions showed that the reduction of ionic conductivity of the gels with respect to that of the solutions is relatively small, and depends primarily on the volume fraction of S micelles.

[1]This work was supported by the National Science Foundation through the MRSEC program at the University of Minnesota.

9:24AM Y41.00008 Fracture Behavior of High-Toughness, Ionically Cross-linked Triblock Copolymer Hydrogels , KEVIN HENDERSON, KATHRYN OTIM, KENNETH SHULL, Northwestern University — Mechanisms for enhancing energy dissipation and hence toughness are important for the generation of robust synthetic soft materials for biomedical applications. Ionic cross-linking in particular has been explored in triblock copolymer hydrogels and affords a remarkable change in mechanical performance comparable to non-cross-linked analogs. Here we employ a physically associated base triblock copolymer network composed of hydrophobic poly(methyl methacrylate) endblocks and a hydrophilic poly(methacrylic acid) midblock capable of complexing with divalent cations. Increases in stiffness and strength have previously been reported, with the extent dependent upon the identity, concentration, and pH of a cross-linking cation solution. We delineate the measured toughness in such systems using tensile tear tests and relate the mechanical performance to a damage zone model reminiscent of loading behavior observed in double network hydrogels.

9:36AM Y41.00009 Origin of the Toughness and the Elastomeric Properties of Gels from Block Copolymers with Semicrystalline Syndiotactic Polypropylene Blocks , FANNY DEPLACE, ZHIGANG WANG, GLENN H. FREDRICKSON, EDWARD J. KRAMER, MC-CAM and the Departments of Materials and Chemical Engineering, UC Santa Barbara, JEFFREY M. ROSE, GEOFFREY W. COATES, Department of Chemistry and Chemical Biology, Baker Laboratory, Cornell University, FUMIHIKO SHIMIZU, Mitsubishi Chemical Group, Science and Technology Research Center, Inc., Yokohama, LIXIA RONG, BENJAMIN S. HSIAO, SUNY Stony Brook, Department of Chemistry, Stony Brook — The exceptional toughness and elastomeric properties of gels from block copolymers with semicrystalline syndiotactic polypropylene blocks have been reported. From results obtained from small angle and wide angle X-ray scattering experiments simultaneously performed with step cycle tensile stretching, the toughness can be attributed to the formation, orientation and elongation of crystalline fibrils along the tensile direction. The evolution of the crystalline structure during deformation is confirmed by FTIR measurements and the crystalline morphology is characterized by polarized microscopy imaging. Both polypropylene crystals and the rubbery phase play a role in the elasticity of the gels. Due to the viscoelasticity of the rubbery phase, an increase in the elastic recovery is observed when the gels are allowed to relax at zero load before starting the next cycle.

9:48AM Y41.00010 Chemomechanical Characterization of Autonomic Polyacrylamide Gels , MATTHEW SMITH, Nanostructured and Biological Materials Branch, AFRL, WPAFB, OH, KEVIN HEITFELD, Renegade Materials Corporation, RYAN KRAMB, MAXIM TCHOUL, DANIEL GALLAGHER, RICHARD VAIA, Nanostructured and Biological Materials Branch, AFRL, WPAFB, OH — Autonomic behavior is a distinctive attribute of complex biological systems. Like biological tissue, self-oscillating hydrogels driven by the Belousov-Zhabotinsky (BZ) reaction can convert chemical signals into a mechanical response. Under appropriate conditions BZ gels exhibit sustained mechanical swell-deswell oscillations; and arrays of these gels have the potential to form networks of coupled oscillators. One of the key challenges to developing criteria for device design and assessing practical performance limits of these materials is the need for detailed knowledge of the chemomechanical characteristics of the BZ gels at various states of autonomic behavior. Recently we developed an easily synthesized BZ gel system based on polyacrylamide. Here in, the swell-deswell amplitude, mechanical forces produced during uniform oscillations, and the chemical response to external loads are discussed in context with current poly(N-isopropylacrylamide)-based systems. These studies establish the parameter space leading to robust chemomechanical oscillations and provide an experimental foundation to refine currently available theoretical models to guide the design of autonomic materials and devices.

10:00AM Y41.00011 Block copolymer photonic crystal gels for mechanochromic sensing , EDWIN CHAN, NIST, JOSEPH WALISH, EDWIN THOMAS, MIT, CHRISTOPHER STAFFORD, NIST — Block copolymer based photonic crystal gels (BCPG) have been previously demonstrated for chemical sensing by taking advantage of dynamic changes in structural color upon interactions with their environment. With their high degree of tunability in structural color and mechanical properties, these materials can function as mechanochromic sensors with the potential application for measuring local mechanical deformation such as cell adhesion and mechanics. In this work, we demonstrate the application of a BCPG for local mechanical sensing by investigating the changes in structural color in response to mechanical deformation. The BCPG consists of a hydrophobic block (polystyrene) – hydrophilic polyelectrolyte (poly(2-vinyl pyridine)) block copolymer that self-assembles into a one- dimensional periodic lamellar structure and functions as a one dimensional Bragg reflector. Contact adhesion testing is used to measure and relate the changes in structural color of the BCPG films as a function of mechanical deformation. We explore the effects of solvent conditions and applied mechanical deformation in determining the relationships between structural color changes and mechanical strain.

10:12AM Y41.00012 Theoretically Informed Coarse-Grained Simulations of Polymer Nanogels , PRATEEK JHA, JOS ZWANIKKEN, Northwestern University, FRANCOIS DETCHEVERRY, JUAN DE PABLO, University of Wisconsin - Madison, MONICA OLVERA DE LA CRUZ, Northwestern University — Nanoscale finite-sized polymer networks (nanogels) are smart responsive materials that undergo large reversible volume changes with moderate changes in environmental conditions such as temperature, pH, light, and electric field. We develop a coarse-grained model of nanogels in terms of experimentally measurable physical quantities, and perform a theoretically informed Monte Carlo simulation that combines ideas from both the particle and continuum approaches of polymer physics. The elastic interactions are treated through beads connected by harmonic springs ("particles"), and the van der Waals and electrostatic interactions are treated by weighted densities ("fields"). Our simulations predict high degrees of swelling and a discontinuous volume phase transition in ionic nanogels, in contrast to moderate swelling and a continuous volume phase transition for the non-ionic case. We analyze the effects of mesh-size, polymer charge fraction, ionic strength, and solvent quality, on the swelling behavior of nanogels. A comparison is made with the results of a simplified continuum model, where the electrostatic interactions are treated using the Poisson-Boltzmann approximation.

Friday, March 25, 2011 8:00AM - 11:00AM –

Session Y42 DPOLY: Focus Session: Dynamics of Polymers–Phenomena due to Confinement–Theory, Wrinkling, and Glass Transitions A302/303

8:00AM Y42.00001 Twinkling Fractal Analysis of Confinement Effects on the Glass Transition of Thin Films , RICHARD WOOL, JOSEPH STANZIONE III, Chemical Engineering, Univ Delaware — The Twinkling Fractal Theory (TFT) of the Glass Transition has recently been verified experimentally [J.F. Stanzione, et al., "Observing the twinkling fractal nature of the glass transition", J. Non-Cryst. Solids (2010), doi:10.1016/j.jnoncrysol.2010.06.041] Here we apply the TFT to understand nanoconfinement effects on T_g for amorphous thin films of thickness h with free and adhered surfaces. The TFT states that T_g occurs when the dynamic clusters percolate rigidity at the rate of testing γ. The lifetime τ of these fractal clusters of size R behaves as $\tau \sim R^{\delta}$ exp $\Delta E/kT$, where $\delta = D_f/d_f$ in which D_f is the fractal dimension and $d_f = 4/3$ is the fracton dimension for the vibrational density of states $g(\omega) \sim \omega^{df}$. The activation energy $\Delta E = \beta[T^{*2}\text{-}T_g^2]$ in which $\beta \approx 0.3$ cal/mol $^oK^2$ and $T^* \approx 1.2T_g$. In confined spaces, only clusters of size R<h can exist and these have a very fast relaxation time compared to the bulk. Thus, for free surfaces, T_g must be dropped at that test rate to percolate rigidity and we obtain the familiar expression $T_g(h)/T_{g\infty} \approx [1\text{-}(B/h)^{\delta}]$ where $\delta \approx 1.8$ when $D_f \approx 2.5$ and B is a known constant. For thin films adhered to solid substrates, T_g increases in accord with the adhesion energyΔA as $\Delta E \rightarrow \Delta E + \Delta A$ and the adhered cluster lifetime increases. As the rate of testing γ increases, the confinement effects diminish as T_g increases in accord with $T_g(\gamma) = T_{go} + (k/2\beta) \ln \gamma/\gamma_o$.

8:12AM Y42.00002 Mechanical properties of thin polymer films close to the glass transition: a mesoscale model , DIDIER R. LONG, ALAIN DEQUIDT, PAUL SOTTA, CNRS/Rhodia — Polymer dynamics slows down in the vicinity of a solid substrate (when interactions are sufficiently strong), as can be evidenced experimentally by measuring the glass transition temperature Tg in thin films. We extend here the Long and Lequeux model which quantitatively accounts for this effect. We describe the mechanical properties of the polymers on the scale of dynamical heterogeneities (of a few nanometers). We propose a constitutive relation regarding the local relaxation time, the local stress, and the deformation history. The mechanical equations coupled to these constitutive relations are solved, allowing to reach a scale of a few tens of nanometers and macroscopic time scales. In particular, we measure the elastic modulus G' as a function of temperature, for various films thicknesses. This measurement allows for measuring the glass transition temperature of the film as a function of thickness. The results show that the glass transition temperature is shifted as compared to the bulk (corresponding to large film thickness), depending on the strength of the polymer/substrates interaction, with values which are consistent with experimental results.

8:24AM Y42.00003 A Simple Approach to Free Volume Transport in Molten/Glassy Material[1] , JANE LIPSON, Dartmouth College, SCOTT MILNER, Penn State University, NICHOLAS TITO, Dartmouth College — A key component of microscopic models for the glass transition, in polymer thin films and more generally, is the local dynamics of free volume, which governs what portions of a near-glassy liquid are mobile at a given instant in time. For example, our recent Delayed Glassification (DG) model implements a proposal of de Gennes that segment-sized kinks of free volume may travel from a free surface into a film along polymeric loops or bridges, helping to plasticize material within some accessible distance from the surface. Recently, we have constructed a simple model for 'the mobility of mobility', i.e., how local mobility is itself transported through a dense liquid slightly above Tg. Our simple model results in growing cooperativity lengths and intermittency timescales as Tg is approached from above. If time permits, we shall also describe how the model may be adapted to describe the approach to glassy behavior in supported and freestanding films.

[1]Support from NSF-DMR is gratefully acknowledged.

8:36AM Y42.00004 Deviations in mechanical properties of ultrathin polymer films via surface wrinkling , CHRISTOPHER M. STAFFORD, Polymers Division, National Institute of Standards and Technology — In ultrathin polymer films (h $<$ 100 nm), the measurement of stress relaxation and Young's modulus is a difficult problem due to the delicate nature of such thin films and the lack of appropriate measurement tools for this length scale. Recent work has shown that the Young's modulus of ultrathin glassy polymer films can be measured by a wrinkling-based metrology. Interestingly, the modulus of such thin films was observed to deviate considerably from their bulk counterparts. Building off these observations, we have shown that the rate of structural relaxation and the temperature dependence of the film modulus can also be obtained by following the 'relaxation' of strain-induced wrinkling patterns back to their flat equilibrium state. By measuring the decay or relaxation of surface undulations in compressed thin films, we demonstrate that the structural relaxation of the polymer film is highly thickness-dependent and obeys Arrhenius temperature dependence with an activation energy that decreases progressively with decreasing film thickness. This gives rise to an overall broadening of glass transition and to a relatively weak temperature dependence of structural relaxation.

9:12AM Y42.00005 Calorimetry of Thin Films – From Single Layer Glass Transitions to Interlayer Diffusion in Double Layers , CHRISTOPH SCHICK, Institute of Physics, University of Rostock, Germany, DONGSHAN ZHOU, State Key Laboratory of Coordination Chemistry, Nanjing University, China, HEIKO HUTH, MATHIAS AHRENBERG, Institute of Physics, University of Rostock — Nanocalorimetry allows studying the glass transition in nanometer thin films. One of the striking results of fast scanning (FSC) as well as alternating current (AC) calorimetry is the commonly observed constant Tg in thin films down to a few nm. Blends of polystyrene and poly(phenylene oxide) (PS/PPO) confined in thin films (down to 6 nm) were investigated by AC nanocalorimetry. For this blend, we see even for the thinnest films (6 nm, corresponding to about half of PPO's radius of gyration Rg) only one unchanged glass transition. The good miscibility between PS and PPO remains even in ultrathin films. Finally, we show that our chip calorimeter is sensitive enough to study the inter-layer diffusion in ultrathin films. The PS chains in a 150 nm PS/PPO double layer that is prepared by spin coating PPO and PS thin films in tandem gradually diffuse into the PPO layer when heated above the Tg of PS, forming a PSxPPO100-x blend. However, on top of the PSxPPO100-x blend, there exists a stable pure PS like layer (ca. 30nm in our case) that does not diffuse into the blend beneath even staying at its liquid state over 10 hours.

9:24AM Y42.00006 T_g depression and segmental dynamics of polystyrene thin films , DANIELE CANGIALOSI, CSIC-CFM, VIRGINIE M. BOUCHER, DIPC, ANGEL ALEGRIA, CSIC-CFM and UPV/EHU, JUAN COLMENERO, CSIC-CFM and DIPC — The glass transition temperature (T_g) of polymer thin films has been a subject of intense debate in the last two decades. (Pseudo)thermodynamic determinations, such as calorimetry and ellipsometry, generally suggest a significant depression of T_g, whereas the dynamic T_g, measured by techniques such broadband dielectric spectroscopy and AC-calorimetry directly probing the molecular mobility, is found to be unchanged. The present study provides a resolution to this controversy on polystyrene by showing that the experimental relaxation time obtained from (pseudo)thermodynamic techniques, and the intrinsic molecular relaxation time can be rescaled on a master curve, only accounting for the thickness of the film. Furthermore the thickness and cooling rate dependence of the (pseudo)thermodynamic T_g is quantitatively captured by the free volume holes diffusion model. In this framework, the T_g depression emerges from the ability of thinner films to maintain equilibrium, due to the shortest distance free volume holes have to diffuse to the polymer interface.

9:36AM Y42.00007 Evidence for Two Simultaneous Mechanisms Causing Tg Reductions in High Molecular-Weight Free-Standing Films Observed as Dual Glass Transitions More Than 30 K Apart in a Single Film , JUSTIN PYE, CONNIE ROTH, Emory University — Glass transition temperature (Tg) changes seen in nanoconfined polymer films have been well documented over the past 15+ years. Supported films exhibit a molecular-weight (MW) independent Tg reduction that manifests itself as a gradient in dynamics emanating from the free surface. Low MW free-standing films show qualitatively the same Tg reduction as supported films, but with the presence of two free surfaces resulting in a Tg reduction that is twice as large for a given film thickness. In contrast, high MW free-standing films exhibit a qualitatively different behavior with a linear reduction in Tg that is MW dependent, potentially described by de Gennes' sliding mode theory. These observations suggest that there may exist two separate mechanisms which can propagate enhanced mobility from the free surface into the film. With ellipsometry measurements over an extended temperature range, we have observed two reduced Tgs more than 30 K apart in individual high MW free-standing polystyrene films suggesting that both mechanisms act simultaneously within a film. These results may explain recent studies on high MW free-standing films using different experimental techniques that contradict the original literature.

9:48AM Y42.00008 Demonstration of Glass Transition Temperature Depression in Thin Supported Polystyrene Films Using Internal Standard , MIKHAIL EFREMOV, PAUL NEALEY, Department of Chemical and Biological Engineering, University of Wisconsin - Madison, Madison, WI 53706 — Clear evidence for glass transition temperature (Tg) depression in $\sim$ 5 nm thick atactic polystyrene (Mw = 212 kg/mol) films supported on silicon substrates is demonstrated by ellipsometry in vacuum [1]. Transition in polystyrene droplets formed by dewetting is used as an internal reference. Both temperature-modulated [2] and linear temperature scanning techniques are utilized; measurements are performed at $10^{-6} - 10^{-8}$ torr residual gas pressure. The method is sensitive enough to observe glass transition in $1 - 2$ nm thick supported polystyrene films. Our recent study shows appreciable reduction of Tg in less than $10 - 20$ nm thick samples; Tg versus thickness function is found to follow a step-like curve originally reported by [3]. The curve is characterized by moderate (about 17 K) constant Tg depression for thickness less than $7 - 8$ nm. References: [1]. M. Y. Efremov, S. S. Soofi, A. V. Kiyanova, C. J. Munoz, P. Burgardt, F. Cerrina, and P. F. Nealey, Rev. Sci. Instrum., 79, 043903 (2008). [2]. M. Y. Efremov, A. V. Kiyanova, and P. F. Nealey, Macromolecules, 41, 5978 (2008). [3] T. Miyazaki, K. Nishida, and T. Kanaya, Phys. Rev. E, 69, 061803 (2004).

10:00AM Y42.00009 Effect of Packing Density on the Measurement of Glass Transition Temperatures in Thin Film , GI XUE, Nanjing University, DEPARTMENT OF POLYMER SCIENCE, NANJING UNIVERSITY TEAM — In the measurement of *Tg* of polymers, a break or jump in some properties is seen at the transition temperature. For bulk polymer, the measurement of *Tg* by different methods has similar result. However, the results reported for thin films have shown quite disagreement among different experimental methods. We used NMR and fluorescence spectroscopy to detect interchain distance and found that the thin film and the freeze-dried polymers show reduced packing densities. And we also found no thickness dependence of *Tg* in thin film and no changes of *Tg* in the freeze-dried polymer measured by calorimetric method or by dynamic mechanical thermal analysis. However the *Tg* in the same samples measured by thermo-mechanical analysis or by positron annihilation lifetime spectroscopy is significantly lower than that in bulk polymers. We argue that the reduction in packing density is a major factor which causes the disagreement among *Tg* measured by different methods for thin films. During the processes of some measurements, an unjamming transition is proposed to take place, which reduces *Tg*.

10:12AM Y42.00010 The Effect of Molecular Weight on the Glass Transition Temperature of Polymer Thin Films , QIANG GU, DONGSHAN ZHOU, GI XUE, Department of Polymer Science and Engineering, The School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, GI XUE TEAM — The thickness dependence of glass transition temperature (Tg) of polymer thin films has attracted considerable attention in both technological and scientific fields. With decreasing polymer film thickness d, the Tg(d) can decrease, increase or remain constant lying on the details of measurement techniques and sample preparation, etc. Using the recently developed differential alternating current chip calorimeter, we directly measured the calorimetric Tg of polystyrene thin films with various molecular weights. We found that when the molecular weight of polystyrene is below the critical chain entanglement, its Tg in a thin film with a thickness of 15 nm can reduce by 20 degrees (compared to bulk sample). However, the Tg of polystyrene film above the entanglement molecular weight remains constant as the film thickness changes. We argue that the molecular weight plays an important role in the thickness dependence of glass transition temperature of polymer thin films.

10:24AM Y42.00011 Glassy dynamics within surface-bound molecular monolayers , L.I. CLARKE, Dept. of Physics, NC State University, Raleigh, NC 27695, M.P. ROMAN, D.R. STEVENS, M.C. SCOTT, J.R. BOCHINSKI — Dynamics within a monolayer collection of surface-bound substituted-alkyl chains are studied with narrow-band dielectric spectroscopy. A transition from independent (intra-molecular) motion in low density systems to complex, glassy (inter-molecular) motion as the density is increased is observed. At high density, both the glassy mode [1,2] and the sub-Tg relaxation [3] have direct analogy to equivalent relaxations in polyethylene. Thus this experimental approach enables observation of the formation of a fragile glass as an explicit function of density; in addition by altering the molecular characteristics and surface arrangement, resultant changes in the nature of the glass transition (its glass transition temperature Tg and fragility m) can be determined. The effects of packing efficiency, chain length, and molecule-molecule interactions, as tuned by altering dipoles within the chain, will be discussed.

[1] M. C. Scott *etal.*, *ACS Nano* **2**, 2392 (2008);
[2] M. Beiner, and H. Huth, *Nature Materials* **2**, 595 (2003);
[3] Q. Zhang *et al.*, *J. Phys. Chem. B* **110**, 4924 (2006).

10:36AM Y42.00012 Interchain Coupling in Thin Polymer Film Studied by Fluorescence Non-radiative Energy Transfer , JIE XU, GI XUE, Nanjing University, NANJING UNIVERSITY TEAM — According to many views, the glass transition temperature (Tg) changes with decreasing polymer film thickness. There is an ongoing debate on the origin of the changes. As an important parameter, however, the interchain distance of thin film was still a challenge. We used Non-radiative energy transfer (NET) method to characterize polymer interchain proximity and association in polymer thin film, by attaching carbazolyl probe (donor) or anthryl probe (accepter) to the side groups of polymethyl methacrylate (PMMA) chain, respectively. We measured the NET results of PMMA films on silicon and found that the NET results decreased with decreasing film thickness. The NET results represented the interchain distance or density. With decreasing film thickness h, the density of the films decreased, which caused an increment of the polymer chain mobility. That might help us to understand the physical nature Tg changes.

10:48AM Y42.00013 Impact of annealing and adsorption on the distribution of segmental mobility and tracer diffusivity of ultrathin films of polystyrene[1] , SIMONE NAPOLITANO, CINZIA ROTELLA, MICHAEL WUBBENHORST, Katholieke Universiteit Leuven — We show experimental evidence that the changes ultrathin films undergo during annealing are strongly correlated to the amount of chains irreversibly adsorbed at the interface. A careful analysis of the time evolution of the dielectric function during annealing steps above Tg revealed three different regimes: at times much shorter than the adsorption time, the thickness of the adsorbed layer is constant and the interface mimics the effect of a free surface (packing frustration); upon increase of surface coverage, the films undergo a series of metastable states characterized by the largest changes in the deviations from bulk behavior; finally, when the thicknesses of the irreversibly adsorbed layer doubles its starting value, the system approach a new equilibrium whose properties are fixed by the new interfacial configurations. Our picture is further confirmed by the effect of annealing on the distribution of glass transition temperatures [1], dielectric relaxation strength and tracer diffusivity at different distances from the adsorbing interface.

[1] Rotella, Napolitano et al. Macromolecules, 2010, 43, 8686-8691

[1]SN acknowledges FWO (Fonds Wetenschappelijk Onderzoeks - Vlaanderen) for a postdoctoral scholarship.

Friday, March 25, 2011 8:00AM - 11:00AM –
Session Y43 DPOLY: Molecules, Solutions, Networks, & Gels A306/307

8:00AM Y43.00001 Distinct Tensile Response of Model Semi-flexible Elastomer Networks[1] , BERNARDO M. AGUILERA-MERCADO, CLAUDE COHEN, FERNANDO A. ESCOBEDO, School of Chemical & Biomolecular Engineering, Cornell University — Through coarse-grained molecular modeling, we study how the elastic response strongly depends upon nanostructural heterogeneities in model networks made of semi-flexible chains exhibiting both regular and realistic connectivity. Idealized regular polymer networks have been shown to display a peculiar elastic response similar to that of super-tough natural materials (e.g., organic adhesives inside abalone shells). We investigate the impact of chain stiffness, and the effect of including tri-block copolymer chains, on the network's topology and elastic response. We find in some systems a dual tensile response: a liquid-like behavior at small deformations, and a distinct saw-tooth shaped stress-strain curve at moderate to large deformations. Additionally, stiffer regular networks exhibit a marked hysteresis over loading-unloading cycles that can be deleted by heating-cooling cycles or by performing deformations along different axes. Furthermore, small variations of chain stiffness may entirely change the nature of the network's tensile response from an entropic to an enthalpic elastic regime, and micro-phase separation of different blocks within elastomer networks may significantly enhance their mechanical strength.

[1]This work was supported by the American Chemical Society.

8:12AM Y43.00002 Elastically tuned defect mode in cholesteric elastomers , JUAN ADRIAN REYES, LAURA OLIVIA PALOMARES, Instituto de Fisica Universidad Nacional Autonoma de Mexico — We consider an axially elongated cholesteric elastomer having a twist defect. We show that its localized mode can be mechanically tuned, and the scaling of the inverse relative line width can be largely enhanced when the values of the deformation and shape anisotropy are near the pseudo isotropic curve. This choice causes a tremendous variation in the behavior of the photon dwell time in the defect mode, which then grows linearly versus the sample thickness. The shift of the defect wavelength, the reflection band width, and the angle between the electric and magnetic fields are also calculated.

8:24AM Y43.00003 Glassy structure and thermal fluctuations of amorphous nematogenic solids , FANGFU YE, BING LU, University of Illinois, XIANGJUN XING, Shanghai Jiao Tong University, PAUL GOLDBART, University of Illinois — Amorphous nematogenic solids (ANS) are media comprising rod-like nematogens that have been randomly linked to form macroscopic, elastically deformable networks. Classes of ANS include chemical nematogen gels (i.e., networks of small molecules) and liquid crystalline elastomers (built from crosslinked nematogen-containing macromolecules), as well as biophysical networks, such as those composed of actin filaments. One common feature of these systems is that the linking process introduces into them a new type of random field, consisting of a conventional static part along with a new, thermal-fluctuation-induced, dynamic part. We develop a phenomenological model of ANS which shows how this composite random field, together with the coupling between the orientational and positional fluctuation that nematogens exhibit, leads to the occurrence of decaying but also oscillatory correlations of the thermal fluctuation, and also shows how these correlations influence the glassy structure of ANS.

8:36AM Y43.00004 Thermal and Mechanical Properties of Sequential and Simultaneous Thiol-Ene-Isocyanate Networks , OLIVIA MCNAIR, DAVIS BRENT, DANIEL SAVIN, School of Polymers and High Performance Materials, University of Southern Mississippi — Ternary networks containing having stoichiometrically balanced thiol /(ene+isocyanate) ranging from 0 to 20 molsynthesized via sequential or simultaneous thiol/ene and thiol/isocyanate click reactions. The effects of cross-link density were studied using three thiols, GDMP (difunctional), 3T (trifunctional) and 4T (tetrafunctional) respectively. TEA catalyzes the isocyanate-thiol coupling and chain extension, while the photoinitiator DMPA initiates a radical thiol-ene crosslinking process. Real-time FTIR was used to study kinetics of both light and dark reactions utilizing thiol, ene and isocyanate peaks which appear independently. It was found that difunctional thiols and isocyanates reacted initially, forming chain extended prepolymers end-capped with thiol functionalities. Upon UV irradiation, thiol functionalized prepolymers reacted with TTT, a trifunctional ene, forming networks containing incorporated thiourethane linkages. Initial DSC results indicated higher Tgs for higher cross-linked networks; however, isocyanate content has significant effects on each system. Films were also be thermally characterized via DMA and mechanical properties measured using MTS.

8:48AM Y43.00005 Computational and Experimental Investigation of Morphology of Polymer Gels , YELENA SLIOZBERG, KENNETH STRAWHECKER, JAN ANDZELM, JOSEPH LENHART, U. S. Army Research Laboratory — Thermo-reversible polymer gels based on block copolymers represent a remarkable class of materials for a wide range of applications. An efficient approach to control and modify the properties of these gels is to use multicomponent mixtures of self-assembling block copolymers differing in architecture, length and chemical nature. As a result of microphase separation, "mixed" or "pure" micelles, containing block copolymers of the same or different types, are developed. Here, we present a dissipative particle dynamics (DPD) study of the morphology of a binary mixture of AB/ABA block copolymers differing in length of the insoluble blocks in B-selective solvent. We have observed numerous morphologies of AB/ABA blends, which are characterized by formation of pure and mixed micelles of various compositions, structures and sizes. We have discovered that changing the copolymer ratio and processing conditions impacts morphology of these blends. Finally, we have established factors that affect an intermicellar distance and a bridge fraction which ultimately determines the mechanical properties of the gels. Results of our computations were compared with our experimental findings based on atomic force microscopy and the other experimental and theoretical studies and demonstrated a good agreement.

9:00AM Y43.00006 Theory of volume phase transitions of polyelectrolyte gels , JING HUA, MITHUN MITRA, MURUGAPPAN MUTHUKUMAR, University of Massachusetts, Amherst — We will present theoretical results for the effect of charge regularization accompanying volume phase transitions of polyelectrolyte gels. Our theoretical formulation of the cascade effect that couples the effective degree of ionization and the polymer density leads to significant deviations from the classical Flory-type theories.

9:12AM Y43.00007 Plasticity and slow relaxation phenomena in reinforced rubbers , PAUL SOTTA, STEPHANE DUPRES, DIDIER LONG, CNRS — Elastomers reinforced with nanometric solid particles or aggregates exhibit remarkable properties: temperature dependent reinforcement of the modulus in the linear regime, non linear effects, irreversibility and hysteretic effects. Important progress has been achieved recently in modeling these properties, based on glassy layers around filler particles. In some cases, reinforcement as a function of temperature and filler volume fraction was explained quantitatively. We shall focus here on the plasticity and related slow relaxation phenomena which occur in these systems. We show that the amplitude of plasticity is correlated to the reinforcement amplitude, and that plasticity relaxes with a very broad distribution of relaxation times (similar to an ageing phenomenon), in the same way as the stress relaxes at high strain amplitude. These experimental observations of long time evolution are well described by the mesoscale model for reinforced rubbers that we have proposed.

9:24AM Y43.00008 Migration of chemical additives in a rubber under UV irradiation , LUDOVIC DEVANT, CNRS, ROLAND BENOIT, MARIE-LOUISE SABOUNGI, EMMANUEL GOMEZ, BENOIT LE ROSSIGNOL — The evolution of the chemical composition of a rubber, in particular that of its surface, is governed by several factors including temperature, oxidation and migration of additives. Oxidation mechanisms alone do not account for all the phenomena observed, for example the appearance of deposits on the surface. We have studied the effects of temperature and photo-oxidation on the migration of chemical additives on a rubber surface. The morphological and chemical evolution were followed by AFM and XPS, respectively. 3D reconstruction with time-of-flight secondary-ion mass spectrometry (TOF-SIMS) combined with the AFM and XPS results enabled us to establish a relation between the oxidizing degradation of the rubber and the surface migration of the additives. This finding is supported by a kinetic study of the surface evolution.

9:36AM Y43.00009 Probing the sliding interactions between bundled actin filaments , ANDY WARD, ZVONIMIR DOGIC, Brandeis University — Assemblies of filamentous biopolymers are hierarchical materials in which the properties of the overall assemblage are determined by structure and interactions between constituent particles at all hierarchical levels. For example, the overall bending rigidity of a two bundled filaments greatly depends on the bending rigidity of, and the adhesion strength between individual filaments. However, another property of importance is the ability for the filaments to slide freely against one another. Everyday experience indicates that it is much easier to bend a stack of papers in which individual sheets freely slide past each other than the same stack of papers in which all the sheets are irreversibly glued together. Similarly, in filamentous structures the ability for local re-arrangement is of the utmost importance in determining the properties of the structures observed. In order to study this phenomenon we create bundles of biopolymers by inducing attractive interactions between actin filaments via the depletion mechanism. We find that bundles of actin filaments to do not slide freely across one another. In order to characterize these sliding interactions, we perform active experiments using laser tweezers to pull one filament across the other at constant velocity.

9:48AM Y43.00010 Apparent Yield Stress and Interfacial Viscoelasticity of Globular Protein Solutions , VIVEK SHARMA, ADITYA JAISHANKAR, Hatsopoulos Microfluids Lab, Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, YING-CHIH WANG, Rheosense Inc, San Ramon, CA 94583, GARETH H. MCKINLEY, Hatsopoulos Microfluids Lab, Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139 — Globular proteins influence the dynamics, phase behavior and transport of biomolecules and drugs in the mammalian body. In conventional rheological studies conducted on torsional rheometers, protein solutions are commonly reported to have a solid-like response at concentrations as low as 0.03% by weight. In this study, we probe the bulk and interfacial viscoelasticity of bovine serum albumin (BSA) solutions as a canonical example of a globular protein system. Using a stress-controlled rotational rheometer, augmented by microfluidic rheometry and interfacial rheometry, we demonstrate that the origin of the yield-like response reported in bulk viscometric flows lies in the formation of a film of adsorbed protein, formed spontaneously at the solution/gas interface. We directly measure the concentration-dependent interfacial viscoelasticity of the adsorbed protein and we describe a coherent means of extracting the interfacial contribution from bulk viscosity measurements. Finally, we demonstrate how the presence of surfactants changes both the interfacial and bulk rheology of pharmaceutical formulations based on protein solutions.

10:00AM Y43.00011 The enhanced bubble formation in short dsDNA loops , O-CHUL LEE, WOKYUNG SUNG[1], Pohang university of science and technology (POSTECH) — Recent experiments have shown the dsDNAs readily bend and loop over the nanometer scale much shorter than its persistence length (50 nm). Motivated by this, we study possibility of enhanced bubble formation in short dsDNA loops by evaluating free energy of bubble formation analytically, and also by simulating the breathing DNA model. We analyze the bubble size distribution and the average bubble size as a function of the loop length, which are compared with those of the linear DNA of the same length. 1) T. E. Cloutier and J Widom, Mol. Cell **14**, 355 (2004). 2) P. A. Wiggins *et al.*, Nat. Nanotechnol. 1, 137 (2006). 3) O. Lee, J. H. Jeon and W. Sung, Phys. Rev. E 81, 021906 (2010)

[1]Corresponding author

10:12AM Y43.00012 Universality in the timescales of internal loop formation in unfolded proteins and single-stranded oligonucleotides[1] , RYAN CHENG, UT Austin, TAKANORI UZAWA, Hokkaido University, Japan, KEVIN PLAXCO, UC Santa Barbara, DMITRII MAKAROV, UT Austin — Understanding the rate at which various parts of a molecular chain come together to facilitate the folding of a biopolymer (e.g., a protein) into its functional form remains an elusive goal. Here we use experiments, simulations, and theory to study the kinetics of internal loop closure in disordered biopolymers such as single-stranded DNA and unfolded proteins. We present theoretical arguments and computer simulation data to show that the relationship between the timescale of internal loop formation and the positions of the monomers enclosing the loop can be recast in a form of a universal master dependence. Our measurements of the loop closure times in single-stranded oligonucleotides, as well the internal loop closure kinetics in unfolded proteins reported by others, are all well described by this theoretically predicted dependence. Experimental deviations from the master dependence can then be used as a sensitive probe of dynamical and structural order in unfolded proteins and other biopolymers.

[1]This work was supported by the NIH, NSF, and Robert A. Welch Foundation. CPU time was provided by the Texas Advanced Computing Center.

10:24AM Y43.00013 Topological interactions between ring polymers , DIETER HEERMANN, University of Heidelberg — The detailed topological and entropic forces between loops still remain elusive. We have quantitatively determined the potential of mean force between the centers of mass of two ring polymers, i.e. loops. We find that the transition from a linear to a ring polymer induces a strong increase in the entropic repulsion between these two polymers. On top, topological interactions such as the non-catenation constraint further reduce the number of accessible conformations of close-by ring polymers by about 50 percent, resulting in an additional effective repulsion.

10:36AM Y43.00014 Modulation of DNA condensation by cation valence , PREETHI CHANDRAN, Section on Tissue Biophysics and Biomimetics, NICHD; NIBIB; National Institutes of Health, Bethesda, MD 20892, EMILIOS DIMITRIADIS, Laboratory of Bioengineering and Physical Science, NIBIB, National Institutes of Health, Bethesda 20892, CANDIDA SILVA, PETER BASSER, FERENC HORKAY, Section on Tissue Biophysics and Biomimetics, NICHD, National Institutes of Health, Bethesda, MD 20892 — Aggrecan is a negatively charged bottlebrush-shaped proteoglycan in the extracellular matrix, with unique polyelectrolyte properties. Aggrecan-hyaluronic acid aggregates are responsible for the compressive resilience of articular cartilage. Unlike linear polyelectrolytes such as DNA, aggrecan is insensitive to the presence of multivalent counterions (e.g., calcium ions) and self-assembles into micro-gels in near-physiological salt solutions. These features are preserved by aggrecan adsorbed on mica surfaces. To probe both the nature of aggrecan assemblies in solution and their surface interactions, we image the aggrecan assemblies adsorbed on mica surface using Atomic Force Microscopy The effect of counterion valence on the hydration-dehydration properties of the aggrecan assemblies will be discussed.

10:48AM Y43.00015 Combining DNA Nanotechnology and Fluorescence Polarization Microscopy to Determine the Orientation of DNA-bound Fluorophores , HUNTER BANKS, CHRISTOPH SCHNEIDER, DEBORAH FYGENSON, UC Santa Barbara — We describe a technique to measure the axis of the transition dipole moment of a fluorophore bound to dsDNA and compare results with existing techniques. We use DNA nanotubes to present the dsDNA in a known orientation and query a variety of intercalating (e.g., YO-YO, TO-TO), groove-binding (e.g. DAPI) or covalently linked (e.g., Fluorescein, Cy3, Cy5) dyes. A de Sénarmont prism in front of the camera generates simultaneous images of fluorescence polarized perpendicular and parallel to the DNA nanotube axis, allowing for ratio measurements that are insensitive to bleaching. We suggest the use of technique to detect helical supertwist, and possibly other nanoscale structural features, of DNA nanostructures.

Friday, March 25, 2011 8:00AM - 11:00AM –

Session Y44 DMP DPOLY: Focus Session: Organic Electronics and Photonics – Exciton and charge separation physics A309

8:00AM Y44.00001 Charge transport studies in organic semiconductors using carrier extraction by linearly increasing voltage (CELIV) technique , ALMANTAS PIVRIKAS, Johannes Kepler University Linz — Organic optoelectronic devices, such as solar cells, light emitting diodes and transistors, share a common feature: their performance critically depends on the efficiency with which charge carriers (electrons and/or holes) move in the material. Understanding and improving the charge transport is the main goal when improving the device performance or designing novel organic compounds through chemical engineering. Due to low carrier mobility in disordered films, as well as due to its time, electric field and carrier density dependence, standard measurement technique like Hall effect and Time-of-Flight are either inapplicable or limited in applicability. Charge Carrier Extraction by Linearly Increasing Voltage (CELIV) technique has become a world standard used by many scientific groups to measure charge transport and recombination in inorganic and organic semiconductors. The method can be used to study the charge carrier mobility dependence on time, carrier concentration, electric field, temperature, film thickness and morphology directly in the operational devices. However, the latest research have shown that CELIV current transients and extraction maximum used for mobility evaluation is strongly dependent on experimental conditions such as carrier density, light absorption profile and electric field. Procedure, allowing estimating the correction factor in mobility relation will be presented. In contrast to inorganic crystalline semiconductors, the long-range disorder in the films of organic devices makes the charge transport properties strongly dependent on the degree of disorder and nanomorphology of the films. Carrier density, electric field and temperature dependent mobility in disordered organic semiconductors is shown to obey Arrhenius-type, Poole-Frenkel-type, Meyer-Neldel rule, and Gill's law. Stochastic transport theories are used to describe charge carrier hopping within localized Density-Of-States as opposed to delocalized band-transport in the crystals.

8:36AM Y44.00002 Direct determination of energy level alignment of organic-organic bulk heterojunction: cases of the P3HT:PCBM and P3HT:FLN-i blend , ZELEI GUAN, ANTOINE KAHN, Department of Electrical Engineering, Princeton University, JONG BOK KIM, HE WANG, YUEH-LIN LOO, Department of Chemical Engineering, Princeton University — Using photoemission spectroscopy (UPS&IPES) combined near edge X-ray absorption fine structure method, we have determined the surface compositions and electronic alignments of the blend films comprising poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl-C61-butyric acid methyl ester. Given the fact that the surface of the blend film is a nearly pure P3HT wetting layer, we use a lift-off method to access the originally buried surface, which is rich in both P3HT and PCBM and thus representative of the BHJ. We show that the donor/acceptor LUMO-HOMO gap is 1.46 eV, implying a 0.5-0.6 eV interface dipole barrier between the two materials. As far as we know, this is the first report of the direct determination of electronic structure of the blend. The combined measurement and lift-off method are standard and can be applied to other organic blend films, like P3HT and FLN-i.

8:48AM Y44.00003 Direct Determination of Energy Level Alignment and Charge Transport at Metal/Alq_3 Interfaces via Ballistic-Electron-Emission Spectroscopy (BEES) , J.S. JIANG, J.E. PEARSON, S.D. BADER, Argonne National Laboratory — In organic electronic devices, the difference between the electrode work function and the organic lowest unoccupied molecular orbital (LUMO) or highest occupied molecular orbital (HOMO) is a crucial parameter in determining the nature of charge transport. However, experimental determination of LUMO is challenging.[1] For the archetypal electroluminescent organic semiconductor tris-(8-hydroxyquinoline) aluminum (Alq_3), various techniques gave significantly different HOMO-LUMO gap values.[2] Using BEES, we directly determined the energy barrier for electron injection at clean interfaces of Alq_3 with Al and Fe to be 2.1 eV and 2.2 eV, respectively. We quantitatively modeled the sub-barrier BEES spectra with an accumulated space charge layer, and found that the transport of non-ballistic electrons is consistent with random hopping over the injection barrier. Supported by U.S. DOE Office of Science Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

[1] J. C. Scott, J. Vac. Sci. Tech, A **21**, 521 (2003).
[2]I. H. Campbell, D. L. Smith, Appl. Phys. Lett. **74**, 561 (1999); I. G. Hill *et al.* Chem. Phys. Lett. **327**, 181 (2000); S. F. Alvarado *et al.* IBM J. Res. Dev. **45**, 89 (2001).

9:00AM Y44.00004 ABSTRACT WITHDRAWN –

9:12AM Y44.00005 Band alignment optimization of bulk rrP3HT/C_{60} heterojunction , ARNAUD MAILLARD, ALAIN ROCHEFORT, Ecole Polytechnique de Montreal, Engineering Physics Department — Organic solar cells could overcome the cost limitation of traditional solar cells by using large-scale fabrication techniques associated with polymers. However, a better understanding of the bulk heterojunctions (BHJs) electronic properties used in these devices is required to reach an efficiency of 10%. DFT and GW computations were used to study BHJs formed by the inclusion of C_{60} in a regioregular poly(3- hexylthiophene) polymer (rrP3HT) crystal. An increasing packing density in the BHJ extent the energy separation between the C_{60}-LUMO and the rrP3HT-HOMO, which is proportional to the open circuit voltage of the device (Voc). This trend is consistent with the induced dipole moment variation observed at a pentacene- C_{60} junction upon reduction of the intermolecular distance [1]. In contrast, an increasing size of rrP3HT crystal domain leads to decrease both Voc and rrP3HT bandgap, in a similar fashion than upon the formation of rrP3HT crystallite along the annealing of BHJs [2].

[1] M. Linares, et al., J. Phys. Chem. C, 114 (2010), 3215.
[2] G. Dennler, et al., Adv. Mater., 21 (2009), 1323.

9:24AM Y44.00006 Strong interface p-doping and band bending in C_{60}[1] , IRFAN IRFAN, HUANJUN DING, YONGLI GAO, MINLU ZHANG, CHING TANG, University of Rochester, DEPARTMENT OF PHYSICS AND ASTRONOMY COLLABORATION, DEPARTMENT OF CHEMICAL ENGINEERING COLLABORATION — C_{60} is a strongly n-type material with its lowest unoccupied molecular orbital very close to the Fermi level, and p-doping C_{60} has been a challenging issue. We measured the electronic energy level evolution of C_{60} on molybdenum oxide (MoO_x)/ conducting indium tin oxide (ITO) interfaces with ultra-violet photoemission spectroscopy (UPS), inverse photoemission spectroscopy (IPES) and atomic force microscopy (AFM). We found that MoO_x strongly p-dopedC_{60}at the interface, resulting in an inversion layer in C_{60}. The energy levels of C_{60}relax gradually as the thickness of C_{60} increases, and the band bending region is observed to be greater than 400 Å in C_{60}. The root mean square (RMS) roughness measured with AFM of 581 Å thick C_{60} film was 68 Å, slightly increased from that of the ITO substrate of 55 Å. We have also investigated the effect of exposing the MoO_x air, and found that it eliminated the doping effect.

[1]NSF DMR- 1006098

9:36AM Y44.00007 Understanding the role of interfaces in small molecule organic photovoltaics , TIM JONES, University of Warwick — This abstract not available.

10:12AM Y44.00008 Photophysics of Poly(3-dodecylthinylenevinylene) with Controlled Regioregularity , EVAN LAFALCE, University of South Florida, Dept. of Physics, XIAOMEI JIANG, University of South Florida, Dept. of Physics — Poly(thienylene vinylene) (PTV) is a conductive polymer with potential applications for use in photovoltaics owing to its low-band gap, good hole-mobility and low oxidation potential. It is generally considered a non-luminescent material and reports suggest its emissive properties are highly dependent upon the excitation, conjugation length, alkyl side group and regio-regularity, complicating the interpretation of the non-radiative decay routes for photo-generated excitations. Better understanding of this behavior could explain the low efficiencies so far observed in PTV based solar cells and lead to improved performance. We have studied photoluminescence of Poly(3-dodedyl -2,5-thienylene vinylene) as a function of regio-regularity in thin films and solutions. By varying the excitation, temperature, and also by controlling the morphology through the use of different solvents, concentrations, and film preparation techniques, we hope to deduce the physical mechanisms competing with radiative recombination. Complimentary characterization of films through XRD and electro-absorption yield detailed information about the semi-crystalline structure and electronic levels, respectively.

10:24AM Y44.00009 Magneto-Optical Studies of Internal Photovoltaic Processes in Organic Solar Cells , HUIDONG ZANG, ZHIHUA XU, BIN HU, University of Tennessee — It has been found that exciton dissociation inevitably forms electron-hole pairs, namely charge-transfer (CT) complexes, at donor-acceptor interfaces due to Coulomb attraction in organic solar cells. In particular, the dissociation of CT complexes is a critical process that is accountable for the generation of photocurrent. However, it is a challenging issue to study the CT complexes formed at donor-acceptor interfaces. Here, we use magneto-optical measurements: magnetic field effects of photocurrent (MFE_{PC}) and light-assisted dielectric response (LADR) as effective experimental tools to experimentally examine the formation of CT complexes and the related photovoltaic processes. Our studies reveal that internal electrical drifting and local Coulomb interaction can largely change the binding energy and dissociation probability of CT complexes through intrinsic electrical polarization in donor-acceptor interpenetrating network. This experimental finding indicates that intrinsic electrical polarization plays an important role in controlling charge dissociation, transport, and collection in organic solar cells.

10:36AM Y44.00010 Photoluminescence Influenced by Chain Conformation in Thin Conjugated Polymer Films by Spin Coating and Dewetting , P.W. LEE, W.C. LI, Y. CHIEN, Department of Materials Science and Engineering, National Tsing Hua University, G. REITER, nstitute of Physics, Albert-Ludwigs-Universität, Freiburg, Germany, A.C.-M. YANG, Department of Materials Science and Engineering, National Tsing Hua University — Motivated by recent observations of photoluminescence (PL) enhancement by molecular constraints, the chain conformation effect was explored. It was found that PL efficiency decreased with film thickness under a constant spin speed but increased under a constant solution concentration indicating that prolonged solvent evaporation, and hence more open entangled coils, improved PL efficiencies. Strong substrate dependence was observed in the ultrathin regime, revealing the role of substrate-polymer interactions during the condensation process. Upon annealing, the thin film dewetted and resulted multi-fold PL enhancement. As revealed by micro-PL spectroscopy, the PL efficiency was about 10 times greater in the residual layer (∼3 nm) than that in the droplets and demonstrated independence of substrate quenching effect, unveiling important optoelectronic features of the molecular constrained states.

10:48AM Y44.00011 ABSTRACT WITHDRAWN –

Friday, March 25, 2011 8:00AM - 11:00AM –

Session Y45 DAMOP: Atom Interactions with Molecules, Surfaces, and X-Rays A310

8:00AM Y45.00001 ABSTRACT WITHDRAWN –

8:12AM Y45.00002 Dissipative Effects on Quantum Sticking[1] , YANTING ZHANG, DENNIS CLOUGHERTY, University of Vermont — Using variational mean-field theory, many-body dissipative effects on the threshold law for quantum sticking and reflection of neutral particles are examined. For the case of an ohmic bosonic bath, we study the effects of the infrared divergence on the probability of sticking and obtain an analytic expression for the rate of sticking as an asymptotic expansion in the incident energy E. The low-energy threshold law for quantum sticking is found to be robust with respect to many-body effects and remains a universal scaling law to leading order in E. Non-universal many-body effects alter the coefficient of the rate law and the exponent of a subdominant term.

[1]We gratefully acknowledge support from NSF under DMR-0814377.

8:24AM Y45.00003 Breaking Quantum Mirrors with Thermal Fluctuations[1] , IAN GOYETTE, DENNIS CLOUGHERTY, University of Vermont — We study ultracold atoms interacting with a surface at finite temperature. For the case where the surface is out of thermal equilibrium with the environment, the asymptotic form of the Casimir-Polder potential decays as an inverse square law and can be either attractive or repulsive, depending on the temperature difference. We analyze the effect of this interaction on the threshold law for quantum sticking, the probability that an atom will stick to the surface $s(E)$ as the incident energy tends to zero. We predict a new threshold law for neutral atoms interacting with a surface out of thermal equilibrium with its environment: $s(E) \sim E^{\gamma}$ as $E \to 0$ where γ $(0 \leq \gamma \leq 1/2)$ depends on the strength of the non-equilibrium Casimir-Polder interaction which can be tuned with temperature.

[1]We gratefully acknowledge support by NSF under DMR-0814377.

8:36AM Y45.00004 ABSTRACT WITHDRAWN –

8:48AM Y45.00005 Temperature dependence of the depolarization rates of $Ne^*(2p_i$ [J=1]) atoms induced by He atom collisions , VAIBHAV KHADILKAR, Dept.of Physics, Lamar University, CHRISTIAN BAHRIM, Dept. of Computer Science, UT Dallas — Our theoretical depolarization rates for the disalignment, disorientation, and alignment relaxation of $Ne^*(2p_i$ [J=1]) atoms at temperatures between 10 K and 3000 K are compared with various experiments. We perform quantum close-coupling many-channel calculations using a new model potential for the interaction between $Ne^*(2p_i$ [J=1]) and He atoms [1]. We analyze isotropic collisions in a gaseous mixture at thermal equilibrium, and find excellent agreement between our calculations and the experimental data above 77 K [1, 2]. We explain the temperature dependence of the depolarization rates using the anisotropy of the collisional channels [2]. For T < 77 K, our disalignment rates for the $Ne^*(2p_2$ [J=1]) and $Ne^*(2p_{10}$ [J=1]) atoms are larger than the experimental data. The experiment predicts a linear variation of the intra-multiplet cross sections to zero-energy. Our calculations indicate that for the $2p_2$ and $2p_{10}$ states, at low collision energies, the nuclear rotation at large atomic separation has a stronger influence in the molecular Hamiltonian than the electrostatic interaction. This situation does not occur for the $2p_5$ and $2p_7$ states, where the agreement between theory and experiment is found even at 20K [1]. [1] Bahrim C and Khadilkar V 2009 *Phys Rev A* **79** 042715. [2] Khadilkar V and Bahrim C 2010 *J Phys B* **43** (in press).

9:00AM Y45.00006 Dipole Transitions for the hydrogen molecule using Fully Nonadiabatic Wavefunctions , STEVEN ALEXANDER, Southwestern University, R.L. COLDWELL, University of Florida — Using variational Monte Carlo and simple, explicitly-correlated fully-nonadiabatic wavefunctions we have computed highly accurate trial wavefunctions for the lowest rovibrational state of several states of the hydrogen molecule. With these wavefunctions we have calculated the transition moments for all possible dipole transitions and we compare our results with those from more traditional calculations.

9:12AM Y45.00007 Formation of the negative molecular ion MH- by radiative association of a neutral molecule M with H- , VIATCHESLAV KOKOOULINE, University of Central Florida, MEHDI AYOUZ, University of Marquette, MAURICE RAOULT, OLIVIER DULIEU, Lab. Aime Cotton, University of Paris XI — We consider the formation of negative molecular ions MH^- through the reaction of radiative association: $M+H^- \to MH^- + ?\omega$, where M is a diatomic or triatomic neutral molecule. We present a theoretical approach to calculate the cross-section and the rate constant for the reaction and apply the theory to study formation of molecular ions from H^- and neutral molecules abundant in the interstellar medium (ISM): We consider H_2, CO, and H_2O as possible candidates to form negative ions. Such ions have never been observed in the ISM. Their eventual observation would serve as a proof of presence of H^- in the ISM too. The H^- ion cannot be detected directly by the photoabsorption spectroscopy. Supported by Triangle de la Physique contract QCCM and the National Science Foundation grant PHY-0855622

9:24AM Y45.00008 Terahertz Time-Domain Spectroscopy of Ices of N_2, CO_2, and Ar[1] , BAGVANTH R. SANGALA, PERRY A. GERAKINES, DAVID J. HILTON, Department of Physics, The University of Alabama at Birmingham, AL 35294-1170, USA — We used Terahertz Time-Domain Spectroscopy (THz- TDS) to study thin ice films of N_2, CO_2, and Ar from 0.1 -1.6THz. We observed an absorption line for N_2 ice films at 1.46THz in the temperature range of 10-28K. Ar ice films have absorption lines at 0.47THz and 0.97THz in the temperature range of 10-30K. We observed no absorption line for CO_2 ice films in the temperature range of 10-40K from 0.1-1.6THz. These results will be helpful in analyzing the data terms from observations of THz radiation from astronomical sources impinging upon interstellar materials.

[1]This research was supported by NASA under the grant NASA NSPIRES 07-APRA07-0110.

9:36AM Y45.00009 Collision-Induced Infrared Absorption by Collisional Complexes in dense Hydrogen-Helium gas mixtures at Thousands of Kelvin[1] , MARTIN ABEL, LOTHAR FROMMHOLD, The University of Texas at Austin, XIAOPING LI, KATHARINE L.C. HUNT, Michigan State University — The interaction-induced absorption by collisional pairs of H_2 molecules is an important opacity source in the atmospheres of the outer planets and cool stars. The emission spectra of cool white dwarf stars differ significantly in the infrared from the expected blackbody spectra of their cores, which is largely due to absorption by collisional H_2–H_2, H_2–He, and H_2–H complexes in the stellar atmospheres. Using quantum-chemical methods we compute the atmospheric absorption from hundreds to thousands of kelvin [1]. Laboratory measurements of interaction-induced absorption spectra by H_2 pairs exist only at room temperature and below. We show that our results reproduce these measurements closely [1], so that our computational data permit reliable modeling of stellar atmosphere opacities even for the higher temperatures [1].

[1] Xiaoping Li, Katharine L. C. Hunt, Fei Wang, Martin Abel, and Lothar Frommhold, "Collision-Induced Infrared Absorption by Molecular Hydrogen Pairs at Thousands of Kelvin", International Journal of Spectroscopy, vol. 2010, Article ID 371201, 11 pages, 2010. doi: 10.1155/2010/371201

[1]This work has been supported in part by the National Science Foundation through Grants AST-0709106 and AST-0708496.

9:48AM Y45.00010 Size dependent ionization dynamics of argon clusters in intense x-ray pulses , SEBASTIAN SCHORB, M. SWIGGERS, R. COFFEE, M. MESSERSCHMIDT, S. MOELLER, G. WILLIAMS, J. BOZEK, SLAC National Accelerator Laboratory / LCLS, T. OSIPOV, Western Michigan University, S. WADA, Hiroshima University, D. RUPP, T. MOELLER, Technische Universitaet Berlin, C. BOSTEDT, SLAC National Accelerator Laboratory / LCLS — Free Electron Lasers open the door for novel experiments in many science areas ranging from ultrafast chemical dynamics to single shot imaging of molecules. For the success of virtually all experiments with free electron lasers a detailed understanding of the light - matter interaction in the x-ray regime is pivotal. The Linac Coherent Light Source (LCLS) free electron laser in Stanford allows for the first time to study innershell ionization dynamics of intense x-ray pulses on a femtosecond time scale. We performed experiments on the ionization dynamics of Argon clusters at different pulse length using the slotted spoiler foil in the second LCLS bunch compressor [1]. The Auger rate of argon clusters is predicted to be size dependent and lower than in atoms due to delocalization of the valence electrons [2]. We observe a dependence of the ionization dynamics on pulse length and cluster size. The results are discussed and also compared to recent atomic and molecular data from LCLS.

[1] P. Emma et al. PRL 92, 074801 (2004)
[2] U. Saalmann, JM Rost PRL 89, 14 (2002)

10:00AM Y45.00011 *Ab initio* **calculations of atomic coherence excited by optical pulses: CEP effects and generation of X-ray radiation** , SUMAN DHAYAL, YURI ROSTOVTSEV, univ of North Texas — Recent progress in ultrashort, e.g. attosecond, laser technology allows to obtain ultra-strong fields which can be of the same order of magnitude as the electric field created by an atomic nucleus. Interaction of such strong and broadband field with atomic systems even under the action of a far-off resonance strong pulse of laser radiation should be revisited. As we have shown, such pulses can excite remarkable coherence on high frequency transitions. We have found and analyzed analitical solutions for various pulse shapes. We have developed new mechanisms of efficient atomic coherent excitation by using two-frequency laser pulses and via tunneling through electric fields. We have done *ab initio* calculations using TDDFT for several atoms and simple molecules interacting with strong optical fields. We compare efficiency generation with the efficiency of high harmonic generation approach, and discuss the CEP effects and possible applications of the results obtained to cooperative generation of XUV radiation. The efficiency of XUV generation is calculated for particular candidates for XUV radiation such as H (100 nm) and He (50 nm) atoms and H-like ions (Li^{2+} (30 nm), as well as Ar^{8+} and Xe^{8+} (30-50 nm).

10:12AM Y45.00012 XAS measurements at LCLS: Investigating Electronic Damage at an X-Ray FEL , CATHERINE GRAVES, DAVID BERNSTEIN, Stanford University, SLAC, JOSHUA TURNER, WILLIAM SCHLOTTER, HERMANN DÜRR, ANDREAS SCHERZ, JOACHIM STÖHR, SLAC — As X-ray FEL sources such as the LCLS ramp up scientific studies, the damage caused by the intense x-ray pulses has become a central question. X-ray FEL investigations of solid-state materials must consider the change in the electronic system during the x-ray pulse, in contrast to proposed biomolecular imaging experiments which must suppress atomic motion.[1] The potential electronic damage to the system is also amplified in many materials investigations which probe absorption edges. Therefore, a key need of all studies involving materials research with X-ray FELs is to mitigate or overcome the electronic damage when probing the system. We report the first x-ray absorption spectroscopy (XAS) results from LCLS, which show significant line shape changes dependent on the fluence and x-ray pulse length. We employ a technique previously developed at FLASH which also allows us to visualize the beam dispersion.[2] Our spectroscopy results from LCLS demonstrate a safe fluence and pulse length regime at which material investigations can be conducted without perturbing the ground state of the system during the probing x-ray pulse.

[1]Neutze, R. et. al. Nature 406, 752 (2000).
[2]Bernstein, D.P. et al. Appl. Phys. Lett. 95, 134102 (2009).

10:24AM Y45.00013 Berry phase-like effect near DOS singularity in continuum models coupled with discrete states , SAVANNAH GARMON, DVIRA SEGAL, University of Toronto, INGRID ROTTER, Max Planck Institute for the Physics of Complex Systems — Threshold effects in a continuum model (cut-off frequency in a waveguide or the band edge in tight-binding chains) may significantly modify the single-particle discrete eigenvalue spectrum resulting from coupled discrete states. Focusing on tight-binding chains as an example we reveal a Berry phase-like effect as the system parameters are adiabatically varied about certain exceptional points (non-analytic points in the eigenvalue spectrum) that are related to the threshold (van Hove) singularity in the density of states. We show that this effect is related to the form of the eigenvalue expansion in the vicinity of the band edge. In particular, for a semi-infinite model with a side-coupled impurity the eigenvalues in this vicinity may be expanded in powers of the coupling g, rather than the more usual g^2. In another example, in the case of an infinite tight-binding chain with a side-coupled impurity (or a two-level atom traveling in an infinite waveguide) the DOS singularity results in a $g^{4/3}$ amplification of the decay width of the resonant state [1, 2].

[1] Phys. Rev. B **73**, 115340 (2006).
[2] Phys. Rev. Lett **94**, 043601 (2005).

10:36AM Y45.00014 A Novel Geometric Effect of the Sunbeam (NGES) and Geometric Spin Hall Effect of Light (GSHEL) due to the Earth Rotation[1] , SANGBOO NAM, Retired — Recently there are reports of NGES[2] based on geometrical optics, and GSHEL[3] based on electrodynamics in vacuum. Here, I discuss the nature of NGES, using the Berry notion of the classical parallel transport,[4] and present GSHEL due to the earth rotation. For both NGES and GSHEL, the observing frame (detecting plane) should be tilted with respect to the light beam propagation direction. Setups to detect simultaneously both GNES and GSHEL are discussed. Descriptions given here are applicable to any beams such as electronic and atomic beams.

[1]sangboonam@mailaps.org

[2]S. B. Nam, arXiv **0910.5767** (2009).

[3]A. Aiello, et al., Phys. Rev. Lett. **103**, 100401 (2009).

[4]M. V. Berry, "Geometric Phases in Physics" (Ed. by A. Shapere and F. Wilczek, Singapore, 1989) **pp7-28**.

10:48AM Y45.00015 Observation of a Passive PT Phase Transition , A. GUO, C. FURROW, VAS. P. KUNETS, S.-Q. YU , G. SALAMO, G.A. SIVILOGLOU, R. EL-GANAINY, K.G. MAKRIS, D.N. CHRISTODOULIDES, D. DUCHESNE, R. MORANDOTTI, M. VOLATIER-RAVAT, V. AIMEZ, DEPT. OF PHYSICS, UNIVERSITY OF ARKANSAS, FAYETTEVILLE, AR, USA TEAM, COLLEGE OF OPTICS & PHOTONICS-CREOL, UNIVERSITY OF CENTRAL FLORIDA, ORLANDO, FL, USA COLLABORATION, INRS-EMT, VARENNES, QUEBEC J3X 1S2, CANADA COLLABORATION, CENTRE DE RECHERCHE EN NANOFABRICATION ET EN NANOCARACTERISATION, UNIVERSITE DE SHERBROOKE, SHERBRO COLLABORATION — In 1998 Bender and Boettcher discovered that the spectrum of a system with PT-symmetric Hamiltonian can still be entirely real. This subject attracts more and more attention during the last few years. One of the intriguing characteristics of PT-symmetric systems is the possibility of a *phase transition* beyond which the spectrum ceases to be entirely real. This symmetry breaking occurs suddenly once the imaginary component of the potential exceeds a certain critical level. Here we report the observation of a phase transition in a passive PT-symmetric optical structure once the loss exceeds a certain critical value. This counterintuitive loss-enhanced transmission is purely an outcome of a spontaneous PT symmetry breaking.

Friday, March 25, 2011 11:15AM - 2:15PM –

Session Z1 DCMP: Solid-State Spin Qubits: Coherence Control and Protection Ballroom A1

11:15AM Z1.00001 Control of single-spin decoherence by dynamical decoupling and spin bath manipulation , RONALD HANSON, Kavli Institute of Nanoscience Delft, Delft University of Technology, The Netherlands — Controlling the interaction of a single quantum system with its environment is a fundamental challenge in quantum science and technology. We dramatically suppress the coupling of a single spin in diamond with the surrounding spin bath by using high-fidelity double-axis dynamical decoupling [1]. The coherence is preserved for arbitrary quantum states, as verified by quantum process tomography. The resulting coherence time enhancement is found to follow a general scaling with the number of decoupling pulses. No limit is observed for the decoupling action up to 136 pulses, for which the coherence time is enhanced more than 25 times compared to spin echo. Furthermore, we have exploited multi-pulse sequences to enhance the sensitivity of single-spin magnetometry and to measure properties of the decoupling sequences themselves [2]. In this talk, I will present an overview of this work combined with our latest results on coherent manipulation of the spin bath environment.

[1] Universal dynamical decoupling of a single solid-state spin from a spin bath, G. de Lange, Z.H. Wang, D. Ristè, V.V. Dobrovitski, and R. Hanson, Science 330, 60 (2010).

[2] Single-spin magnetometry with multi-pulse sequences, G. de Lange, D. Ristè, V. V. Dobrovitski, R. Hanson, arXiv:1008.4395 (2010).

11:51AM Z1.00002 Control of electron spin decoherence in nuclear spin baths[1] , REN-BAO LIU, The Chinese University of Hong Kong — Nuclear spin baths are a main mechanism of decoherence of spin qubits in solid-state systems, such as quantum dots and nitrogen-vacancy (NV) centers of diamond. The decoherence results from entanglement between the electron and nuclear spins, established by quantum evolution of the bath conditioned on the electron spin state. When the electron spin is flipped, the conditional bath evolution is manipulated. Such manipulation of bath through control of the electron spin not only leads to preservation of the center spin coherence but also demonstrates quantum nature of the bath. In an NV center system, the electron spin effectively interacts with hundreds of ^{13}C nuclear spins. Under repeated flip control (dynamical decoupling), the electron spin coherence can be preserved for a long time ($>$1 ms). Therefore some characteristic oscillations, due to coupling to a bonded ^{13}C nuclear spin pair (a dimer), are imprinted on the electron spin coherence profile, which are very sensitive to the position and orientation of the dimer. With such finger-print oscillations, a dimer can be uniquely identified. Thus, we propose magnetometry with single-nucleus sensitivity and atomic resolution, using NV center spin coherence to identify single molecules. Through the center spin coherence, we could also explore the many-body physics in an interacting spin bath. The information of elementary excitations and many-body correlations can be extracted from the center spin coherence under many-pulse dynamical decoupling control. Another application of the preserved spin coherence is identifying quantumness of a spin bath through the back-action of the electron spin to the bath. We show that the multiple transition of an NV center in a nuclear spin bath can have longer coherence time than the single transition does, when the classical noises due to inhomogeneous broadening is removed by spin echo. This counter-intuitive result unambiguously demonstrates the quantumness of the nuclear spin bath.

[1]This work was supported by Hong Kong RGC/GRF CUHK402207, CUHK402209, and CUHK402410. The author acknowledges collaboration with Nan Zhao, Jian-Liang Hu, Sai Wah Ho, Jones T. K. Wan, and Jiangfeng Du.

12:27PM Z1.00003 Single spin qubits in self-assembled quantum dots , RICHARD WARBURTON, Department of Physics, University of Basel, Switzerland — The search for a highly coherent electronic spin in the solid state has led most spectacularly to the NV colour centre in diamond. Have self-assembled quantum dots, InGaAs in GaAs, been left behind? The advantages of self-assembled quantum dots are considerable - there is a strong optical transition, advanced heterostructure technology and post-growth processing techniques - but so far the spin coherence has been at best modest. This talk will present some possible ways to out fox the decoherence processes in a semiconductor with the goal of creating a highly coherent spin.

1:03PM Z1.00004 Preserving electron spin coherence in solids by optimal dynamical decoupling , JIANGFENG DU, University of Science and Technology of China — To exploit the quantum coherence of electron spins in solids in future technologies such as quantum computing, it is first vital to overcome the problem of spin decoherence due to their coupling to the noisy environment. Dynamical decoupling, which uses stroboscopic spin flips to give an average coupling to the environment that is effectively zero, is a particularly promising strategy for combating decoherence because it can be naturally integrated with other desired functionalities, such as quantum gates. Errors are inevitably introduced in each spin flip, so it is desirable to minimize the number of control pulses used to realize dynamical decoupling having a given level of precision. Such optimal dynamical decoupling sequences have recently been explored. The experimental realization of optimal dynamical decoupling in solid-state systems, however, remains elusive. Here we use pulsed electron paramagnetic resonance to demonstrate experimentally optimal dynamical decoupling for preserving electron spin coherence in irradiated malonic acid crystals at temperatures from 50K to room temperature [1]. Using a seven-pulse optimal dynamical decoupling sequence, we prolonged the spin coherence time to about 30 ms; it would otherwise be about 0.04 ms without control or 6.2 ms under one-pulse control. By comparing experiments with microscopic theories, we have identified the relevant electron spin decoherence mechanisms in the solid. Recently, we demonstrate experimentally that dynamical decoupling can preserve bipartite pseudo-entanglement in phosphorous donors in a silicon system [2]. In particular, the lifetime of pseudo entangled states is extended from 0.4 us in the absence of decoherence control to 30 us in the presence of a two-flip dynamical decoupling sequence.

[1]. Jiangfeng Du, Xing Rong, Nan Zhao, Ya Wang, Jiahui Yang and R. B. Liu, Preserving electron spin coherence in solids by optimal dynamical decoupling, Nature 461, 1265-1268 (2009).
[2] Ya Wang, Xing Rong, Pengbo Feng, Wanjie Xu, Bo Chong, Ji-Hu Su, Jiangbin Gong, and Jiangfeng Du, Preservation of bipartite pseudo-entanglement in solids using dynamical decoupling, submitted to Phys. Rev. Lett.

1:39PM Z1.00005 Theory of qubit dephasing in a large nuclear spin bath , SANKAR DAS SARMA, Univ of Maryland-College Park — This abstract not available.

Friday, March 25, 2011 11:15AM - 2:15PM –
Session Z2 DCMP: Pseudogap in High Tc Cuprates Ballroom A2

11:15AM Z2.00001 Loop-Current Order in Several Families of Cuprates , PHILIPPE BOURGES, LLB-CEA Saclay — In high temperature copper oxides superconductors, a novel long range 3D magnetic order associated with the pseudogap phase has been identified in two different cuprate families - $YBa_2Cu_3CuO_{6+x}$ (YBCO),[1] $HgBa_2CuO_4$ (Hg1201)[2] - over a wide region of temperature and doping. That magnetic order, evidended using polarized neutron diffraction, respects the translation symmetry of the lattice and can be described as a Q=0 antiferromagnetism with active role of in-plane oxygens atoms. Such a magnetic order can be associated with orbital moments in the circulating currents phase proposed by C. Varma. Similar magnetic ordering is observed in the archetypal cuprate $La_{2-x}Sr_xCuO_4$ (LSCO) system below 120 K for x=0.085.[3] In contrast to the previous reports, the magnetic ordering in LSCO is **only** short range with an in-plane correlation length of $\sim$ 10 Å and is bidimensional (2D). Such a less pronounced order suggests an interaction with other electronic instabilities. In particular, LSCO also exhibits a strong tendency towards stripes ordering at the expense of the superconducting state. Additional polarized neutron diffraction measurements have been performed in YBCO.[4] At lower doping (8.5 %), the magnetic order is observed at lower temperature ($\sim$ 150 K) than the generally assumed value for the pseudogap. It tends to vanish for dopings where the nematic electronic liquid crystal phase sets up. Recently, two others cuprates families have been studied: $Bi_2Ca_2SrCu_2O_{8+\delta}$ (Bi2212) and electron doped $Nd_{2-x}Ce_xCuO_4$ (NCCO). In both families, a magnetic order related to the pseudogap phase has been also observed. The recent results will be discussed during the talk.

[1]B. Fauqué, Y. Sidis, V. Hinkov, S. Pailhès, C.T. Lin, X. Chaud, and P. Bourges, *Phys. Rev. Lett.* **96**, 197001 (2006).
[2]Y. Li, V. Balédent, N. Barisić, Y. Cho, B. Fauqué, Y., Sidis, G. Yu,, X. Zhao, P. Bourges, and M. Greven, *Nature* **455**, 372 (2008).
[3]V. Balédent, B. Fauqué, Y. Sidis, N. B. Christensen, S. Pailhès, K. Conder, E. Pomjakushina, J. Mesot, and P. Bourges *Phys. Rev. Lett.* **105**, 027004 (2010).
[4]V. Balédent, D. Haug, Y. Sidis, V. Hinkov, C.T. Lin and P. Bourges, preprint

11:51AM Z2.00002 Novel magnetic excitations in a model cuprate high-T_c superconductor[1] , YUAN LI, Max Planck Institute for Solid State Research, Germany — Magnetic fluctuations might be essential to the mechanism of high-temperature superconductivity in the cuprates. For a long time, such fluctuations have been theoretically regarded as arising from the antiferromagnetic correlations within the copper-oxygen layers, and experimental studies of magnetic excitation spectrum have mainly been carried out near the corresponding wave vector (1/2, 1/2). Following neutron diffraction experiments which demonstrated the universal existence of a "$q = 0$ antiferromagnetic order" in the pseudogap phase of three different cuprates [1-3], our recent inelastic neutron scattering experiments on the model compound $HgBa_2CuO_{4+\delta}$ (Hg1201) revealed the existence of unusual magnetic excitations that weakly disperse throughout the entire Brillouin zone [4,5]. Like the $q = 0$ antiferromagnetic order, the new excitations are observed in the pseudogap phase and therefore appear to be associated with the order. The excitations possess very large spectral weights at well-defined characteristic energies that are comparable to the resonance energy [6] and to those of electron-boson-coupling features observed in a wide range of cuprates, highlighting their possible influence on the electronic structure. These findings demonstrate that the pseudogap state is a distinct phase of matter rather than a mere crossover. They furthermore cast doubt on the presumed predominant importance of the wave vector (1/2, 1/2) in the magnetic excitation spectrum, and have the profound implication that a single-band description of the cuprates is insufficient.

[1] B. Fauque *et al.*, *Phys. Rev. Lett.* **96**, 197001 (2006).
[2] Yuan Li *et al.*, *Nature* **455**, 372 (2008).
[3] V. Baledent *et al.*, *Phys. Rev. Lett.* **105**, 027004 (2010).
[4] Yuan Li *et al.*, *Nature* **468**, 283 (2010).
[5] Yuan Li *et al.*, unpublished.
[6] G. Yu *et al.*, *Phys. Rev. B* **81**, 064518 (2010).

[1]Project was funded by DOE and NSF grants. The author achnowledges the Alexander von Humboldt Foundation.

12:27PM Z2.00003 Collective Modes in Cuprates and their coupling to Fermions , CHANDRA VARMA, University of California, Riverside, CA. — The quantum-critical fluctuations of the loop current order observed universally in underdoped Cuprates have been derived and shown to be local in space and power law in time. The coupling of these fluctuations to fermions are shown to promote d-wave pairing as well as to give the Marginal Fermi liquid single particle spectra in the normal state [1]. Three collective fluctuations modes in the loop order modes are derived [2]. They are massive weakly dispersive magnetic modes. Two of these branches have been discovered. Experiments are suggested to discover the third branch.

[1] V. Aji, A. Shekhter and C.M. Varma, Phys. Rev. B. 81, 06451 (2010).
[2] Yan He and C.M. Varma, arXiv:1008.3182.

1:03PM Z2.00004 Disentangling Cooper-pair formation above T_c from the pseudogap state in the cuprates , TAKESHI KONDO, Ames Laboratory, Iowa State University — The discovery of the pseudogap in the cuprates created significant excitement amongst physicists as it was believed to be a signature of pairing, in some cases well above room temperature. This was supported by a number of experiments detecting phase-fluctuating superconductivity above T_c. However, several recent experiments reported that the pseudogap and superconducting state are characterized by different energy scales, and likely compete with each other, leaving open the question of whether the pseudogap is caused by pair formation. To address this issue, we investigate the spectral weights, which are easier to quantify and in many cases interpret than the spectral feature, which is traditionally used. A key such measure is the density of states at the Fermi energy $D(E_F)$. In conventional, clean superconductors this weight is zero below T_c, but can be finite if there are strong impurity scattering effects. In such cases $D(E_F)$ reflects the pair breaking states. A separate scenario is a generic "density wave state" in the absence of pairing, which leads to a decrease of the $D(E_F)$ due to the opening of the density wave gap. In addition there is also the possibility of the coexistence of superconductivity and the density wave state - inhomogeneous superconductors such as the cuprates, where superconducting and non-superconducting patches coexist in the sample. One can then expect that the temperature dependence of $D(E_F)$ can be used to distinguish between these scenarios and disentangle the electronic ground states of the cuprates. Since the spectral gap in the cuprates displays significant momentum dependence, in our study we use the intensity of the spectral function at E_F, $I(E_F, k)$, which when integrated over all momenta equals $D(E_F)$. This allows us to isolate the behavior at a specific k-point and avoid smearing due to averaging. In this talk, we report the discovery of a spectroscopic signature of pair formation and demonstrate that in a region commonly referred to as the "pseudogap", two distinct states coexist: one that persists to an intermediate temperature T_{pair} and a second that extends up to T^*. The first state is characterized by doping independent scaling behavior and is due to pairing above T_c, but significantly below T^*. The second state is the "proper" pseudogap - characterized by the loss of low energy spectral weight, anomalies in transport properties and the absence of pair formation. T_{pair} has a universal value around 120-150K even for materials with very different T_c and it likely sets limit on the highest attainable T_c in the cuprates.

1:39PM Z2.00005 Phenomenology of electronic nematic and smectic states in STM studies of high T_c cuprates[1] , EUN-AH KIM, Cornell University — Electronic liquid crystals are phases in which electronic structure of a material breaks the spatial symmetries of its crystal lattice: electronic nematic only breaks the point group symmetry, while smectic (stripe) additionally breaks the translational symmetry. Here I define two independent order parameter fields for nematic and smectic that can be constructed from STM data. Using these order parameters we find long range intra-unit cell nematicity in the pseudogap states [1]. In contrast, we observe many topological defects that disorder the smectic fields. However, these defects reveal a remarkable coupling between smectic tendency and fluctuations in the nematic order. From these observations, we propose a Ginzburg-Landau free energy describing the quantum nematic/smectic coupling and demonstrate how it can explain the coexistence of these states and correctly predict their interplay [2]. In principle, this understanding may enable us to disentangle the complexities of the system specific cuprate phase diagrams.

[1] M. J. Lawler, K. Fujita, Jhinhwan Lee, A. R. Schmidt, Y. Kohsaka, Chung Koo Kim, H. Eisaki, S. Uchida, J. C. Davis, J. P. Sethna, Eun-Ah Kim, "Intra-unit-cell electronic nematicity of the high Tc copper-oxide pseudogap states", Nature **466**, 347 (2010).
[2] A. Mesaros, K. Fujita H. Eisaki, S. Uchida, J.C. Davis, S. Sachdev, J. Zaanen, M.J. Lawler, and Eun-Ah Kim, "How topological defects couple the smectic and nematic electronic structure of the cuprate pseudogap states", submitted (2010).

[1]This work was supported in part by NSF Grant DMR-0520404 to the Cornell Center for Materials Research and by NSF Grant DMR-0955822

Friday, March 25, 2011 11:15AM - 2:15PM –
Session Z9 DFD: Complex Fluids, Polymers, Gels D220

11:15AM Z9.00001 An anisotropic continuum model for flow, aggregation and microstructure evolution in magnetorheological fluids , MURAT OCALAN, GARETH MCKINLEY, Massachusetts Institute of Technology — The complexities associated with the transport of magnetorheological (MR) fluids under non-uniform magnetic and flow fields pose unresolved problems for generating accurate computational models. The evolutions of the electromagnetic and rheological properties of MR fluids are strong functions of the suspension microstructure; however, the geometrical features that lead to the field non-uniformities are often of a much larger length scale. To address these commonly occurring flow problems, we develop an anisotropic continuum model for MR fluids in which the electromagnetic stress is incorporated into the constitutive model for the viscoplastic stress generated in the bulk fluid by considering the generation and distortion of suspension microstructure under flow. The new model is incorporated into both a single-phase and a two-phase continuum description of the suspension. The aggregation dynamics and the evolution of MR fluid microstructure are observed in unique ferromagnetic microfluidic channels that replicate flow conditions of practical interest. The predictions of the newly developed models are verified with the experimental observations of microstructure evolution and macroscopic measurements of fluid rheology.

11:27AM Z9.00002 Electrorheological response of dense strontium titanyl oxalate suspensions , CARLOS ORELLANA, JINBO HE, HEINRICH JAEGER, James Franck Institute and Department of Physics, The University of Chicago, Chicago, IL 60637, USA — Strontium Titanyl Oxalate (STO) particles were synthesized using a new method of precipitating the STO out of a water solution by adding alcohol. When dispersed in silicon oil, dense STO suspensions exhibit a high static yield stress in the presence of an electric field (200kPa at 5kV/mm), high shear stress at high shear rates and low current densities. We also find that the yield stress increases roughly linearly with applied field. This behavior is a key characteristic of a polar molecule dominated electrorheological effect. We also observed stress stiffening with time under low shear, stress oscillations, and stress reduction with strain. These effects can be accounted for by the interaction of permanent dipoles with the particles, the creation of shear bands of a few particles in width and the lack of self-diffusion in the samples.

11:39AM Z9.00003 Molecular Simulations of Particle Nanorheology , MIR KARIM, RAJESH KHARE — Over the past few years, experimental and theoretical developments in the field of microrheology have enabled determination of the local mechanical properties of complex materials. In this presentation, we will extend this approach to determine the local viscoelastic properties of polymeric materials using molecular dynamics (MD) simulations. Molecular simulations provide the unique ability to explicitly account for the intermolecular interactions in the system. Thus an approach based on molecular simulations allows for the determination of the viscoelastic properties at the nanoscale. The specific system that is studied in this work consists of a polymeric melt in which the polymers are modeled as bead-spring chains. We will present a comparison of the results obtained from the passive and the active nanorheology approaches. A discussion of the parameter (e.g. amplitude and frequency) ranges that allow usage of these techniques will also be presented.

11:51AM Z9.00004 Microscopic Approach for the Friction on a Spherical Particle in Dense Liquids: Hydrodynamics and Beyond , UMI YAMAMOTO, KENNETH SCHWEIZER, University of Illinois, Urbana-Champaign — We propose a new microscopic, non-mode-coupling, statistical dynamical approach to deriving the Stokes-Einstein (SE) friction coefficient of a large spherical particle dissolved in a dense fluid. The real space method is based on including as a slow variable the force exerted on a particle by the surrounding fluid. By exploiting the appropriate separation of time and length scales, and the Kirkwood superposition approximation for multi-point correlations, the SE result is obtained including the slip and stick limits plus the crossover function. This advance provides the foundation for developing a unified theory of friction for nanoparticles that includes both hydrodynamics and the non-hydrodynamic contribution associated with material-specific particle-fluid and particle-particle forces. Applications to nanoparticles in unentangled and entangled polymer solutions and melts, under various interfacial polymer-particle structure conditions, will be reported. Questions of particular interest include how the non-hydrodynamic friction contribution scales with particle radius, the role of length-scale-dependent viscosity in polymer liquids, and the conditions required for crossover to the hydrodynamics-dominated regime.

12:03PM Z9.00005 Rheology of bacterial flagella suspensions , SEVIM YARDIMCI, THOMAS GIBAUD, DANIEL CHEN, EDWARD BARRY, ZVONIMIR DOGIC, Physics Department, Brandeis University — The mechanical behavior of a suspension of rigid and semiflexible filaments has been studied in great detail. In comparison the effect of the filament geometry has been relatively unexplored. We present experimental results on the rheological behavior of suspensions of curly and straight flagella with an identical average contour length. We find that both suspensions are trapped in a glassy state and exhibit a solid-like behavior. We observe that the scaling of viscoelastic moduli is highly dependent on filament geometry. Taken together, this highlights the role of filament geometry in suspension mechanics.

12:15PM Z9.00006 Brownian Dynamics simulations of dilute graphene solutions under flow , YUEYI XU, MICAH GREEN, Department of Chemical Engineering, Texas Tech University — Many graphene-based materials (such as thin conductive films and nanocomposites) are processed in the liquid phase and require the conformation and alignment of graphene in solution to be precisely controlled. However, prior studies of conformation dynamics of sheetlike macromolecules such as graphene have been limited to equilibrium behavior, and there have been no studies of the dynamics of sheetlike macromolecules on flow processing timescales. Here we develop Brownian Dynamics (BD) algorithms in order to quantify the effects of flow processing on graphene conformation. The method is conceptually similar to those used for linear polymers; we coarse-grain the sheet using a bead-rod lattice of arbitrary 2-D connectivity and develop a novel theoretical framework for bending and metric forces. Using this technique, we simulate the conformation dynamics of dilute sheetlike macromolecule solutions in shear flow and compute the corresponding solution properties as a function of flow strength, sheet size, and solvent quality.

12:27PM Z9.00007 Orientation Dependent Gelation of Platelet Suspensions , YA-WEN CHANG, ANDRES MEJIA, ZHENGDONG CHENG[1], Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX 77832 — Gelling behavior of colloidal suspensions of disk-shaped particles has long been used as an ideal system for studying the formation of arrested state of matter. High aspect ratio synthetic α-Zirconium phosphate (α–ZrP) monolayer platelets have recently received our attention as a new type of liquid crystal building blocks. We report the phase diagram of charged α-Zirconium phosphate platelet suspensions across the isotropic (I) –nematic (N) region versus salt concentrations. Typical electrostatic screening induced flocculation and gelation of platelet suspensions were observed. The morphological and rheological characteristics of liquid crystalline and colloidal gel phases were studied with polarized optical imaging and rotational/oscillatory rheometer. At high ionic strengths (>10mM), a re-entrance of fluidic liquid crystal phase occurs when particle volume fractions are above the arrested gel phase. We contribute this behavior to the competition between the driving forces for isotropic/nematic and sol/gel transitions of attractive colloidal platelets. Strong particle alignment hinders gelation, which usually demonstrates the "house of card" configuration in platelet suspensions; Isotropic suspensions flocculate and gel easily, as we confirmed experimentally.

[1]Material Science and Engineering Program, Texas A&M University, College Station, TX 77832

12:39PM Z9.00008 Dynamic separation of macromolecules under temperature gradient[1] , YUSUKE MAEDA, The Rockefeller University, Center for Studies in Physics and Biology, AXEL BUGUIN, Institut Curie, Centre de recherche, CNRS/UMR, ALBERT LIBCHABER, The Rockefeller University — Thermophoresis is a motion of suspensions in a fluid that are subjected to a temperature gradient. Although its effect is widely studied in case of single solute in water, little is known about how the mixture of different solutes is affected. We heated water with an infrared laser by $\Delta T_{\max}$=5C and ∇T=0.25C/um to induce thermophoresis of polyethylene glycol (PEG) and DNA. PEG is depleted from the hot region and results in a stationary gradient of its high volume fraction ϕ. Under this high concentration of PEG, DNA of small concentration is submitted to thermophoresis and osmotic pressure difference. The DNA shows regime of depletion, ring-like localization and accumulation as the volume fraction of PEG increases. As the osmotic force depends on the size of trapped solutes, DNA of different size accumulates at different regions. Depending whether the DNA size is below or above 5kbp a different scaling of position versus DNA size is observed. Thermal separation is a general phenomenon. It applies also to RNA and microbeads.

[1]YTM is supported by JSPS fellowship and M.Josee-H.Kravis fellowship from the Rockefeller University.

12:51PM Z9.00009 Non-affine deformations in flexible and semi-flexible polymer gels[1] , ANINDITA BASU, Physics and Astronomy, University of Pennsylvania, QI WEN, Institute for Medicine and Engineering, University of Pennsylvania, XIAOMING MAO, TOM LUBENSKY, Physics and Astronomy, University of Pennsylvania, PAUL JANMEY, Institute for Medicine and Engineering; Physics and Astronomy, University of Pennsylvania, ARJUN YODH, Physics and Astronomy, University of Pennsylvania — We test the validity of affine deformation assumption in flexible and semi-flexible polymer networks by embedding different-sized fluorescent tracer beads within model polymer networks and quantifying their displacements under shear. A conventional rheometer is used with a confocal microscope for this purpose. Non-affinity is quantified as a function of applied strain, polymer chain density, cross-link concentration, network morphology, reaction kinetics and size of probe particles used. Non-affinity measurements in flexible polymer gels are in qualitative agreement with current theories in rubber elasticity. For semi-flexible bio-polymer gels, measurements indicate that non-affine deformations are small for networks of thinner, relatively flexible filaments and get smaller as strain increases into non-linear elastic regime. These small measures are consistent with the entropic model for non-linear elasticity of semi-flexible gels. However, as filament stiffness and mesh size increase, the deformations become more non-affine, as predicted by the enthalpic bending and stretching models of non-linear elasticity.

[1]MRSEC DMR-0520020, DMR-0505048, and DMR- 0079909

1:03PM Z9.00010 Drying of polymer films: study of demixing phenomena , JULIE FICHOT, RODOLPHE HEYD, CNRS, MARIE-LOUISE SABOUNGI, CHRISTOPHE JOSSEREND, EMILIE COMBARD, JEAN FRANCOIS TRANCHANT — Understanding the mechanisms that control the stability of polymeric films is important in beauty care. We have prepared films starting from a water-soluble organic polymer, a preservative and water. We study the drying of these films as a function of several physicochemical parameters that control their interfaces such as temperature, humidity and the nature of the support. The viscoelastic properties of the solutions before spreading out are analyzed with a rheometer in order to adjust the temperature. The topography of the films is observed by optical microscopy and the evolution of the drying is determined with a precision gravimetric balance. The behavior of the films on a nanometric scale is followed by AFM. During the drying process, droplets appear on the surface of the film, made up of water surrounded by a shell of preservative. As the films dries, the water evaporates from the droplets and the preservative spreads on the surface of the film, leading to the formation of craters on the surface of the dried film. The dimensions and numbers of the craters depend strongly on the type and concentration of the preservative employed.

1:15PM Z9.00011 Multiple Particle Collision Dynamics Simulations of the Effect of Catenation on the Structural and Dynamic Properties of Ring Polymers in Solution , GOVIND HEGDE, RAJESH KHARE, Department of Chemical Engineering, Texas Tech University — Multiple particle collision dynamics (MPCD) is a particle based mesoscale simulation technique that coarse-grains the solvent while preserving the hydrodynamics, thus enabling simulations over longer length and time scales as compared to molecular dynamics (MD) simulations. In this work, MPCD is used to study the effect of topology on the structural and dynamic behavior of complex fluids. The systems of interest in this work are the dilute solutions of ring and catenated ring polymers. MPCD simulation results are compared with those obtained from MD simulations in which the hydrodynamic interactions are governed by the explicit intermolecular interactions. Different chain topologies are considered such as catenated as well as multi-catenated rings. Results will be presented for the effect of chain length on the radius of gyration and chain diffusion coefficient for the various topologies studied. Our results will also be compared with previous theoretical and experimental work reported in literature.

1:27PM Z9.00012 Strongly anisotropic polymer networks , STEPHAN ULRICH, University of Goettingen, ANNETTE ZIPPELIUS, University of Goettingen, Max Planck Institute for Dynamics and Self-Organization, PANAYOTIS BENETATOS, Cavendish Laboratory, University of Cambridge — We investigate a network of worm-like chains, which are strongly oriented along a preferred direction due to an external field, boundary conditions, or a nematic environment. We discuss the effects of random permanent cross-links, whose density may follow an arbitrary distribution along the alignment direction. We show that the tilt modulus is unaffected by cross-links. As the cross-link density is increased beyond the gel point, the network develops a stiffness to in-plane shear deformations. Results for the shear elasticity and fluctuations of the polymer chains are presented. The case of cross-linking the chains on one end only is highlighted, it constitutes a simple model for polymer brushes. Moreover force-extension curves are presented for a toy model that consists of two cross-linked chains.

1:39PM Z9.00013 Structure and Dynamics of Water Absorbed in Polyamide , MARCO LAURATI, PAUL SOTTA, DIDIER LONG, LUDOVIC ODONI, VERONIQUE BOSSENEC, THIERRY BADEL, Laboratoire Polymeres et Materiaux Avances, UMR5268, CNRS/Rhodia Recherches et Technologies, 85 Rue des freres Perret, 69192 Saint-Fons Cedex, ARANTXA ARBE, ANGEL ALEGRIA, JUAN COLMENERO, Centro de Fisica de Materiales (CSIC-UPV/EHU), Paseo Manuel de Lardizabal 5, 20018 Donostia/San Sebastian, Spain — We present results of elastic and inelastic neutron scattering, dielectric spectroscopy and MD simulations concerning the structural organization and the dynamics of water absorbed in an amorphous polyamide material. We find that, different from predictions of available models of water absorption in polyamide, only a small fraction of water binds to the amide groups while most of it organizes into aggregates. Such structural model is supported by results on the microscopic dynamics of water, which can be described as diffusive motions with a relaxation time following a VFT dependence on temperature, similarly to bulk water. Measured average diffusion coefficients of water absorbed in Polyamide are approximately two orders of magnitude smaller than in bulk water, revealing the confinement effect of the polymer matrix.

1:51PM Z9.00014 Order parameter defining liquid-liquid transition in water[1] , J. RAUL GRIGERA, OSVALDO CHARA, ANDRES MCCARTHY, IFLYSIB (UNLP-CONICET), c.c. 565, La Plata, Argentina — Water presents both open tetrahedral and compact hexagonal structures. Although several order parameters have been proposed to quantify this, all of them are only applicable to data produced by simulation. We present an order parameter (P_r) that is calculated from the radial distribution function $g(r)$, also available from experiment. We hereby extract the tetrahedral and hexagonal components from the $g(r)$, each one reconstructed as the sum of a Freundlich distribution for the first peak, two subsequent Gaussian distributions, and a sigmoidal to account for the rest. The order parameter can be calculated from the relative contribution of tetrahedral over hexagonal contribution. We obtained the P_r for SPC/E water model from molecular dynamics simulations of water at different pressures and temperatures. At 300K, the pressure in which both, tetrahedral and hexagonal contributions become equal (P_r= 0), a structural crossover is found in the vicinity of 2kbar, close to the pressure at which the ''anomalous'' behavior manifests. Having computed P_r for this wide range of pressure and temperature we then calculate the HDL spinodal, the coexistence line, the second critical point, and the Widom line.

[1]Supported by CONICET, UNLP, and CIC Prov.BsAs.

2:03PM Z9.00015 Particle and fluid diffusivity of non-colloidal suspensions , EMMANOUELA FILIPPIDI, ALEXANDRE FRANCESCHINI, CHUI-LAI CHEUNG, JACOB TUTMAHER, SEAN PARADISO, TARUN JAIN, DAVID PINE, Center for Soft Matter Research, New York University — Suspensions of non-colloidal spheres at moderate volume fractions (0.2-0.4) under slow periodic strain undergo a phase transition from an absorbing to an active fluctating state. Particle trajectories change from reversible below the critical strain to irreversible above. We measure the fluid diffusivity of the fluorescently labelled fluid and compare it with the particle diffusivity in order to obtain a measure of the coupling between the two. Of particular interest is how the fluid diffusivity changes near the onset of irreversibility of the particle trajectories.

Friday, March 25, 2011 11:15AM - 2:03PM –

Session Z10 DCMP: Novel Instrumentation and Techniques in Surface Science D221

11:15AM Z10.00001 Development of a device-oriented UHV scanning probe microscope based on quartz sensors[1] , JACOB TOSADO, WILLIAM G. CULLEN, MICHAEL S. FUHRER, University of Maryland — Scanning tunneling microscopy (STM) provides atomic-scale spatial resolution and performs local electronic spectroscopy of conducting materials. The recent emergence of graphene has highlighted the ability to tune carrier density by applying a gate voltage. However, preparation of samples as field-effect-transistors necessitates a dielectric substrate below the device, which is problematic for STM. Driven by the need to carry out high resolution imaging in ultrahigh vacuum, we are now developing an instrument which combines STM with atomic force microscopy (AFM) using a quartz sensor. This combination allows AFM approach and navigation, with uncompromised STM performance due to the very high stiffness of the quartz sensor. Primary features of the microscope design include in-situ exchange of probes and samples, with flexibility in probe and sample geometries and multiple contacts to both probe and sample. The microscope is housed in a UHV chamber with complete surface preparation and analysis capability. This talk will cover unique design features as well as testing of the microscope concept.

[1]Supported by a NRI supplement to the UMD-NSF-MRSEC grant #DMR 0520471, with infrastructure support from the Center for Nanophysics and Advanced Materials.

11:27AM Z10.00002 Low-temperature STM/STS study on superconducting FeSe films[1] , XUCUN MA, CANLI SONG, YILIN WANG, PENG CHENG, LILI WANG, KE HE, XI CHEN, QIKUN XUE, INSTITUTE OF PHYSICS, CHINESE ACADEMY OF SCIENCES TEAM, DEPARTMENT OF PHYSICS, TSINGHUA UNIVERSITY TEAM — By using molecular beam epitaxy (MBE) technique, we have prepared single crystalline and atomically flat FeSe thin films on graphene-terminated SiC substrate. Low temperature scanning tunneling microscopy/spectroscopy (STM/STS) measurements reveal that the local superconducting gap in the quasiparticle density of states remains robust down to two triple layers ($\sim$1.1 nm), and that the FeSe films show a novel thickness-dependent superconductivity transition behavior. We show that the superconductivity of the FeSe films can be manipulated by concise control of their surface structures. *dI/dV* mapping of the vortex lattice confirms that FeSe is a typical type II superconductor. Understanding these properties may help us to unravel the mechanism of the recently discovered Fe-based superconductors and even the long-term studied cuprates.

[1]The work was financially supported from NSF and MOST of China.

11:39AM Z10.00003 In situ coherent x-ray scattering and STM studies of hexagonally reconstructed Au(001) in Electrolytes[1] , MICHAEL S. PIERCE, Materials Science Division, Argonne National Laboratory, VLADIMIR KOMANICKY, Faculty of Science, Safarik University, ANDI BARBOUR, DANIEL HENNESSY, Materials Science Division, Argonne National Laboratory, JUNDAR SU, ALEC SANDY, Advanced Photon Source, Argonne National Laboratory, HOYDOO YOU, Materials Science Division, Argonne National Laboratory — We have studied the dynamics of Au(001) and Au(111) surfaces in situ in 0.1 M HClO4 electrolyte solution using coherent x-ray scattering experiments and STM microscopy. Our coherent x-ray scattering experiments measure a correlation time for the surface as a function of applied potentials. Coherent x-ray scattering differs from the ordinary x-ray diffraction in sensitivity to the structural and temporal details. The correlation times were obtained from measurements conducted while the surface is in equilibrium and the ordinary surface scattering intensity is constant. The correlation time changes from high 10^3 seconds to low 10^2 seconds. The correlation times of reconstructed surfaces at low potential are at least an order of magnitude smaller than those measured at the reconstructed surfaces in vacuum. The correlation times also change dramatically in response to the applied potential. These experiments also represent the first successful application of coherent x-ray scattering to the study of electrochemical interfaces in situ.

[1]Work at ANL is supported by DOE-BES and work at SU by VEGA.

11:51AM Z10.00004 Local transport measurements at mesoscopic length scales on epitaxial graphene using scanning tunneling potentiometry , WEIGANG WANG, KO MUNAKATA, MICHAEL ROZLER[1], FRANCOISE KIDWINGIRA[2], MALCOLM BEASLEY, Stanford University — By contrast to quantum transport measurements across nanostructures (single molecular, carbon nanotube, or lithographically manufactured), local transport measurements on macroscopic samples at mesoscopic length scales are relatively uncharted territory. Scanning tunneling potentiometry (STP) is the natural tool to perform such measurements. Due to its characteristic materials parameters, thin epitaxial graphene on silicon carbide is an attractive model system for search of quantum mechanical effects in local transport. We report results of STP measurements on epitaxial graphene at room temperature. In addition to the expected residual resistivity dipoles, we have observed features in the measured potential that are counter intuitive to classical diffusive considerations. Based on these results, we conclude that a more complete theoretical description of STP measurement is necessary. Work supported by AFOSR.

[1]Present address: Rush University
[2]Present address: KLA-Tencor Corporation

12:03PM Z10.00005 Possible microscopic origin of large broadening parameter in point Andreev reflection spectroscopy[1] , JIAN WEI[2], GOUTAM SHEET[3], VENKAT CHANDRASEKHAR, Northwestern University — We report on the low frequency noise in ballistic point-contacts between a silver tip and a niobium foil. The ballistic nature is confirmed by point-contact Andreev reflection (PCAR) spectroscopy. As has been found by others, a broadening parameter Γ needs to be introduced to fit the PCAR spectra. For contacts with higher resistance, a larger Γ is required to fit the PCAR spectra, and we find that random two level fluctuations dominate the noise spectra. This finding suggests that two level fluctuations contribute to the broadening of the gap features.

[1]This research was conducted with support from U.S. Department of Energy through Grant No. DE-FG02-06ER46346.
[2]Now at Peking University, PR China
[3]Now at Argonne National Laboratory

12:15PM Z10.00006 Scanning SQUID measurements of the superconducting state of δ-doped $SrTiO_3$ heterostructures , JULIE A. BERT, Stanford University, MINU KIM, CHRIS BELL, HAROLD Y. HWANG, University of Tokyo, KATHRYN A. MOLER, Stanford University — The discovery of interface superconductivity in complex oxide heterostructures has generated significant excitement. We used scanning SQUID microscopy to investigate the magnetic properties of one such heterostructure, δ-doped structures in $SrTiO_3$ thin films. We have observed a diamagnetic response and imaged vortices providing further evidence of a two-dimensional superconducting state. Finally we measured the magnetic susceptibility from which we observe spatial inhomogeneities in the superconducting response and can estimate the temperature dependence of the magnetic penetration depth.

12:27PM Z10.00007 Probing Transient Structures during interfacial charge transfer mimicking solar cells and heterogeneous catalysis[1] , LIN CHEN, Argonne National Lab./Northwestern U., XIAOYI ZHANG, Argonne National Lab., GRIGORY SMOLENTSEV, Southern Federal University, JIANCHANG GUO[2], KLAUS ATTENKOFER, ANDREW B. STICKRATH, DI-JIA LIU, Argonne National Lab, NOSHEEN GOTHARD, Northwestern University — Photoinduced charge transfer at interfaces is a key process in photocatalysis and dye sensitized solar cells (DSSCs). Using X-ray transient absorption (XTA) spectroscopy, we extracted metal center surrounding transient structural information in a DSSC mimic, namely the RuN3 dye on the TiO_2 nanoparticle surfaces. Structural evolution of the adsorbed dye sensitizer and the rearrangement of the nanocrystal surface associated with the electron density shift during and after the interfacial charge injection were investigated. The other interfacial charge transfer system is a suspension of Pt nanoparticles on TiO_2 where the photoexcitation induces redox reactions and generate hydrogen fuel. The preliminary XTA results demonstrate the feasibility of the method in probing heterogeneous catalytic systems.

[1]The work was supported by the US Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.
[2]Current address: Oak Ridge National Lab

12:39PM Z10.00008 Composition of CuAu alloy and changes upon corrosion studied by Hard X-ray Photoelectron Spectroscopy , PARASMANI RAJPUT, BLANKA DETLEFS, ESRF, Grenoble, France, AJAY GUPTA, UGC-DAE Consortium for scientific research, Indore 452017, India, DIETER KOLB, University Ulm, Germany, JORG ZEGENHAGEN, ESRF, Grenoble, France — Metals and their alloys are highly susceptible to corrosion in wet environment. Dealloying is a particular type of corrosion, attacking practically all metals in industrial use: When an alloy is coming into contact with an electrolyte, the less noble metal may go into solution, typically causing crack formation and subsequent material failure upon stress. We used bulk sensitive Hard X-ray photoelectron spectroscopy (HAXPES) with an excitation energy of 6 keV as a new powerful tool to investigate the chemical composition of alloys and changes upon dealloying, studying Cu_xAu (with x = 4.1) alloy films of 9 to 50 nm thickness. Morphology, structure and composition were further characterized by atomic force microscopy, X-ray reflectivity and quantitative X-ray fluorescence. The HAXPES analysis revealed that chemical shifts of metal core-levels, i.e. Au4f and Cu3s, can be used as a benchmark for the alloy composition. HAXPES as a function of electron emission angle allowed depth sensitive determination of the chemical composition before and after dealloying in sulphuric acid.

12:51PM Z10.00009 X-Ray Characterization of Electrodeposited Alloy Thin Films[1] , NICHOLAS WOZNIAK, DANIEL MCNEEL, ALYSSA FREY[2], JENNIFER HAMPTON, Hope College — Particle-Induced X-ray Emission (PIXE) was used to measure the composition of electrodeposited NiFe and NiFeCu thin films. The thin films were deposited on gold-plated silicon wafers, and PIXE spectra were analyzed to obtain the Ni, Fe, Cu, and Au content in each sample. By comparing the Ni, Fe, and Cu content in a sample to the Au content in the same sample, the relative amounts of deposited material between samples could be measured. The effect of the deposition solution, deposition parameters and duration of deposition was explored. The results were compared to those measured with Energy Dispersive Spectroscopy. The results show that PIXE can measure the total deposited metal in a sample over at least four orders of magnitude with similar fractional uncertainties. The technique is also sensitive enough to observe the variations in alloy composition due to sample non-uniformity or variations in deposition parameters.

[1]This work is supported by the National Science Foundation under REU Grants No. PHY/DMR-1004811 and. PHY-0969058, the Hope College Dean for the Natural and Applied Sciences Office, and the Hope College Department of Physics.
[2]University of Wisconsin-Eau Claire

1:03PM Z10.00010 Thermal conductance of interfaces with molecular layers - low temperature transient absorption study on gold nanorods supported on self assembled monolayers , WEI WANG, JINGYU HUANG, CATHERINE MURPHY, DAVID CAHILL, UNIVERSITY OF ILLINOIS AT URBANA CHAMPAIGN, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING TEAM, DEPARTMENT OF CHEMISTRY COLLABORATION — While heat transfer via phonons across solid-solid boundary has been a core field in condense matter physics for many years, vibrational energy transport across molecular layers has been less well elucidated. We heat rectangular-shaped gold nanocrystals (nanorods) with Ti-sapphire femtosecond pulsed laser at their longitudinal surface plasmon absorption wavelength to watch how their temperature evolves in picoseconds transient. We observed single exponential decay behavior, which suggests that the heat dissipation is only governed by a single interfacial conductance value. The "RC" time constant was 300ps, corresponding to a conductance value of 95MW/m^{2}K. This interfacial conductance value is also a function of ambient temperature since at temperatures as low as 80K, which are below the Debye temperature of organic layers, several phonon modes were quenched, which shut down the dominating channels that conduct heat at room temperature.

1:15PM Z10.00011 Contact voltage-induced softening transition of gold-on-gold contacts at cryogenic temperatures , DIANA BERMAN, MATTHEW WALKER, JACQUELINE KRIM — A series of experiments were performed in vacuum environments to investigate the impact of contact voltage on the surface softening transition for gold-on-gold contacts at cryogenic temperatures [1]. The purpose of this work was twofold: (1) To examine whether asperity heating models already validated for high temperature contacts were also applicable at cryogenic temperatures, and (2) to explore the implications and validity of prior suggestions that contact temperatures between 338 and 373 K are high enough to dissociate adsorbed film and/or push them aside, but low enough to prevent asperities from becoming soft and adherent. Measurements on two distinct RF MEMS switch types were performed in the temperature range 79 - 293K and for contact voltages ranging from 0.01 to 0.13 V. Contact resistance values at all temperatures were observed to be lower for higher contact voltages associated with increased heating and softening effects. In-situ removal of adsorbed species by oxygen plasma cleaning resulted in switch adhesive failure. Switches that had not been cleaned meanwhile exhibited distinct reductions in resistance at contact temperatures close to 338 K, consistent with suggestions that films begin to desorb, disassociate, and/or be pushed aside at that temperature. Funding agencies: AFOSR, DARPA, and NSF DMR. [1] D. Berman, M. Walker, J. Krim, J. Appl. Phys., 108, 044307 (2010).

1:27PM Z10.00012 Reduction of a polar oxide surface in a strong DC-field[1] , WOLFRAM STEURER, SVETLOZAR SURNEV, Institute of Physics, University of Graz, Universitaetsplatz 5, Graz, A-8010, Austria, GIOVANNI BARCARO, ALESSANDRO FORTUNELLI, IPCF/CNR, via G. Moruzzi 1, Pisa, I-56124, Italy, FALKO P. NETZER, Institute of Physics, University of Graz, Universitaetsplatz 5, Graz, A-8010, Austria — Polar oxide surfaces are of fundamental scientific interest because of their inherent instability in bulk samples on electrostatic grounds. Here we report first experimental evidence of field-induced reduction of a polar oxide surface by applying homogeneous external DC-fields. Ultrathin Ni-oxide nanostructures immersed into an Ag(100) substrate have been grown by reactive evaporation and have subsequently been exposed to electric fields in the range of 0.5-1.6 V/nm. We achieve such high fields in a setup resembling a plate capacitor where the Ag(100) substrate (with the deposited NiO film) acts as the cathode with a counter electrode placed 800nm apart. For fields exceeding the threshold of 0.9 V/nm, oxygen atoms are torn away from the surface, thus, efficiently reducing the initially highly-ordered Ni-oxide film. The remaining Ni atoms on the surface are highly mobile and cluster together. No oxide reduction occurs if the field polarity is inverted.

[1]This work is supported by the ERC Advanced Grant "SEPON."

1:39PM Z10.00013 Interference between Surface and Bulk Scattering in Nanoscale Conductors , SWARBHANU CHATTERJEE, ALEXANDER MEYEROVICH, University of Rhode Island — We analyze the quasiclassical and quantum interference between the bulk and boundary scattering channels in thin high quality films. The effective transport time is calculated beyond the Matthiessen's approximation as an expansion in inverse bulk mean free path. The interference corrections to resistivity exhibit a crossover between two regimes that are characterized by distinct dependences on temperature and/or impurity concentration. In our quasiclassical approximation the results reduce to a transparent analytical expression. We discuss differences between quantum and quasiclassical approaches and experimental implications of our results.

1:51PM Z10.00014 Quantitative Transmission Electron Microscopy of Nanoparticles and Thin-Film Formation in Electroless Metallization of Polymeric Surfaces[1] , ANIRUDDHA DUTTA, HELGE HEINRICH, STEPHEN KUEBLER, CHRIS GRABILL, University of Central Florida, ANIKET BHATTACHARYA — Gold nanoparticles(Au-NPs) act as nucleation sites for electroless deposition of silver on functionalized SU8 polymeric surfaces. Here we report the nanoscale morphology of Au and Ag nanoparticles as studied by Transmission Electron Microscopy (TEM). Scanning TEM with a high-angle annular dark-field detector is used to obtain atomic number contrast. From the intensity-calibrated plan-view scanning TEM images we determine the mean thickness and the volume distribution of the Au-NPs on the surface of the functionalized polymer. We also report the height and the radius distribution of the gold nanoparticles obtained from STEM images taking into consideration the experimental errors. The cross sectional TEM images yield the density and the average distance of the Au and Ag nanoparticles on the surface of the polymer.

[1]Supported by grant NSF, Chemistry Division.

Friday, March 25, 2011 11:15AM - 2:15PM –

Session Z13 GSNP DFD: Granular Materials II D225/226

11:15AM Z13.00001 Perfect fluid flow from the impact of a dense granular jet , WENDY W. ZHANG, JAKE ELLOWITZ, NICHOLAS GUTTENBERG, University of Chicago, HERVE TURLIER, Institut Curie, SIDNEY R. NAGEL, University of Chicago — Axisymmetric collision of a cylindrical water jet with a circular target generates a thin conical sheet, also known as a water bell [Cheng et al. Phys. Rev. Lett. 99, 2007]. Intriguingly, recent experiments on granular jet impact in the regime of dense inertial flow reveal similar behavior: the angles by which the collimated sheets of particles are ejected from the target agree closely with the angles measured in the water-bell experiments [Clanet, C. J. Fluid Mech. 430, 2001] . This quantitative correspondence suggests that the collective granular motion during impact can be modeled as an incompressible, continuum fluid. Since viscous effects are weak in water-jet impact and the granular jet is comprised of non-cohesive particles (hence possessing zero surface tension), the simplest scenario is that the continuum motion corresponds to the flow of a perfect fluid. We show an exact solution of 2D perfect fluid impact agrees quantitatively with 2D discrete-particle simulation results. Therefore, the emergence of a highly collimated outgoing sheet does not necessarily signal the creation of a thermodynamic liquid phase. Such a coherent outcome results generically when the motion is nearly incompressible and dominated by inertia.

11:27AM Z13.00002 Jet-Induced Granular 2-D Crater Formation with Horizontal Symmetry Breaking[1] , ABE CLARK, ROBERT BEHRINGER, Duke Physics — We investigate the formation of a crater in a 2-D bed of granular material by a jet of impinging gas, motivated by the problem of a retrograde rocket landing on a planetary surface. As the strength and height of the jet are varied, the crater is characterized in terms of depth and shape as it evolves, as well as by the horizontal position of the bottom of the crater. The crater tends to grow logarithmically in time, a result which is common in related experiments. We also observe an unexpected horizontal symmetry breaking at certain well-defined conditions. We present data on the evolution of these asymmetric states and attempt to give insights into the mechanism behind the symmetry-breaking bifurcation. This horizontal symmetry breaking is highly suggestive of a pitchfork bifurcation, and we give evidence to classify it as forward or backward in different regimes of operation. As we will demonstrate, the formation of an asymmetric crater could be of considerable practical concern for lunar or planetary landers, particularly in the case of a backward pitchfork bifurcation, which is characterized by hysteresis and very rapid transitions.

[1]supported by ORBITEC (contract # OTC-GS-02381), subcontracted from USAF (contract # NNX09 CF72P) and by NASA contract

11:39AM Z13.00003 Simulations of granular jet impact deadzone formation , NICHOLAS GUTTENBERG, JAKE ELLOWITZ, WENDY ZHANG, University of Chicago, HERVE TURLIER, Univ. Pierre & Marie Curie, SIDNEY NAGEL, University of Chicago — Motivated by granular experiments showing the emergence of continuum-like dynamics when a dense jet hits a target, we simulate the impact of 2D and 3D granular jets of frictional, cohesion-less grains upon a fixed target. This is a inertial, dense jet regime where the motion is essentially incompressible. Impact deflects the material in the jet into a hollow conical sheet. The cone angles measured in simulation are consistent with previous experimental studies of the 3D granular jet impact. In addition, experiments have revealed the formation of a "dead zone," a region where the grain motion is negligibly small. The simulation shows that this dead zone can only form when a no-slip boundary condition is enforced at the target. The presence or absence of the dead zone leads to a change in cone angle consistent with the experimentally observed differences in cone angle between the 3D granular flow and the corresponding water bell flow.

11:51AM Z13.00004 Endless penetration in impact cratering[1] , J. CARLOS RUIZ-SUAREZ, Cinvestav-IPN, Unidad Monterrey, FELIPE PACHECO-VAZQUEZ, Cinvestav-IPN, Unidad Merida, J. MANUEL SOLANO-ALTAMIRANO, Cinvestav-IPN, Unidad Monterrey, GABRIEL CABALLERO-ROBLEDO, Cimav-Unidad Monterrey — The phenomena of impact cratering have been in the minds of physicists at least for two decades; the reason being the interest for elucidating the intriguing rheological response produced by granular systems when they are penetrated. With the great amount of work done in this regard, one could think that the problem is reasonably well understood. However, we study here a fascinating phenomenon never observed before in granular penetration experiments: depending on the mass of a projectile colliding onto a granular bed, it either stops at a given depth like normally expected, or keeps sinking with a terminal velocity as if the medium were a newtonian fluid. Understanding this intriguing behaviour could help us to know the subtleties of intrusion phenomena in granular media.

[1]Grant 101384, Conacyt México

12:03PM Z13.00005 Avalanches of Singing Sand in the Laboratory , SIMON DAGOIS-BOHY, Kamerlingh Onnes Laboratorium, Universiteit Leiden, SYLVAIN COURRECH DU PONT, STÉPHANE DOUADY, Laboratoire M.S.C., Univ. Paris Diderot — The song of dunes is a natural phenomenon that has arisen travellers' curiosity for a long time, from Marco Polo to R.A. Bagnold. Scientific observations in the XXth century have shown that the sound is emitted during a shear flow of these particular grains, the free surface of the flow having coherent vibrations like a loud speaker. The sound emission is also submitted to a threshold effect with many parameters like humidity, flow speed, surface of the grains. The sound has been reproduced in laboratory avalanche experiments close to the natural phenomenon on field, but set in a channel with a hard bottom and a few centimeters of sand flowing, which contradicts explanations of the sound that involve a sand dune under the avalanche flow. Flow rates measurements also show the presence of a plug region in the flow above the sheared band, with the same characteristic length as the coherence zones of the sound. Finally we show experimentally that the Froude number, once modified to take into account the height of this plug band, is the parameter that sets the amplitude of the sound, and produces a threshold that depends on the grain type.

12:15PM Z13.00006 Shear strength of vibrated granular/granular-fluid mixtures , BRIAN UTTER, RALPH HERMAN, BEN FOLTZ, James Madison University — The behavior of dense granular materials can be characterized by the continuous forming and breaking of a strong force network resisting flow. This jamming/unjamming behavior is typical of a variety of systems and is influenced by factors such as grain packing fraction, applied shear stress, and the random kinetic energy of the particles. We present experiments on shear strength of granular and granular-water mixtures under the influence of external vibrations, one parameter that leads to unjamming. We use low vibration (< 1g) and slow shear and measure avalanching statistics in a rotating drum and the torque required to move a stirrer through a sand/water mixture. We find that external vibration (i) increases granular strength at small vibrations in the dry system, (ii) removes history dependence (memory), and (iii) decreases shear strength at all accessible saturation levels in the sand-fluid system. Additionally, shear strength is found to be smallest for both dry and completely saturated mixtures. Additional ongoing experiments probe beyond a dimensionless acceleration of 1 and explore jamming and surface chemistry effects in the avalanching flow of granular/fluid mixtures.

12:27PM Z13.00007 Collisions between solitary waves in granular alignments[1] , SURAJIT SEN, SUNY Buffalo, DIANKANG SUN, New Nexico Resonance — Solitary waves arise naturally when an unloaded alignment of elastic spheres, that is held between fixed end walls, is perturbed at one end. Unlike most known classes of solitary waves, those in granular materials are special and tend to break down and reform during any collision. Here we present what happens when two solitary waves of unequal magnitude suffer head-on and overtaking types of collisions. We will show that these collisions provide ways for solitary waves to not only become smaller but also become larger (within bounds) and that they are the underlying reason behind the emergence of the quasi-equilibrium phase.

[1]Research Support: Army Research Office

12:39PM Z13.00008 Oil in Water Emulsion Flow in a 2D Hopper[1] , XIA HONG, DANDAN CHEN, KENNETH DESMOND, ERIC WEEKS, Physics Dept., Emory University — Granular flows are still somewhat poorly understood. One such case is the flow of 2D disks through a hopper. In a prior experiment by To (K. To, et al. PRL 86(1) 2001), they found that as 2D disks flow through a hopper they may jam due to arch formations at the hopper exit, and that the jamming probability can be increased by enhancing the static friction between the disks. In our study we remove the effects of static friction by using quasi-2D oil in water emulsion droplets flowing through a hopper to understand the role of friction in jamming. The droplets feel a viscous friction, but no static friction. Similar to the granular experiment, our oil droplets flow due to gravity. We have observed the transition between jammed and unjammed flows in our setup, and we are currently investigating its nature as the hopper size changes. In our experiments, jamming seems to occur only for very small hopper openings, and arches are always unstable.

[1]the Petroleum Research Fund (47970-AC9)

12:51PM Z13.00009 Water Retention of Mixed Hydrogel Particles and Sandy Soil , YULI WEI, DOUGLAS DURIAN, University of Pennsylvania — We study the water-holding capacity of mixed hydrogel particles and a model sandy soil. To probe static behavior, we develop a custom pressure plate method that measures the expelled water per unit pressure increment per unit cross-sectional area; results are analyzed in terms of the water-accessible pore areas in the granular packing. To probe dynamic behavior, we build a raindrop impingement set-up that measures the retained water inside a dry granular packing during steady rain at a fixed rate. The percentage saturation of the granular packing is deduced. In both studies, we first determine the influence of the packing height and then of the gel concentration and size. Results from pressure plate method show that the swollen hydrogel particles partially clog the pores in the sandy soil, so that less water could be expelled for a given pressure increment. The total water-accessible area determined from the expelled water curve decreases exponentially as the gel concentration increases. Large hydrogel particles are less efficient in clogging the pores when no extra confinement is applied on the packing. Results from the raindrop impingement measurements also show that the water-holding capacity of sandy soil is improved by addition of hydrogel particles.

1:03PM Z13.00010 Granular "electrophoresis": in situ measurement of charge and size of freely-falling grains , SCOTT WAITUKAITIS, The University of Chicago, GUSTAVO CASTILLO, Universidad de Chile, SEBASTIAN GONZALEZ, University of Twente, HEINRICH JAEGER, The University of Chicago — We present measurements of tribocharged, chemically identical grains falling from a hopper. Tribocharging is the transfer of electrical charge between contacting surfaces. Granular interactions are governed by contacts, and not-surprisingly tribocharging can have important effects on bulk granular behavior. What is surprising is that this occurs even in grains of the same material. Typically same chemistry tribocharging (SCT) correlates with the particle size distribution: larger particles charge positively and smaller particles negatively. However, the detailed mechanism of SCT remains elusive. We have developed an experimental technique to make *in situ* measurements of the particle size and charge on small ($\sim$100-500 μm) grains. With high speed videography of freely-falling grains we resolve particle sizes down to a few microns, charges as small as a few thousand electrons, and forces as small as a few picoNewtons. Our results confirm the qualitative charge segregation observed in previous SCT experiments and provide quantitative measurement for theoretical comparison.

1:15PM Z13.00011 Strain-stiffening in random packings of granular chains , HEINRICH JAEGER, ALICE NASTO, DYLAN MURPHY, ERIC BROWN, University of Chicago — We report on triaxial compression experiments performed to characterize the mechanical response of random packings of granular particles. For a wide variety of particle shapes, the packings yield when the shear stress exceeds a value on the order of the confining pressure. In contrast, granular chains consisting of flexibly connected beads exhibit strain stiffening (i.e., the effective modulus increases with strain), sustain stresses far beyond the confining pressure, and do not yield until the chains break. The critical chain length required for significant strain-stiffening to occur corresponds to the minimum circumference of closed loops the chains are able to form during the formation of the packings. This strain-stiffening behavior is similar to that found in polymer materials, and chain packings therefore may serve as a model system to quantify the contribution of pure entanglement effects to the strength of polymer materials in the absence of Brownian motion.

1:27PM Z13.00012 Anisotropic diffusion of vibrated semi-flexible granular rods , VIKRANT YADAV, ARSHAD KUDROLLI, Clark University — We discuss the diffusive dynamics of semi-flexible granular rods as a function of their concentration in a vertically vibrated container. These rods are composed of short beaded chains and are tracked with a camera, and their trajectories used to analyze the rotational and translational displacement as a function of area fraction ϕ. We observe that the diffusion in the parallel and perpendicular direction in the body frame of reference deviate from those calculated for thermally excited elastic polymer rods. In particular we find that the diffusion perpendicular to the major axis in dilute regime is observed to be greater than that in the parallel direction due to rotation about the major axis of the rod. The motion is observed to become sub-linear above $\phi = 0.48$ and 0.54 in the perpendicular and parallel directions, respectively, both lower than for spherical particles. Rotational diffusion is also investigated and found to deviate systematically from exponential decays with increase in ϕ.

1:39PM Z13.00013 Vibrofluidized melting of geometrically cohesive granular media , NICK GRAVISH, GEOFFREY RUSSELL, Georgia Tech, SCOTT V. FRANKLIN, Rochester Institute of Technology, DAVID HU, DANIEL I. GOLDMAN, Georgia Tech — Dry granular media composed of particles of special shapes (e.g. long rods or c-shaped particles) can display cohesive effects through particle geometry alone. We study the solid to gas transition in piles of c-shaped particles under vertical vibration as we vary acceleration and frequency. A cylindrical solid of particles is formed with wall angles near 90° and is placed on a solid surface. For fixed frequency as acceleration increases, the pile undergoes two transitions. The first is from the solid-like state to a liquid-like state in which the wall angles relax but the mobile particles remain spatially localized. The second is from the liquid-like state to the gaseous state in which particles become separated (not entangled). Using video and accelerometer measurements, we record the temporal evolution of the spatial density and pile-plate collisional impulse. A critical energy scale, set by the particle geometry and gravitational potential energy, governs the liquid-gas transition.

1:51PM Z13.00014 Switchable capillary bridges in sphere packings , CHRISTOPH GÖGELEIN, MARTIN BRINKMANN, MATTHIAS SCHRÖTER, STEPHAN HERMINGHAUS, Max-Planck-Institute for Dynamics and Self-Organization — If one adds a small amount of water to a heap of sand, it becomes paste-like since the grains get interconnected by capillary bridges. Due to this effect, we can easily sculpture wet sand (e.g., building a sand castle), whereas a heap of dry grains ripples away and cannot sustain any shape. In the present work, we use a non-Brownian suspension of glass spheres immersed in a binary liquid mixture. The suspending water-lutidine mixture exhibits a well studied lower critical point slightly above ambient temperature. Hence, the mixture starts to phase separate upon heating. Since the water-rich phase wets the hydrophilic glass spheres, capillary bridges are formed between adjacent particles. If the system is cooled below the demixing temperature, the bridges disappear within a few seconds by intermolecular diffusion. Thus, this systems offers the opportunity to switch the capillary bridges on and off by altering the temperature. In this presentation, we will show the temperature-induced formation of capillary bridges using confocal and bright light microscopy [1]. Furthermore, we will discuss the effect of capillary bridges on random sphere packings using a fluidized bed setup.

[1] C. Gögelein, M. Brinkmann, M. Schröter, and S. Herminghaus, Langmuir 26 (2010) 22, 17184.

2:03PM Z13.00015 Stable Solitary Waves in Granular Alignments[1] , YOICHI TAKATO, SURAJIT SEN, SUNY Buffalo — We study the propagation of an impulse in a loaded chain of elastic spheres where the spheres are held between fixed walls. We show that for a certain critical loading, propagating impulses develop into solitary waves and these solitary waves are not measurably affected by wall collisions, the latter being typically the case with granular solitary waves. The properties of these special solitary waves and of possible connections between this problem and the Fermi-Pasta-Ulam problem will be addressed.

[1]Supported by Army Research Office

Friday, March 25, 2011 11:15AM - 2:15PM –

Session Z14 GSNP: Focus Session: Statistical Mechanics of Complex Networks III D227

11:15AM Z14.00001 Frequency of Relevant Nodes with Different Function Classes in Critical Boolean Networks[1] , SHABNAM HOSSEIN, MATTHEW REICHL, KEVIN E. BASSLER, University of Houston — Boolean networks have two phases of dynamical behavior, fixed and chaotic, depending on the update functions of the nodes. Boolean functions can be categorized by their symmetry properties, which are related to their canalization properties. Canalization is a type of network robustness, which was first introduced to explain the stability of phenotype expression of biological systems. For networks with 3 inputs per node, the 256 possible Boolean functions can be divided into 14 classes that correspond to the group orbits of rotation plus parity. For critical networks at the boundary of the fixed and chaotic phases, we analytically derive the frequency of the different types of Boolean functions among the relevant nodes that control the dynamics. By setting up a set of differential equations that determines the relevant nodes through a pruning process, we can find the average number of nodes in each of the classes. Then, considering the effects of fluctuations, the probability distribution of the number of relevant nodes is accurately derived. We find that in critical networks the frequency of relevant nodes is inversely correlated with canalization.

[1]This work is supported by NSF Grant No. DMR-0908286.

11:27AM Z14.00002 Two-Component Diffusion[1] , ANNA STEPHENSON, JAYANTA RUDRA, Oklahoma School of Science and Mathematics — When two diffusing components propagate through the same material, the space that is occupied by one component may not be occupied by the other. This interaction, which is purely geometrical and non-chemical in nature, plays an important role in the dynamics of two-component flow. It redefines the diffusing space for each of them and each component sees its surrounding space being constrained by the other. We use a novel approach to describe the diffusion of two components through a discrete lattice of a narrow channel. Specially, we look at the influence of a fast component on a slow one and vice versa. We express the time evolution of the joint probability distribution of two diffusing components in terms of a modified Master equation such that both of these may not occupy the same lattice site at the same time. From this restricted time evolution of the joint probability distribution we then calculate relative flow rate of the component and infer whether such a channel could be used as a molecular sieve to separate a slow component from a fast one.

[1]Supported by OSSM Foundation

11:39AM Z14.00003 Backbones and borders from shortest-path trees , DANIEL GRADY, CHRISTIAN THIEMANN, DIRK BROCKMANN, Northwestern University — One of the most important tasks in complex network research is to distinguish between vertices and edges that are topologically essential and those that are not. To this end, a variety of vertex and edge centrality measures have been introduced, ranging from measuring local properties (degree, strength) to quantities that depend on the global structure of the graph (betweenness). Here we introduce a novel technique based on the family of shortest-path trees, which is applicable to strongly heterogeneous networks. This approach can identify significant edges in the network, distinct from conventional edge betweenness, and these edges make up a network backbone relevant to dynamical processes that evolve on such networks. We will show that important network structures can be extracted by investigating the similarity and differences of shortest-path trees and show that tree dissimilarity in combination with hierarchical clustering can identify communities in heterogeneous networks more successfully than ordinary reciprocal-weight distance measures. We demonstrate the success of this technique on complex multi-scale mobility networks.

11:51AM Z14.00004 Interactive Network Exploration using Shortest-Path-Tree Tomography , CHRISTIAN THIEMANN, DIRK BROCKMANN, Northwestern University — The shortest-path tree of a node contains information on the whole network as observed from a specific node, thus combining local and global information in a two- dimensionally embeddable sub-network. We developed new visualization software that reduces a complex network to its nodes' shortest-path trees and allows for interactive exploration of this network in a structured way. In this talk I will present various example networks and also briefly talk about off-spring projects that have been sparked by looking at networks in this way, including a simplified view on disease spreading on networks.

12:03PM Z14.00005 Searching for the extreme values of the mutual information between two interacting subsystems , ILYA GRIGORENKO, VINCENT CRESPI, Penn State University — We have considered two interacting subsystems represented by classical spins with a long-range interaction immersed in a thermal reservoir. We searched for maxima and minima of the mutual information between the subsystems by tuning the interaction parameters within only one subsystem: the parameters of the second subsystem - which can be thought of as an environment for the first one - and the interaction parameters between the first subsystem and the environment remain unchanged. We have identified the conditions leading to maximisation and minimisation of the mutual information between the subsystems, and their relation to a degeneracy of the energy spectrum that is spontaneously engineered by the optimisation procedure. We interpret the spatially inhomogeneous structure of the optimised subsystem in terms of information heterogeneity.

12:15PM Z14.00006 Synchronization Dynamics of Coupled Anharmonic Plasma Oscillators , JOHN LAOYE, Department of Physics, Olabisi Onabanjo University, PMB 2002, Ago-Iwoye, Nigeria, UCHECHUKWU VINCENT, Department of Physics, Lancaster University, Lancaster LA1 4YB, United Kingdom, TAIWO ROY-LAYINDE, Department of Physics, University of Ibadan, Ibadan Nigeria — The synchronization of two identical mutually driven coupled plasma oscillators modeled by anharmonic oscillators was investigated. Each plasma oscillator was described by a nonlinear differential equation of the form: $\ddot{x} + \epsilon(1 + x^2)\dot{x} + x + \kappa x^2 + \delta x^3 = F \cdot \cos(\omega t)$. The model employed the spring-type coupling. Numerical simulations, including Poincaré sections, time series analysis, and bifurcation diagram were performed using the fourth-order Runge-Kutta scheme. The numerical value of the threshold coupling K_{th} was determined to be approximately 0.15.

12:27PM Z14.00007 Visual analytics for discovering node groups in complex networks[1] , TAKASHI NISHIKAWA, Clarkson University — Given the abundance of relational data from a variety of sources, it is becoming increasingly more important to be able to discover hidden structures in the topology of real-world complex networks. In this talk, I will extend the usual definition of groups as densely connected sets of nodes and show that many real networks have groups distinguished by a diverse combinations of node properties, but not by the density of links alone. To overcome the virtually unlimited ways to potentially distinguish groups, we have developed an **exploratory** analysis tool that exploit human visual ability. In this visual analytical approach, the user input from **visual interaction** is integrated into the analysis to discover unknown group structures, rather than simply detecting a known type of structure. I will also address the problem of determining an appropriate number of groups, when it is not known *a priori*. I will demonstrate that our method can effectively find and characterize a variety of group structures in model and real-world networks, including community and k-partite structures defined by link density, as well as groups distinguished by combinations of other node properties.

[1]Funded by FODAVA NSF-DMS-0808860

1:03PM Z14.00008 A Network Approach to Rare Disease Modeling , SUSAN GHIASSIAN, SABRINA RABELLO, AMITABH SHARMA, CCNR Northeastern University, OLAF WIEST, University of Notre Dame, ALBERT-LASZLO BARABASI, CCNR Northeastern University — Network approaches have been widely used to better understand different areas of natural and social sciences. Network Science had a particularly great impact on the study of biological systems. In this project, using biological networks, candidate drugs as a potential treatment of rare diseases were identified. Developing new drugs for more than 2000 rare diseases (as defined by ORPHANET) is too expensive and beyond expectation. Disease proteins do not function in isolation but in cooperation with other interacting proteins. Research on FDA approved drugs have shown that most of the drugs do not target the disease protein but a protein which is 2 or 3 steps away from the disease protein in the Protein-Protein Interaction (PPI) network. We identified the already known drug targets in the disease gene's PPI subnetwork (up to the 3rd neighborhood) and among them those in the same sub cellular compartment and higher coexpression coefficient with the disease gene are expected to be stronger candidates. Out of 2177 rare diseases, 1092 were found not to have any drug target. Using the above method, we have found the strongest candidates among the rest in order to further experimental validations.

1:15PM Z14.00009 Flavor network and the principles of food pairing , YONG-YEOL AHN, Northeastern University, SEBASTIAN AHNERT, Cambridge University, JAMES BAGROW, ALBERT-LASZLO BARABASI, Northeastern University — We construct and investigate a flavor network capturing the chemical similarity between the culinary ingredients. We found that Western cuisines have a statistically significant tendency to use ingredient pairs that share many flavor compounds, in line with the food pairing hypothesis used by some chefs and molecular gastronmists. By contrast, East Asian cuisine tend to avoid compound sharing ingredients. We identify key ingredients in each cuisine that help us to explore the differences and similarities between regional cuisines.

1:27PM Z14.00010 Relationship between structural and functional networks in complex systems with delay , TONI PEREZ, Lehigh University, VICTOR EGUILUZ, IFISC, JAVIER BORGE-HOLTHOEFER, ALEX ARENAS, Universitat Rovira i Virgili — Functional networks of complex systems are usually obtained from the analysis of the temporal activity of their components, and are often used to infer their unknown underlying connectivity. Here we investigate on this challenge from a fundamental physical perspective, analyzing the functional network resulting from the simplest dynamical system with delay presenting a synchronous dynamics on a given topology. We have found the conditions for the emergence of locked dynamical states and the equations relating topology and function in a system of diffusively delay-coupled elements in complex networks. We solve exactly the resulting equations in motifs (directed structures of three nodes), and in directed networks. The mean-field solution for directed uncorrelated networks shows that the clusterization of the activity is dominated by the in-degree of the nodes, and that the locking frequency decreases with increasing average degree. We find that the exponent of a power law degree distribution of the structural topology, γ, is related to the exponent of the associated functional network as $\alpha = (2 - \gamma)^{-1}$, for $\gamma < 2$.

1:39PM Z14.00011 Why hubs may not be the most efficient spreaders , LAZAROS GALLOS, City College of New York, MAKSIM KITSAK, CAIDA, University of California-San Diego, SHLOMO HAVLIN, Bar-Ilan University, FREDRIK LILJEROS, Stockholm University, LEV MUCHNIK, New York University, H.E. STANLEY, Boston University, HERNAN MAKSE, City College of New York — The origin of a spreading process in a complex network can drastically influence the extent of the area that spreading can reach. In principle, the network hubs should be the most efficient spreaders. Here, we find that, in contrast to common belief, there are plausible circumstances where the best spreaders do not correspond to the best connected nodes or to the most central nodes (high betweenness centrality). Using the SIR model we find that: *(i)* The most efficient spreaders are those located within the core of the network as identified by the k-shell decomposition analysis. *(ii)* When multiple spreaders are considered simultaneously, the distance between them becomes the crucial parameter that determines the extent of the spreading. Similarly, we find that, in the SIS model, infections persist in the high k-shells of the network. Our analysis provides a plausible route for an optimal design of efficient dissemination strategies.

1:51PM Z14.00012 Finite size scaling theory for discontinuous percolation transitions , B. KAHNG, Y.S. CHO, Seoul National University, S.W. KIM, J.D. NOH, University of Seoul, D. KIM, KIAS — Finite-size scaling (FSS) theory has been useful for characterizing phase transitions. When the phase transition is continuous, the critical behavior of a system in the thermodynamic limit can be extracted from the size-dependent behaviors of thermodynamic quantities. However, FSS approach for discontinuous transitions arising in disordered systems has not been studied yet. Here, we develop a FSS theory for the discontinuous PT in the modified Erdös-Rényi model under the Achlioptas process. A scaling function is derived based on the observed fact that the derivative of the curve of the order parameter at the critical point t_c diverges with system size in a power-law manner, which is different from that for continuous percolation transitions. Numerical simulation data for different system sizes are well collapsed onto a scaling function.

2:03PM Z14.00013 Monte Carlo Simulations of Metastable Decay in the Ising Model on the Hyperbolic Plane[1] , HOWARD L. RICHARDS, Physics, Marshall University, MALLORY A. PRICE, Math, Marshall University, JULIE E. LANG, Physics, Morehead State University — Consider a regular network of Ising spins with short-ranged, ferromagnetic interactions and a weak, negative magnetic field. The system evolves under single-spin-flip Metropolis dynamics from an initial state of all spins "up" ($s_i = +1, \forall i$). For Euclidean networks in less than 6 dimensions, decay from the "metastable" state occurs in a finite time (measured in Monte Carlo steps per spin) through the nucleation and growth of one or more finite critical droplets. For networks on the hyperbolic plane, however, we show that the size of a critical droplet diverges at a nonzero magnetic field – the spinodal field. We then use Monte Carlo simulations on the $\{5, 4\}$ grid to demonstrate the divergence of the lifetime of the metastable state at nonzero spinodal fields.

[1]Supported by Marshall University's REU in Scientific Computing, NSF grant OCI-1005117. For information, see www.marshall.edu/reu/.

Friday, March 25, 2011 11:15AM - 1:27PM –
Session Z22 DCMP: Properties of Semiconducting Nanosystems D163

11:15AM Z22.00001 ABSTRACT WITHDRAWN –

11:27AM Z22.00002 Conductivity of Thin Film Structures Fabricated by E-Beam Lithography from Gold Nanoparticle Resists[1] , STEFAN DICKERT, MYOUNG-HWAN PARK, COLIN JERMAIN, VINCENT M. ROTELLO, MARK T. TUOMINEN, University of Massachusetts Amherst — Drop- and spin-coated solutions of ligand coated nanoparticles act as a novel "direct write" e-beam resist, which can be prepared with metallic, magnetic and semiconducting nanoparticles (Y.Ofir. et. al, Adv. Mater. 20, 2561-2566 (2008)). We prepared thin films from gold nanoparticles in which we varied the ligand length, ligand type and the film thickness. Small angle X-Ray scattering experiments as well as SEM imaging of the samples were performed to determine structural properties of the nanoparticle films at various stages of the fabrication process, after drop coating, ebeam exposure and annealing. We further performed resistance measurements in the 2-350K temperature range and report different conductivity mechanisms based on the ligand type and film thickness, ranging from insulating to Mott hopping conduction to metallic. We observed different results for Thioalkylated trimethyl ammonium (TMA) and thioalkyl tetra (ethylene glycol)ated trimethyl ammonium (TTMA) ligands.

[1]This research is supported by NSF grant CMI-0531171.

11:39AM Z22.00003 Terahertz Ionization of Highly Charged InGaAs Quantum Posts , CHRISTOPHER MORRIS, DOMINIK STEHR, TUAN-ANH TRUONG, HYOCHUL KIM, PIERRE PETROFF, MARK SHERWIN, University of California Santa Barbara, CRAIG PRYOR, University of Iowa — Quantum posts (QPs) are quantum dot based nanostructures grown by MBE. They form short $In_{.4}Ga_{.6}As$ cylinders embedded in an $In_{.1}Ga_{.9}As$ quantum well (QW). Terahertz absorption measurements are performed on 30 nm high QPs with ∼6 electrons per post and a charge density of $\sim 2.4 \times 10^{11}/cm^2$ in the surrounding well. Comparison of spectra from QP and reference QW samples shows an absorption feature due to the QPs absent in the QW sample. Temperature dependent measurements show this absorption is due to electrons in the QPs. 8 band k.p calculations of post and well energies are performed as a function of the number of electrons in the posts, and the absorption is determined to be due to an "ionizing" transition from the posts to the well. The highest filled QP state absorbs a terahertz photon, transitioning to a weakly bound unfilled post state ∼20 meV higher. From there, the electron quickly scatters into the two dimensional electron gas in the quantum well matrix. Coulomb repulsion from QP electrons locally depopulates the quantum well states, leaving open states for the QP electrons. QPs represent a promising structure for investigation of Coulomb blockade physics and ionizing transitions in artificial atom systems.

11:51AM Z22.00004 The dipole moments of ZnO nanorods , SEFA DAG, SHUZHI WANG, LIN-WANG WANG, Lawrence Berkeley National Laboratory — A self-consistent linear scaling three dimensional fragment (LS3DF) method is used to study the dielectric properties of large ZnO nanorods. Our ab initio calculations show that the ZnO nanorod with unpassivated (10-10) side surface has a large dipole moment which is caused by both surface and interior bulk dipoles. An systematic analysis is carried out, and we found that the biggest contribution to the total dipole moment is from the (10-10) surface. Dielectric screening model is used to illustrate how the dipole moment changes with nanostructure size and geometry. We also show the effect of the dipole moment on the interior electronic structure of the nanorod.

12:03PM Z22.00005 Natural interface states in coherent and isovalent III-V heterostructures[1] , VOICU POPESCU[2], National Renewable Energy Laboratory, Golden, CO, ALEX ZUNGER, National Renewable Energy Laboratory — Interface states occur in semiconductor heterojunctions whenever a significant perturbation is present, caused by interface defects, lattice mismatch, discontinuities in the effective mass or sharp variations in the potential across the interface. We discuss the natural interface states appearing in perfectly coherent and isovalent III-V heterojunctions when a Γ-well and an X-anti-well coexist in the conduction band. We use empirical pseudopotential calculation to illustrate this type of states for a few III-V heterostructures. For InP/GaP the interface localised states lie energetically in the band-gap and possess, because of their mixed $\Gamma - X$ character, a strong optical signature. This allows us to provide a different interpretation of the photoemission data existent in the literature for InP/GaP quantum wells and dots. We further discuss the presence of the interface localised states in other III-V heterojunctions, investigating the conditions under which they might be experimentally observed.

[1]Funded by DOE, EFRC for Inverse Design, NREL Subcontract XGC-0-40445-01
[2]Present address: Colorado School of Mines, Golden, CO

12:15PM Z22.00006 Electronic Phase Diagram of Single-Element Silicon "Strain" Superlattices[1] , ZHENG LIU, University of Utah, WENHUI DUAN, JIAN WU, Tsinghua University, MAX LAGALLY, University of Wisconsin-Madison, FENG LIU, University of Utah — The evidence that the band gap of Si changes significantly with strain suggests that by alternating regions of strained and unstrained Si one creates a single-element electronic heterojunction superlattice (SL), with the carrier confinement defined by strain rather than by the chemical differences in conventional compositional SLs. Using first-principles calculations, we map out the electronic phase diagram of a one- dimensional pure-silicon SL. It exhibits a high level of phase tunability, e.g., tuning from type I to type II. Our theory rationalizes a recent observation of a strain SL in a Si nanowire and provides general guidance for the fabrication of single-element strain SLs.

[1]This work is supported by DOE-BES (Grants No. DEFG02-03E46027 and No. 46028). We thank DOE-NERSC for providing the computing resources. M.G. L. acknowledges facilities support from UW NSF/MRSEC.

12:27PM Z22.00007 Quantum Boundary Effect in Nanomaterials: Undo the Quantum Size Effect by Surface Passivation of Silicon Nanofilms , YIYANG SUN, XIN LIU, SHENGBAI ZHANG, Rensselaer Polytechnic Institute — It is well known that when the size of a semiconductor is reduced, its band gap will increase due to the increased kinetic energy of the electrons and holes. However, first-principles calculations reveal that there should also be a quantum boundary effect (QBE), which can drastically change the band gap to the extent that the quantum size effect (QSE) is completely erased. It is found that, for Si(001) nanofilms, surface passivations could show such a strong QBE. While the films are passivated by hydrogen, they show a clear QSE with significant increase in band gap. When some of the hydrogen atoms are replaced by =NH ligands, however, the band gap recovers to that of bulk silicon even for film size as small as two nanometers. The concept of zero confinement state for semiconductors will be introduced. It elucidates why it is possible to remove the seemingly universal QSE. The finding here could be highly desirable for certain applications of nanostructured semiconductors where gap increasing due to QSE is detrimental.

12:39PM Z22.00008 Excitation energy dependence of the exciton inner ring , YULIYA KUZNETSOVA, JASON LEONARD, LEONID BUTOV, University of California at San Diego, JOE WILKES, ALEX IVANOV, Cardiff University, ARTHUR GOSSARD, University of California at Santa Barbara — We report on the excitation energy dependence of the inner ring in the emission pattern of indirect excitons. The contrast of the inner ring is found to increase with excitation energy until it reaches the direct exciton plus LO phonon energy and saturate at higher excitation energies. The data show that excitation by low-energy laser light tuned to the direct exciton resonance can effectively suppress the laser-induced heating of the exciton gas. The observed dependence is explained in terms of exciton transport and cooling.

12:51PM Z22.00009 Dynamic coherent exciton condensates in a semiconductor planar microcavity[1] , CHIH-WEI LAI, KYAW ZIN LATT, Michigan State University, YI-SHAN LI, SHENG-DI LIN, National Chiao Tung University — We observed a coherent exciton state with a long decay time $\sim$1000 ps in a semiconductor planar microcavity structure. The lifetime of cavity polariton condensates previously reported has been limited to $\sim$10 ps. The sample consists of InGaAs quantum wells positioned near anti-nodes of the photon field in a GaAs λ-cavity sandwiched by GaAs/AlAs-based Bragg mirrors. Under a pulsed excitation above the stop-band of the Bragg mirrors (excess energy $>$150 meV), spatially coherent exciton emissions were observed to last for $\sim$1 ns. Conventional dynamic exciton-polariton condensates with a $\sim$10 ps lifetime were observed under a near-resonant (excess energy $\sim$ 6 meV) ps pulsed excitation. Dynamics of spatial coherence, energy relaxation, and spin polarization were characterized by time-resolved spectroscopies, including double-slit and polarimetry experiments. The fluctuation of excitonic emissions was characterized by a photon-correlation measurement. The existence of such a long-lived coherent exciton state is attributed to formation of dark excitons under an excitation with significant excessive energy.

[1]Supported by NSF CAREER Award DMR-0955944.

1:03PM Z22.00010 Amplitude oscillations in a non-equilibrium polariton condensate , RICHARD BRIERLEY, PETER LITTLEWOOD, University of Cambridge, PAUL EASTHAM, Trinity College Dublin — Like cold atomic gases, semiconductor nanostructures provide new opportunities for exploring non-equilibrium quantum dynamics. In semiconductor microcavities the strong coupling between trapped photons and excitons produces new quasiparticles, polaritons, which can undergo Bose-Einstein condensation. Quantum quenches can be realised by rapidly creating cold exciton populations with a laser [Eastham and Phillips, PRB 79 165303 (2009)]. The mean field theory of non-equilibrium polariton condensates predicts oscillations in the condensate amplitude due to the excitation of a Higgs mode. These oscillations are the analogs of those predicted in quenched cold atomic gases and may occur in the polariton system after performing a quench or by direct excitation of the amplitude mode. We have studied the stability of these oscillations beyond mean field theory. We show that homogeneous amplitude oscillations are unstable to decay into lower energy phase modes at finite wavevectors, suggesting the onset of chaotic behaviour. The resulting hierarchy of decay processes can be understood by analogy to optical parametric oscillators in microcavities. Polariton systems thus provide an interesting opportunity to study the dynamics of Higgs-like modes in a solid state system.

1:15PM Z22.00011 Coherence dynamics of a long-lived excitonic condensate in an optical microcavity[1] , KYAW ZIN LATT, Michigan State University, YI-SHAN LI, SHENG-DI LIN, National Chiao Tung University, CHIH-WEI LAI, Michigan State University — We report dynamics of long-range spatial coherence of an excitonic condensate with a $\sim$1000 ps life-time in a planar Fabry-Perot microcavity. The sample consists of three sets of three InGaAs(8nm)/GaAs (14nm) quantum wells positioned near anti-nodes of the photon field in a GaAs λ-cavity sandwiched by two GaAs/AlAs-based Bragg mirrors. Conventional dynamic exciton-polariton condensates with a $\sim$10 ps lifetime were observed under a near-resonant (excess energy $\sim$ 6 meV) ps pulsed excitation at a 50 degree incident angle. Under an excitation above the stop-band of the Bragg mirrors (excess energy $\sim$170 meV), an excitonic state with 100-μeV luminescence linewidth was observed to last for $\sim$1 ns. Coherence dynamics were characterized by time-resolved double-slit experiment in a confocal geometry with a ps streak camera system as a function of excitation intensity (fluence) and temperature. The visibility of interference fringes reached above 0.3 within 40 ps and remained above 0.1 up to $\sim$1ns for a double-slit-distance of 12 μm.

[1]Supported by NSF CAREER Award DMR-0955944.

Friday, March 25, 2011 11:15AM - 1:27PM –
Session Z23 DCMP: Superconductivity: Thermodynamics, etc. D165

11:15AM Z23.00001 Evolution of ground state and upper critical field in $R_{1-x}Gd_xNi_2B_2C$ (R = Lu, Y): Coexistence of superconductivity and spin-glass state[1] , S.L. BUD'KO, V.G. KOGAN, H. HODOVANETS, S. RAN, S.A. MOSER, M.J. LAMPE, P.C. CANFIELD, Ames Laboratory and Dept. of Physics and Astronomy, Iowa State University — We report effects of local magnetic moment, Gd^{3+}, doping ($x \leq 0.3$) on superconducting and magnetic properties of the closely related $Lu_{1-x}Gd_xNi_2B_2C$ and $Y_{1-x}Gd_xNi_2B_2C$ series. The superconducting transition temperature decreases and the heat capacity jump associated with it drops rapidly with Gd-doping; qualitative changes with doping are also observed in the temperature-dependent upper critical field behavior, and a region of coexistence of superconductivity and spin-glass state is delineated on the $x - T$ phase diagram. The evolution of superconducting properties can be understood within the Abrikosov-Gor'kov theory of magnetic impurities in superconductors taking into account the paramagnetic effect on upper critical field and the details of the $x - T$ phase diagrams.

[1]Supported by the US DOE - BES under Contract No. DE-AC02-07CH11358.

11:27AM Z23.00002 Micro-Calorimeter for Heat Capacity Studies of Sub-Microgram Superconducting Crystals[1] , CARLOS CHAPARRO, U. WELP, L. FANG, W.K. KWOK, Argonne National Laboratory, Argonne, IL 60439, USA, M. ESKILDSEN, Department of Physics, University of Notre Dame, Notre Dame, IN 46556, USA — A steady-state ac-temperature micro-calorimeter for heat capacity measurement of sub-microgram superconducting samples is presented. It utilizes thermocouple thermometers nano-patterned onto 150 nm thick Si_3N_4 membranes. Theoretical models, mathematical relations describing the operation of the calorimeter and calibration procedures are discussed. The system achieves a resolution of 10^{-4}; and allows for measurements from 5 K to room temperature. The calorimeter can be continuously rotated in a split-coil magnet generating up to 8 T. To demonstrate the performance of our device we present measurements of the specific heat of single crystals of $SmFeAsO_{0.85}F_{0.15}$ (120 μm wide and 10 μm thick, crystal w1) and of $BaFe_2(As_{1-x}P_x)_2$ (150 μm wide and 30 μm thick).

[1]This work was supported by DOE-BES under Contact No. DE-AC02-06CH11357.

11:39AM Z23.00003 Search for quantum critical behavior in the specific heat of HTS cuprates[1] , JEFFERY TALLON, MacDiarmid Institute, Industrial Research Ltd, FELIX BARBER, Industrial Research Ltd, JOHN COOPER, JOHN LORAM, Cavendish Lab., Cambridge University — Much evidence has been accumulated suggesting the presence of a quantum critical point in the lightly overdoped regime for high-T_c superconductors, around p=0.19 holes per Cu. It is however not decisive. In the neighborhood of a quantum critical point the normal-state electronic specific heat should contain a $T\ln(T)$ term. While this would be concealed by the onset of superconductivity it is in principle recoverable using the entropy balance that exists in a second-order phase transition. This paper reviews the data for $Y_{0.8}Ca_{0.2}Ba_2Cu_3O_{7-d}$ and $Bi_2Sr_2CaCu_2O_{8+d}$ and places limits on the magnitude and doping evolution of a $T\ln(T)$ term in the specific heat across the phase diagram.

[1]Work supported by the Marsden Fund of New Zealand.

11:51AM Z23.00004 Thermodynamic effects in superconducting hybrid devices , LAETITIA PASCAL, SUKUMAR RAJAURIA, HUNG NGUYEN, BERNARD PANNETIER, Neel Institute, CNRS, Grenoble, France, FRANK HEKKING, LPMMC, Grenoble, France, HERVE COURTOIS, Neel Institute, CNRS, Grenoble, France — Investigating thermal transport in hybrid superconducting nanostructures can yield a better understanding of such devices and give access to new and useful phenomena. Sub-gap biased superconducting-insulator-normal metal (SIN) junctions exhibit electron cooling, which is useful for achieving electronic temperatures below the cryostat bath temperature. We have designed an experiment to allow independent monitoring of the electron and phonon populations temperatures. An electronic cooler was studied under out-of-equilibrium conditions, in both cooling and heating regimes. The results are interpreted using a thermal model, which takes into account the electron, phonon and photon heat transfer. The Kapitza and electron-phonon couplings, along with a generalized circuit theory approach for the photon heat transfer, will be discussed.

12:03PM Z23.00005 Caloric determination of the anisotropic phase diagram of $BaFe_2(As_{1-x}P_x)_2$ crystals[1] , WAI-KWONG KWOK, ULRICH WELP, CARLOS CHAPARRO, LEI FANG, ALEXEI KOSHELEV, Argonne National Laboratory — We report specific heat measurements on a series of $BaFe_2(As_{1-x}P_x)_2$ single crystals with phosphorous contents ranging from optimal doping (x$\sim$0.3, T_c = 29.5 K) to highly overdoped (x$\sim$0.6, T_c = 11K). We find a sharp superconducting transition at T_c for all doping levels, a suppression of the ΔC-step at $T_c$with increasing doping and enhanced magnetic field dependence at higher doping. The phase diagrams determined from specific heat data show a decrease of dH_{c2}/dT with increasing doping and a nearly constant superconducting anisotropy of $\Gamma \sim$2.5. Our results will be compared with the proposed "universal" scaling of $\Delta C_p/T_c$ and dH_{c2}/dT due to quantum criticality and non Fermi liquid behavior [1] and due to strong pair-breaking and non-magnetic interband scattering [2], respectively.

[1] J. Zaanen, Phys. Rev. B 80, 212502 (2009)
[2] V. G. Kogan, Phys. Rev. B 80, 214532 (2009)

[1]This work was supported by DOE-BES under Contract No. DE-AC02-06CH11357.

12:15PM Z23.00006 Growth of thin superconducting films and heterostructures by atomic layer deposition , JEFFREY KLUG, THOMAS PROSLIER, NICHOLAS BECKER, JEFFREY ELAM, JAMES NOREM, Argonne National Laboratory, JOHN ZASADZINSKI, Illinois Institute of Technology, MICHAEL PELLIN, Argonne National Laboratory — We report the use of atomic layer deposition (ALD) to synthesize thin superconducting films and superconductor-insulator (S-I) heterostructures. ALD uses sequential self-saturating surface chemical reactions to produce uniform coatings with atomic scale control on substrates with arbitrary shape. The ALD process therefore offers the possibility of conformally coating complex shapes with precise, layered structures with tightly constrained morphology and chemical properties. Among other applications, such coatings may enable the production of superconducting radio frequency (SRF) structures with significantly better performance and yield than those obtained from bulk niobium. Furthermore, the atomic-scale thickness control afforded by ALD enables the study of superconductivity and associated phenomena in homogeneous layers in the ultra-thin film limit. In this respect, we will present results of ALD-grown $Nb_{1-x}Ti_xN$-based films and S-I heterostructures. Our program looks both at the metallurgy and superconducting properties of these coatings, and also their performance in working SRF structures.

12:27PM Z23.00007 Laser Processing on the Surface of Niobium Superconducting Radio-Frequency Accelerator Cavities , SENTHILRAJA SINGARAVELU, Old Dominion University, MICHAEL KLOPF, GEOFFREY KRAFFT, Jefferson Laboratory, MICHAEL KELLEY, College of William and Mary — Superconducting Radio frequency (SRF) niobium cavities are at the heart of an increasing number of particle accelerators. Their performance is dominated by a several nm thick layer at the interior surface. Maximizing its smoothness is found to be critical and aggressive chemical treatments are employed to this end. We describe laser-induced surface melting as an alternative "greener" approach. Modeling guided selection of parameters for irradiation with a Q-switched Nd:YAG laser. The resulting topography was examined by SEM, AFM and Stylus Profilometry.

12:39PM Z23.00008 Charge order phase diagrams of hole-doped cuprates , ROBERT MARKIEWICZ, Northeastern University, JOSE LORENZANA, U Rome, La Sapienza, GOETZ SEIBOLD, U. Cottbus, ARUN BANSIL, Northeastern University — "Stripe"-like phases in the cuprates can be dominated by either spin or charge fluctuations. We calculate the phase diagram of charge-order phases stabilized by a lattice distortion using Gutzwiller approximation (GA) + RPA, and compare it to the magnetic phase diagrams [1]. The stripe periodicity is determined by Fermi surface [double] nesting, and hence is very similar for charge or magnetic stripes. A detailed analysis of the susceptibility reveals that the leading charge instability in Bi2201 and Bi2212 is an electronically driven phonon soft mode associated with a "Pomeranchuk wave." This instability has the pseudogap doping dependence and shares many properties with the phase seen in scanning tunneling microscopy (STM) Work supported in part by the USDOE and by a Marie Curie Grant.

[1] R.S. Markiewicz *et al.*, Phys. Rev. B**81**, 014509 (2010).

12:51PM Z23.00009 Using Disorder to Detect Locally Ordered Electron Nematics via Hysteresis , ERICA CARLSON, Purdue University, KARIN DAHMEN, University of Illinois at Urbana Champaign — The interplay between charge, orbital, and lattice degrees of freedom in correlated electron systems has resulted in many proposals for new electronic phases of matter. An electron nematic breaks the point group symmetry of the host crystal, often from C_6 or C_4 rotational symmetry to C_2. Electron nematics have been reported in several condensed matter systems including cuprate and iron arsenic based high temperature superconductors, and they have been proposed to exist in many other materials. However, the combination of reduced dimensionality and material disorder typically limits the spatial range over which electron nematic order persists, rendering its experimental detection extremely difficult. Despite the tantalizing possible connection between the phase and high temperature superconductivity, there is surprisingly little guidance in the literature about how to detect the remaining disordered electron nematic. We propose a general method for detecting disordered electron nematics in bulk condensed matter systems using nonequilibrium methods.

1:03PM Z23.00010 Superconducting-to-Normal State Switching Experiments using Graphene-based Josephson Junctions , JOSEPH LAMBERT, STEVEN CARABELLO, ROBERTO RAMOS, Department of Physics, Drexel University — We report results of ongoing superconductor-to-normal state switching experiments using graphene-based Josephson junctions. These devices consist of a single-layer graphene flake contacted by two superconducting parallel leads separated by a few hundred nanometers. Through the proximity effect, the superconducting state is induced in the graphene region below the leads and the Josephson supercurrent is mediated through the normal graphene region by multiple Andreev reflections. The Josephson effect has been firmly demonstrated in these devices, where supercurrents in the hysteretic current-voltage characteristic, Shapiro steps, the Fraunhofer-like diffraction pattern in the critical current versus external magnetic field, and the current-phase relationship have been observed. We report on work in progress, in measuring I-V characteristics, thermal activation and microwave resonant activation in graphene-based junctions, at various temperatures below 1 Kelvin. We modulate the density of charge carriers using a back-gate voltage, which tunes the critical current. This provides another knob for studying these state switching properties.

1:15PM Z23.00011 Noise spectroscopy: a sensitive probe to explore hot electron effect in highly correlated systems[1] , SUDESHNA SAMANTA, ARUP K. RAYCHAUDHURI, S N Bose National Centre for Basic Sciences, Block-JD, Sector-3, Salt Lake, Kolkata, India — Non-linear electrical conductance in ferromagnetic insulating (FMI) state of manganites can give rise to reversible colossal electro-resistance and current induced resistance change due to heating of the electrons in the system. In FMI state (<120K), the temperature of the lattices or phonon (T_{ph}) and electrons (T_e) in the sample can decouple by high input power density giving rise to heating of the electronic bath. We investigated whether white noise like Nyquist noise can be used to measure T_e (which is expected to be larger than T_{ph}) when the two baths get decoupled. The use of the Nyquist noise to measure T_e assumes that the electron bath forms a proper temperature bath in equilibrium. A dc stressing current was used to heat the electron bath while a small ac signal was used to measure the noise. With enhanced power input to the electron system, the white noise enhances and there is a large deviation from the simple estimate of Nyquist relation ($4k_BT_eR_{sample}$) indicating that the electron system is not in thermal equilibrium and is a non-ergodic system where Fluctuation Dissipation Theorem has broken down.

[1]Department of Science and Technology, Govt. of India

Friday, March 25, 2011 11:15AM - 2:15PM –
Session Z25 DCMP: Novel Superconductors II D166

11:15AM Z25.00001 Momentum-dependent multiple gaps of MgB_2 probed by electron tunneling spectroscopy on MgB_2/native oxide/Pb junctions[1] , KE CHEN, Temple University, WENQING DAI, QI LI, The Pennsylvania State University, X.X. XI, Temple University — Distinct multi-band superconductivity is a unique feature that distinguishes MgB_2 from all other phonon-mediated Bardeen-Cooper-Schrieffer (BCS) superconductors. According to a first-principles calculation employing an anisotropic Eliashberg formalism [Choi *et al.* Nature 418, 758 (2002)], there is a distribution of superconducting energy gap values on the Fermi surface of MgB_2 (two σ bands and two π bands). However, only two distinct gaps have been observed experimentally, leading to the suggestion that consideration of the fully anisotropic electron-phonon interaction may not be necessary for real MgB_2 samples. Here, we present an electron tunneling spectroscopy study on MgB_2/native oxide/Pb junctions that clearly shows the distribution of energy gaps. By deconvoluting the tunneling spectrum based on the density of state of Pb, we derive the momentum-dependent energy gaps of MgB_2, which are in good agreement with the anisotropic Eliashberg calculation. The result affirms the importance of the anisotropic electron-phonon interaction in MgB_2 as well as its important impact on device applications.

[1]The work is partially funded by ONR and by DOE.

11:27AM Z25.00002 Non-Cuprate Superconductor with Cubic Structure and T_c = 85 K , J.M. ESTRADA, E. CHAVIRA, I. ROSALES, O. NOVELO, E. FREGOSO, Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico, D.F., Mexico, E.E. MARINERO, M. NISHIOKA, Hitachi GST San Jose Research Center, 3404 Yerba Buena Rd, San Jose, CA 95135, USA, V. GARCIA-VAZQUEZ, Instituto de Fisica, Benemerita Universidad Autonoma de Puebla, Puebla, Mexico, M. SUCHOMEL, Argonne National Laboratory, 9700 Cass Ave., Argonne, IL 60439-4856, USA — We have synthesized a new superconductor material, namely: **Ba(Yb**$_{0.38}$ **In**$_{0.10}$**Sn**$_{0.42}$ **Pb**$_{0.10}$**)O**$_{2.66}$, by solid-state reaction in air and ambient pressure. The new compound is determined to have a T_c of 85 K, which is new record for a non-cuprate structure. Employing synchrotron XRD and Rietveld refinement, 5 structural phases are identified in the reaction products. The phases identified are: $BaTb_{0.5}Sb_{0.5}$ O_3 (41.3%), Yb_2BaCuO_5 (26.1%), CuO (22.6%), $Yb_2Cu_2O_5$ (4.4%) and $Ba_{1.99}Y_{1.01}$ Cu_3O_8 (5.6%). The microstructure exhibits cubic morphology (SEM) and EDX analysis is utilized to determine the stoichiometry of the new superconducting material, **Ba(Yb**$_{0.38}$ **In**$_{0.10}$**Sn**$_{0.42}$ **Pb**$_{0.10}$**)O**$_{2.66}$, which is isostructural to the cubic $BaTb_{0.5}Sb_{0.5}$ O_3 phase. Magnetic and Resistance measurements vs T indicate a superconducting transition at T_c at 85 K.

11:39AM Z25.00003 Suppression of time reversal symmetry breaking superconcutivity in $Pr(Os,Ru)_4Sb_{12}$ and $(Pr,La)Os_4Sb_{12}$[1] , LEI SHU, UCSD, W. HIGEMOTO, JAEA, Japan, Y. AOKI, TMU, Japan, A.D. HILLIER, ISIS, UK, K. OHISHI, K. ISHIDA, KU, Japan, R. KADONO, A. KODA, KEK, Japan, O.O. BERNAL, CSU, D.E. MACLAUGHLIN, UCR, Y. TUNASHIMA, Y. YONEZAWA, S. SANADA, D. KIKUCHI, H. SATO, TMU, Japan, H. SUGAWARA, UT, Japan, T.U. ITO, JAEA, Japan, M.B. MAPLE, UCSD — Zero-field muon spin relaxation (μSR) experiments have been carried out in the $Pr(Os_{1-x}Ru_x)_4Sb_{12}$ and $Pr_{1-y}La_yOs_4Sb_{12}$ alloy systems to investigate broken time-reversal symmetry (TRS) in the superconducting state, signaled by the onset of a spontaneous static local magnetic field B_s. In both alloy series B_s initially decreases linearly with solute concentration. Ru doping is considerably more efficient than La doping ,with a $\sim$50% faster initial decrease. The data suggest that broken TRS is suppressed for Ru concentration larger than 0.6, but persists for essentially all La concentrations. Our data support the theory of TRS-breaking superconductivity via crystal-field excitonic Cooper pairing of Koga, Matsumoto, and Shiba.

[1]This work was supported by the U.S. NSF 0422674, 0801407, 0604015, and 0802478, the U.S. DOE, DE-FG-02-04ER46105, and by the Grant-in-Aid for Scientific Research Priority Area "Skutterudite" No. 15072206.

11:51AM Z25.00004 Signatures of half-quantum vortices in magnetoresistance of perforated samples[1] , VICTOR VAKARYUK, VALERII VINOKUR, Argonne National Laboratory — Recent cantilever magnetometry measurements of annular micron-size samples of Sr_2RuO_4 [1] have revealed evidence for the existence of half-quantum vortices (HQVs) in this material. Here we suggest to look for HQVs at temperatures close to T_c in magnetoresistance of "punctured" (perforated) Sr_2RuO_4 samples which consist of an array of regularly spaced micron-size holes in an otherwise uniform superconducting matrix. Due to the dissipative nature of resistive measurements signatures of HQVs might be seen even if their thermodynamic stability is not expected. We analyze the dependence of magnetoresistance on the thermodynamic stability of HQVs and point out features which may help to identify them.

[1] J. Jang, D.G. Ferguson, V. Vakaryuk, R. Budakian, S.B. Chung, P.M. Goldbart, Y. Maeno (2010).

[1]Supported by the Department of Energy under the Contract No. DE- AC02-06CH11357.

12:03PM Z25.00005 Nonintegral flux penetration in superconductors with broken time-reversal symmetry via bent domain walls , DAVID FERGUSON, PAUL GOLDBART, University of Illinois at Urbana-Champaign — Sr_2RuO_4 is a candidate material for realizing a superconducting state that spontaneously breaks time-reversal symmetry [1]. In such a state, the spatial pattern of the superconductivity may be broken up into regions of differing chirality, separated by domain walls. Here, we show that, near to bends in such domain walls, nonintegral (and even nonquantized) multiples of the superconducting magnetic flux quantum would penetrate the system [2]. We discuss the implications of this "bend flux" effect for various experimental probes that are sensitive to time-reversal symmetry breaking. For the example of scanned-probe magnetic imaging, the observation of localized-nonquantized flux penetrating a z-axis surface of the sample, could be interpreted in terms of the presence of bent walls between domains of opposing chirality, and hence would be suggestive of time-reversal symmetry-breaking superconductivity. Alternatively, if observations should reveal localized but only *quantized* flux, this would suggest either (i) the absence of domain walls or (ii) their presence, but as a parallel array of straight walls.

[1] C. Kallin and A. J. Berlinsky, J. Phys. Cond. Mat.**21**, 164210 (2009).
[2] D. G. Ferguson and P. M. Goldbart, arXiv:1011.2765v1 (2010).

12:15PM Z25.00006 Scenarios for half-integer fluxoid behavior of annular rings of Sr_2RuO_4 , RAFFI BUDAKIAN, DAVID FERGUSON, PAUL M. GOLDBART, JOONHO JANG, University of Illinois at Urbana-Champaign, VICTOR VAKARYUK, Argonne National Laboratory — Recently, cantilever torque magnetometry experiments on annular rings of superconducting Sr_2RuO_4 have revealed half- height steps in the magnetization [1]. These features are suggestive of the existence, in these annular samples, of half- quantum fluxoid states (i.e., the coreless analogs of half- quantum vortices). We consider the existence and energetic stability (for various forms of triplet superconductivity) of half-quantum fluxoid states in annular samples. We also consider alternative scenarios that could give rise to magnetization steps. One particular scenario requires the presence, in the bulk of the sample, of thermodynamically stable "wall vortices" By analyzing the equilibrium state of the superconductor, as a function of the applied magnetic field, we conclude that any wall-vortex scenario consistent with the observations of Ref. [1] would require a (to date, unexplained) fine tuning of various material parameters.

[1] J. Jang, D. Ferguson, V. Vakaryuk, R. Budakian, S. Chung, P.Goldbart, and Y. Maeno, (2010 unpublished)

12:27PM Z25.00007 The Atomic-Scale Onset of Charge Density Waves in $NbSe_2$, CHOCKALINGAM S P, L. ZHAO, C. ARGUELLO, E. ROSENTHAL, C. GUTIERREZ, J. KANG, A. PASUPATHY, Columbia University, S. JIA, R. CAVA, Princeton University — Many modern complex materials exhibit spatially ordered electronic states such as charge and spin density waves, and scanning tunneling microscopy (STM) has recently been used successfully to visualize some of these phases. Unfortunately such phases often occur simultaneously in a single sample making the interpretation of experimental data difficult. In order to gain insight into the nature of spatial order in a simple material, we study the transition-metal dichalcogenide $NbSe_2$, which displays a 2D charge density wave (CDW) phase at low temperature. How does this CDW phase manifest itself in real space at the atomic scale? In order to answer this question, we have performed variable-temperature STM experiments on $NbSe_2$single crystals at various temperatures around T_c (33.5 K). We discover that static, short-range CDW order exists around crystal defects and impurities at temperatures up to $3T_c$. We will describe the temperature evolution as well as the energy dependence of the short-range CDW using spectroscopic mapping. Our experiments provide a high-resolution measurement of the changes in electronic structure caused by the formation of CDW in the dichalcogenides.

12:39PM Z25.00008 Multiband Superconductivity in $2H$-$NbSe_2$ Probed by Cryomagnetic STM Spectroscopy[1] , IGOR FRIDMAN, J.Y.T. WEI, University of Toronto and Canadian Institute for Advanced Research, C. KLOC, Nanyang Technological University, Singapore, V. LUKIC, Department of Bioengineering, University of Pennsylvania, RONGWEI HU[2], C. PETROVIC, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory — Using a novel magnetic field geometry, we study multiband pairing in single crystals of superconducting $2H$-$NbSe_2$ under finite superfluid momentum. Spectroscopy and conductance imaging were performed with a scanning tunneling microscope (STM) at 300 mK and in a field of up to 9 T, applied in the ab-plane. We observed multiple spectral features that evolve systematically with field, and a two-sloped zero-bias conductance that dips anomalously at 0.7 T. Our analysis yields distinct evidence for multiple gaps coming from the various Fermi-surface sheets, and has possible implications on the origin of the coexisting charge density wave order.

[1]Work supported by NSERC, CFI/OIT, CIFAR, U.S. DOE and Brookhaven Science Associates (No. DE-Ac02-98CH10886).
[2]Present address: Ames Laboratory and Iowa State University

12:51PM Z25.00009 Spin density in UCoGe , JONATHAN TAYLOR, STFC RAL UK, JONATHAN DUFFY, MATTHEW BUTCHERS, Warwick university UK, CHRIS STOCK, NIST, E. BAUER, Los Alomos — Below T = 0.8K, superconductivity and ferromagnetism (T_C = 3K) coexist in UCoGe. The total magnetic moment is 0.03 μ_B at low temperatures. UCoGe is considered to be a weak itinerant ferromagnet. Recent theoretical studies Predict UCoGe indicate that UCoGe is ferromagnetic, but that the small total magnetic moment arises from the near cancellation of large U $5f$ spin and orbital moments. Theory also predicts there to be a Co spin moment. However, the total moment is predicted to be considerably larger than observed experimentally. Using magnetic Compton scattering experiments together with KKR electronic structure calculations we have measured the spin density of the ferromagnetic superconductor UCoGe and determined that at 1.3K the U$5f$ and Co$3d$ spin moments are antiparallel, in agreement with theory, but disagreeing with polarized neutron diffraction results. The measured total spin moment is determined to be -0.35$\mu_B FU^{-1}$, and the orbital moment hence determined to be 0.5$\mu_B FU^{-1}$. These moments are reduced with respect to the LDA calculations. The small ratio of U orbital to spin moments indicates that the 5f moment is itinerant.

1:03PM Z25.00010 Interplay of charge density modulations and superconductivity[1] , JASON W. SADOWSKI, K. TANAKA, Dept. of Physics & Engineering Physics, University of Saskatchewan — Although charge density waves (CDW) in transition metal dichalcogenides (TMDs) have been studied for over three decades, there is yet no consensus on the mechanism for CDW in two-dimensional TMDs. Moreover, the layered 2H-type TMDs which exhibit coexistence of CDW order and superconductivity (SC) present an intriguing opportunity for studying the interplay of SC and charge density modulations. In particular, 2H-$NbSe_2$ is most suitable for such investigation as its transition temperatures for CDW and SC are well separated, and as it is easy to cleave is ideal for surface-sensitive measurements. The relation between CDW and SC in this material is still under debate, with one experiment indicating an enhancement of SC by CDW [1] and another implying a competition of the two kinds of orders [2]. Motivated by these experiments, we study the effects of Fermi surface structure on CDW and its interplay with SC in terms of the Bogoliubov-de Gennes formalism.

[1] Kiss *et al.*, Nat. Phys. **3**, 720 (2007).
[2] Borisenko *et al.*, Phys. Rev. Lett. **102**, 166402 (2009).

[1]NSERC, Canada Foundation for Innvation

1:15PM Z25.00011 First-principles study of the noncentrosymmetric superconductors Li_2Pt_3B and Li_2Pd_3B , TATSUYA SHISHIDOU, ADSM, Hiroshima Univ, TAMIO OGUCHI, ISIR, Osaka Univ — Effect of spin-orbit coupling (SOC) associated with lack of space-inversion symmetry has been a central issue in condensed-matter physics. Li_2Pt_3B and Li_2Pd_3B are superconducting below 2.7 K and 7 K, respectively, and have the same crystal structure (cubic $P4_332$, No. 212), which is noncentrosymmetric and is characterized by highly distorted corner-sharing BPt(Pd)$_6$ octahedra. Despite the same valency and structure, they show quite different superconducting behavior. NMR measurements [1] indicate that Li_2Pt_3B would be a spin-triplet superconductor with line nodes in the gap function while Li_2Pd_3B is a conventional spin-singlet s-wave superconductor. SOC would be a key to understand this difference. To clarify the electronic band structure and Fermi surface of these compounds, we performed density-functional (GGA PBE) calculations with FLAPW method. Relativistic effects were fully taken into account. The band structures calculated are in good accordance with previous work[2] and the spin splitting due to SOC is quite significant in Li_2Pt_3B. This work was supported by a MEXT KAKENHI on Innovative Areas "Topological Quantum Phenomen". [1] M. Nishiyama, Y. Inada, and G.-q. Zheng, PRL **98**, 047002 (2007); PRB **71**, 220505(R) (2005). [2] K.-W. Lee and W. E. Pickett, PRB **72**, 174505 (2005).

1:27PM Z25.00012 The electron-boson spectral density function of underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ and $YBa_2Cu_3O_{6.50}$, JUNGSEEK HWANG, Pusan National University — We investigate the electron-boson spectral density function, $I^2\chi(\omega,T)$, of CuO_2 plane in underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi-2212) and underdoped $YBa_2Cu_3O_{6.50}$ (Y-123) systems using the Eliashberg formalism. We apply a new (in-plane) pseudogap model to extract the electron- boson spectral function. For extracting the spectral function we assume that the spectral density function consists of two components: a sharp mode and the broad Millis-Monien-Pines (MMP) mode. We observe that both the resulting spectral density function and the intensity of the pseudogap show strong temperature dependences: the sharp mode takes most spectral weight of the function and the peak position of the sharp mode shifts to lower frequency and the depth of pseudogap, $1-\tilde{N}(0,T)$, is getting deeper as temperature decreases. We estimate fictitious (maximum) superconducting transition temperatures, $T_c(T)$, from the extracted spectral functions at various measured temperatures using a generalized McMillan formula. The estimated (maximum) T_c also shows a strong temperature dependence; it is higher than the actual T_c at all measured temperatures and decreases with temperature lowering. Since as lowering temperature the pseudogap is getting stronger and the maximum T_c is getting lower we propose that the pseudogap may suppress the superconductivity in cuprates.

1:39PM Z25.00013 Modulation of Spin-Orbit interaction and superconductivity in two-dimensional electron gas at the Mott-Insulator - Band-Insulator interface: LaTiO3 - SrTiO3 , JOHAN BISCARAS, N. BERGEAL, LPEM, A. KUSHWAHA, ITT Kanpur, T. WOLF, LPEM, A. RASTOGI, ITT Kanpur, RAMESH CHANDRA BUDHANI, Low Dimensional Systems Laboratory, Department of Physics, Indian Institute of Technology Kanpur, Kanpur 208016, India, JEROME LESUEUR, LPEM-UMR8213/CNRS - ESPCI ParisTech, 10 rue Vauquelin - 75005 Paris — It has been shown recently that a two-dimensional electron gas could form at the interface of two insulators such as $LaAlO_3$ and $SrTiO_3$ [1], or $LaTiO_3$ (a Mott insulator) and $SrTiO_3$ [2]. We present low temperature transport and magneto-transport measurements on $LaTiO_3/SrTiO_3$ hetero-structures, whose properties can be modulated by field effect using a metallic gate on the back of the substrate. The corresponding phase diagram has been investigated, and superconductivity evidenced for the first time in this system which involves a Mott insulator [3]. We will discuss the role of the confinement potential and the $SrTiO_3$ band structure on the phase diagram, and show the specific role of the spin-orbit coupling measured by localization corrections to the magnetoconductivity. Finally, the superconducting to insulator transition will be analyzed. [1] N. Reyren et al, Science 317, 1196 (2007) [2] A. Ohtomo et al, Nature 419, 378 (2002) [3] J. Biscaras et al, Nature Commun, DOI: 10.1038/ncomms1084 (2010)

1:51PM Z25.00014 Upper Critial Field Calculations in p-Wave Tripet Ferromagnetic Superconductors , CHRISTOPHER LÖRSCHER, RICHARD KLEMM, University of Central Florida — We report $H_{c2}(T)$ calculations for novel triplet ferromagnetic superconductors using a uniaxially anisotropic pairing interaction, obtained by means of the linearized Gor'kov gap equation. In addition to the intrinsic anisotropy of the p-wave states, we also include effective mass anisotropies in our calculations. We investigate the $H_{c2}(T)$ phase diagrams for several combinations of anisotropy, leading to novel $H_{c2}(T)$ properties, including upward curvature. We discuss the relevance of our results to experiments on UCoGe.

2:03PM Z25.00015 Identifying d-vectors in spin-orbit coupled multi-orbital superconductors , CHRISTOPH PUETTER, HAE-YOUNG KEE, University of Toronto — In multi-orbital systems, Hund's interaction has been recognized to play a significant role in spin-triplet pairing. On the other hand, spin-orbit coupling has been treated as a perturbation, which is not a good approximation in 4d or 5d transition metal compounds. We have treated both effects on an equal footing in t2g orbital systems and studied their combined effect on spin-triplet superconductivity. We also discuss the implications of our results for spin-triplet candidate materials.

Friday, March 25, 2011 11:15AM - 2:15PM –

Session Z26 DMP DCOMP: Focus Session: Iron Based Superconductors – Electronic Anisotropy D162/164

11:15AM Z26.00001 In-plane electronic anisotropy of underdoped iron arsenide superconductors , IAN FISHER, Department of Applied Physics, Stanford University — Common to the high Tc cuprates, superconductivity in the Fe arsenides and related compounds is associated with suppression of an antiferromagnetic ground state. On the underdoped side of the phase diagram, in addition to the antiferromagnetic transition, the materials also suffer a phase transition that breaks the 4-fold rotational symmetry of the high-temperature crystal structure, this occurring at either the same or higher temperature than the Neel transition. Emerging evidence based on measurements of detwinned single crystals reveals a dramatic in-plane electronic anisotropy associated with this nematic transition.[1]

[1]In collaboration with: J.-H. Chu, H.-H Kuo, J. Analytis, M. Yi, D. H. Lu, Z. X. Shen, A. P. Sorini, A. F. Kemper, S.-K. Mo, T. P. Devereaux, R. G. Moore, M. Hashimoto, W. S. Lee, Z. Hussain, K. De Greve, P. L. McMahon, Y. Yamamoto (Stanford); Z. Islam (APS,ANL); A. Dusza, A. Lucarelli, F. Pfuner & L. Degiorgi (ETHZ).

11:51AM Z26.00002 Superconducting properties and the interplay between magnetism and superconductivity in 1111 Fe arsenides as revealed by torque magnetometry , GANG LI, GAEL GRISONNANCHE, BENJAMIN CONNER, National High Magnetic Field Lab, NIKOLAI ZHIGADLO, SERGIY KATRYCH, ZBIGNIEW BUKOWSKI, JANUSZ KARPINSKI, Laboratory for Solid State Physics, ETH Zürich, CH-8093 Zürich, Switzerland, LUIS BALICAS, National High Magnetic Field Lab — We performed a study of the angular dependence of the magnetic torque in $LaFeAsO_{0.9}F_{0.1}$ single crystals. We developed a method to separate the magnetic and the superconducting components inherent to the FeAs layers and which are superimposed onto the reversible torque signal $\tau_{\rm rev}(\theta, H, T)$. We show that by exploring the amplitude of the superconducting component in $\tau_{\rm rev}(\theta)$ as a function of H, it is possible to extract the thermodynamic value of the superconducting upper critical field H_{c2}. This so obtained value can be used to extract the field and the temperature dependencies of respectively, the superconducting anisotropy and the superfluid density through the Kogan formalism. We observe a strong temperature and field dependence of the superconducting anisotropy as expectable within a multi-band superconducting scenario. The resulting T-dependence of the superfluid-density resembles the behavior previously reported for LaFePO and which was ascribed to nodal superconductivity.

12:03PM Z26.00003 Properties of de-twinned iron-arsenide $SrFe_2As_2$, ERICK BLOMBERG, M.A. TANATAR, A. KREYSSIG, N. NI, A. THALER, R.W. HU, P.C. CANFIELD, S.L. BUD'KO, A.I. GOLDMAN, R. PROZOROV, Department of Physics & Astronomy and The Ames Laboratory, Iowa State University, Ames, IA 50011, USA — The iron-pnictides, AFe_2As_2 (A = alkali earth metal), undergo a tetragonal to orthorhombic structural transition below T_s, which is in the range between 130 K to 210 K depending on the compound. To release elastic deformation the orthorhombic phase is spontaneously divided into four degenerate, equally populated, structural domains. This makes any measurements of in-plane anisotropy extremely difficult. Unlike high$-T_c$ Y-Ba-Cu-O which is orthorhombic already at room temperature, detwinning of pnictides is more difficult, because of lower T_s. We developed a technique of mechanical de-twinning of these materials that allows transport, x-ray and direct optical measurements [1]. Here we report polarized light microscopy, synchrotron X-ray analysis and AC transport measurements on $SrFe_2As_2$, which represents a clean case of first-order magnetic/structural transition.

[1] M. A. Tanatar, et al. Phys. Rev. B **81** 184508 (2010).

12:15PM Z26.00004 Magnetic Field Effect on the In-plane Electrical Resistivity of $FeTe_{1-x}Se_x$ Single Crystals , YIMIN XIONG, AMAR KARKI, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803-4001, BRIAN SALES, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, RONGYING JIN, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803-4001 — The in-plane electrical resistivity (ρ_{ab}) of $FeTe_{1-x}Se_x$ single crystals is measured as a function of temperature (T), magnetic field (H), and the angle (θ) between H and electric current (I). The results reveal that ρ_{ab} strongly depends on both H and θ, indicating the participation of spin scattering in the electrical transport. The underlying physics will be discussed.

12:27PM Z26.00005 Anisotropy of normal and superconducting states of FeSeTe , M.A. TANATAR, Ames Laboratory, Ames, IA, E.C. BLOMBERG, Department of Physics and Astronomy, Iowa State University and Ames Laboratory, Ames, IA, J.-PH. REID, Departement de Physique, Universite deSherbrooke, Sherbrooke, Quebec, Canada, J. HU, J. QUIAN, Z.Q. MAO, Department of Physics and Engeenering Physics, Tulane UNiversity, New Orleans, Louisiana, USA, LOUIS TAILLEFER, Departement de Physique, Universite deSherbrooke, Sherbrooke, Quebec, Canada, R. PROZOROV, Department of Physics and Astronomy, Iowa State University and Ames Laboratory, Ames, IA 50011, USA — We report anisotropic electrical and thermal transport measurements in non-superconducting parent FeTe and superconduicting optimally doped FeTeSe. Intrinsic in- plane anisotropy of the electrical resistivity was measured in mechanically detwinned crystals of the parent compound [1]. In-plane and inter-plane heat transport was used to probe the symmetry of the superconducting gap in the material close to optimal doping (Tc=15 K). The results are compared to those of superconducting FeSe [2] and doping evolution of thermal conductivity in BaFe2As2 doped with cobalt [3,4]. [1] M.A. Tanatar, *et al.* Phys. Rev. B **81**, 184508 (2010). [2] J. K. Dong, *et al.* Phys. Rev. B **80**, 024518 (2009). [3] M. A. Tanatar, *et al.* Phys. Rev.Lett. **104**, 067002 (2010). [4] J.-Ph. Reid, *et al.* Phys. Rev. B **82**, 064501 (2010).

12:39PM Z26.00006 Pulsed-field contactless mapping of the anisotropic upper critical field in LiFeAs superconducting crystals , K. CHO, H. KIM, M.A. TANATAR, R. PROZOROV, Ames Laboratory, USA, Y.J. SONG, Y.S. KWON, Sungkyunkwan University, Rep. of Korea, W.A. CONIGLIO, C.C. AGOSTA, Clark University, USA, A. GUREVICH, National High Magnetic Field Laboratory, USA — Angle - resolved measurements of the upper critical field were performed using a tunnel diode resonator in the stoichiometric iron arsenide superconductor LiFeAs (T_c=18 K) in pulsed magnetic fields up to 50 T at temperatures down to 0.6 K. Complete $H_{c2}^{\|c}(T)$ and $H_{c2}^{\perp c}(T)$ curves with $T \to 0$ extrapolated values of $H_{c2}^{\|c}(0) = 17 \pm 1$ T and $H_{c2}^{\perp c}(T) = 26 \pm 1$ T were obtained. The anisotropy, $\gamma_{H_{c2}} \equiv H_{c2}^{\perp c}/H_{c2}^{\|c} \approx 2$, close to T_c has revealed the essentially three-dimensional electronic structure of the material. Both temperature - dependent $H_{c2}(T)$ can be well fit within a single set of band structure, magnetism and scattering parameters. In a configuration with $H \parallel c$, $H_{c2}^{\|c}(T)$ is limited by orbital effects with modest scattering. In the perpendicular orientation, $H_{c2}^{\perp c}(T)$ shows a notable low-temperature saturation and a strong departure from the orbital Werthamer-Helfand-Hohenberg model. Instead, fitting results suggest paramagnetic Pauli limiting and the development of a spatially - modulated superconducting state.

12:51PM Z26.00007 Symmetry breaking orbital anisotropy observed in detwinned $Ba(Fe_{1-x}Co_x)_2As_2$ above the spin density wave transition , MING YI, Stanford University, D.H. LU, J.-H. CHU, J.G. ANALYTIS, A.P. SORINI, A.F. KEMPER, S.-K. MO, R.G. MOORE, M. HASHIMOTO, W.-S. LEE, Z. HUSSAIN, T.P. DEVEREAUX, I.R. FISHER, Z.-X. SHEN — Nematicity has recently been observed in the competing phases in proximity to the superconducting phase in the cuprates. Similarly, the iron pnictides exhibit symmetry breaking competing phases in the form of a tetragonal to orthorhombic structural transition and a collinear spin density wave (SDW) transition in the underdoped regime. Evidence for strong in-plane anisotropy in the SDW state has been reported by neutron scattering, scanning tunneling microscopy, and transport measurements, but the nature of this nematic behavior is still elusive. Here we present the results of an ARPES study of detwinned single crystals of underdoped $Ba(Fe_{1-x}Co_x)_2As_2$, resolving single domain electronic structure in the orthorhombic SDW state which exhibits strong in-plane anisotropy consistent with other probes. The anisotropy is evident in a large splitting of the dxz and dyz bands, which is seen to develop almost fully above the onset of the long range magnetic order.

1:03PM Z26.00008 Nematic spin fluid in the tetragonal phase of $BaFe_2As_2$, LELAND HARRIGER, University of Tennessee, HUIQIAN LUO, MENGSHU LIU, TOBY PERRING, CHRIS FROST, JIANGPING HU, MIKE NORMAN, PENGCHENG DAI — We use inelastic neutron scattering to demonstrate the presence of a large spin anisotropy above T_N in the unstressed tetragonal phase of $BaFe_2As_2$. In the low-temperature orthorhombic phase, we find highly anisotropic spin waves with a large damping along the AF a-axis direction. On warming the system to the paramagnetic tetragonal phase, the low-energy spin waves evolve into quasi-elastic excitations, while the anisotropic spin excitations near the zone boundary persist. These results strongly suggest that the spin nematicity we find in the tetragonal phase of $BaFe_2As_2$ is the source of the electronic and orbital anisotropy observed above T_N by other probes, and has profound consequences for the physics of these materials.

1:15PM Z26.00009 Reconstructed electronic structure from orbital ordering and antiferromagnetism in the iron pnictides , WEICHENG LV, PHILIP PHILLIPS, Department of Physics, University of Illinois — Recent experimental developments have unambiguously demonstrated the in-plane electronic and magnetic anisotropy of the iron-based superconductors. It has been argued that this nematic state can arise from orbital ordering physics. Including an energy splitting term that breaks the degeneracy of the Fe d_{xz} and d_{yz} orbitals, we solve the multi-orbital Hubbard model within a mean-field approximation. Despite sensitivity of the resulting state to the input parameters, we find that a weak orbital order that places the d_{yz} orbital slightly higher in energy than the d_{xz} orbital, along with the interactions U and J being of intermediate strength, is compatible with current experimental results. In this regime, the stripe antiferromagnetism is further stabilized and the existence of the Dirac cones is preserved. Furthermore, this anisotropic electronic state leads to the observed resistivity anisotropy and STM interference patterns. Finally the relation between orbital order and superconductivity is discussed.

1:27PM Z26.00010 Magnetic Torque Evidence for Broken Rotational Symmetry in the Tetragonal Phase of $BaFe_2(As_{1-x}P_x)_2$ Single Crystals , SHIGERU KASAHARA, HONGJIE SHI, RYUJI OKAZAKI, KENICHIRO HASHIMOTO, MINORU YAMASHITA, TAKASADA SHIBAUCHI, TAKAHITO TERASHIMA, YUJI MATSUDA, Kyoto University — The emergence of broken four-fold symmetry is found in the tetragonal phase of $BaFe_2(As_{1-x}P_x)_2$ single crystals [1] by in-plane anisotropy measurements of magnetic susceptibility. Magnetic torque detects a spontaneous growth of two-fold oscillations under in-plane field rotations, whose amplitude is linked to an order parameter of an electronic "nematic" phase. Our findings reveal that the spontaneous rotational symmetry breaking sets in far above the tetragonal to orthorhombic structural transition, which might be also linked to the unconventional superconductivity of this system [2,3].

[1] S. Kasahara, et al., Phys. Rev. B 81, 184519 (2010).
[2] K. Hashimoto, et al., Phys. Rev. B 81, 220501(R) (2010).
[3] Y. Nakai, et al., Phys. Rev. B 81, 020503(R) (2010).

1:39PM Z26.00011 Interplay of orbital ordering and magnetism in the parent compounds of the iron pnictides , ANDRIY NEVIDOMSKYY, Physics and Astronomy, Rice University — The neutron scattering experiments on the parent compounds of the 122 family of the iron pnictide superconductors show a pronounced orhthorhombic anisotropy in the spin wave spectra [1], also observed in resistivity measurements on detwinned crystals [2,3]. Orbital ordering of the d_{xz} and d_{yz} orbitals may be a possible explanation for this behaviour [4]. In this work, we establish the effect of orbital ordering on the magnetism and study their interplay through a combination of the first-principles band theory calculations and phenomenological analysis in the framework of the Landau theory. This enables us to establish the coupling between the orbital and magnetic degrees of freedom in these materials. Consequences for the symmetry of the superconducting order parameter are discussed.

[1] J. Zhao et al., Nature Phys. **5**, 555 (2009)
[2] M.A. Tanatar at al., Phys. Rev. B **81**, 184508 (2010).
[3] J.-H. Chu et al., Science **329**, 824 (2010).
[4] C.-C. Chen et al., Phys. Rev. B **82**, 100504(R) (2010).

1:51PM Z26.00012 Orbital-ordering and In-plane Anisotropy in Low-moment Ground-state of Parent Compounds of Iron-based Superconductors[1] , MASAHIKO MACHIDA, HIROKI NAKAMURA, Japan Atomic Energy Agency — Since the discovery of the iron-based superconductor, a large discrepancy between experimental observations and first-principles calculations in the magnetic moment of the antiferromagnetic state of the parent compounds has been intensively debated. The observed moment values are about 3 to 5 times smaller than those of the calculation although there is a variety of the difference depending on the materials. Very recently, an interesting calculation data fully reproducing the observed low moment has been suggested by F. Cricchio et al., (Phys. Rev. B 81 (2010) 140403) who performed first-principles calculations using a LDA+U scheme. In this study, we suggest that the new state is a possible candidate to well explain the other data, e.g., strong anisotropy in spatial patterns measured by STM and magnetic excitations found by neutron scattering. Furthermore, we compare the result with other theoretical works reproducing similar low moment in terms of orbital ordering.

[1] CREST(JST)

2:03PM Z26.00013 Conductivity Anisotropy in the Antiferromagnetic State of Iron Pnictides , BELEN VALENZUELA, ELENA BASCONES, MARIA J. CALDERON, Inst. Ciencia de Materiales de Madrid-CSIC — Recent experiments on iron pnictides have uncovered a large in- plane resistivity anisotropy with a surprising result: the system conducts better in the antiferromagnetic x direction than in the ferromagnetic y direction [1]. We address this problem by calculating the ratio of the Drude weight along the x and y directions, D_x/D_y, for the mean-field $\mathbf{Q} = (\pi, \mathbf{0})$ magnetic phase diagram of a five-band model for the undoped pnictides [2,3]. We find [4] that D_x/D_y ranges between $0.2 < D_x/D_y < 1.7$ for different interaction parameters. Large values of the orbital ordering favor an anisotropy opposite to the one found experimentally. On the other hand, D_x/D_y is strongly dependent on the topology and morphology of the reconstructed Fermi surface. Our results point against orbital ordering as the origin of the observed conductivity anisotropy, which may be ascribed to the anisotropy of the Fermi velocity. [1] J.-H. Chu et al., Phys. Rev. B 81, 214502 (2010); J.-H. Chu et al., Science 329, 824 (2010); M. Tanatar et al., Phys. Rev. B 81, 184508 (2010). [2] M.J.Calderon, B. Valenzuela, E. Bascones, Phys. Rev. B 80, 094531 (2009). [3] E.Bascones, M.J. Calderon, B. Valenzuela, Phys. Rev. Lett. 104, 227201 (2010). [4] B.Valenzuela, E. Bascones, M.J. Calderon, Phys. Rev. Lett. 105, 207202 (2010).

Friday, March 25, 2011 11:15AM - 1:51PM –

Session Z27 GQI: Focus Session: Semiconductor Qubits - Theory and Experiment C155

11:15AM Z27.00001 Quantum dot charge stability diagram from a generalized Hubbard model[1]

, XIN WANG, SHUO YANG, SANKAR DAS SARMA, Condensed Matter Theory Center, Department of Physics, University of Maryland — We develop a theory for the charge stability diagram in solid state quantum dot spin qubits using a general form of the Hubbard model. We argue that the extended Hubbard model (with both on-site and inter-site Coulomb repulsion) is the minimal model to describe the system. The appropriate parameters of the Hubbard model can be read off by comparing our theoretically derived results with the experimental charge stability plots. We make predictions on how the charge stability diagram depends on various parameters of the Hubbard model, especially the spin-exchange and hopping energies.

[1]This work is supported by IARPA, LPS-CMTC, and CNAM.

11:27AM Z27.00002 Microscopic theory for the charge stability diagram of coupled quantum dot systems[1]

, SHUO YANG, XIN WANG, SANKAR DAS SARMA, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, MD 20742 — We present a quantitative microscopic theory for the charge stability diagram of coupled quantum dot systems. Using the configuration interaction method we obtain a generalized Hubbard model, from which the charge stability diagram is calculated and compared with experiments. We establish an exact connection between experimental measurements and the microscopic theory, and predict some experimentally observable quantum effects. We also map the classical capacitance model to the extended Hubbard model, and argue that the effect of spin-exchange and various hopping terms cannot be expressed in the capacitance model.

[1]This work is supported by LPS-CMTC, IARPA, and CNAM.

11:39AM Z27.00003 Formation and electrical characterization of directed self-assembled Ge/Si quantum dot[1]

, DONGYUE YANG, U. Pittsburgh, CHRIS PETZ, U. Virginia, JEREMY LEVY, U. Pittsburgh, JERROLD FLORO, U. Virginia — Directed self-assembly of sub-10 nm Ge islands is a candidate for producing laterally coupled quantum dot molecules with geometrically-defined spin exchange couplings. The islands are created by the nucleation of Ge islands on nanoscale SiC templates defined by direct-write electron-beam lithography.[2] Ge islands are coupled through ohmic contacts to the Si capping layer, and geometries can be defined that are suitable for either vertical or lateral transport.We describe low-temperature magneto-transport measurements on individual and small arrays of Ge islands grown on semi-insulating silicon substrates.

[1]This work is supported by DOE DE-FG02-07ER46421.

[2]O. Guise, J. Ahner, J. John T. Yates, V. Vaithyanathan, D. G.Schlom, J. Levy, Appl. Phys. Lett. 87, 1902 (2005).

11:51AM Z27.00004 The Kondo Effect in a Double Quantum Dot

, SAMI AMASHA, ILEANA RAU, ANDREW KELLER, Stanford University, JORDAN KATINE, Hitachi Global Storage Technologies, HADAS SHTRIKMAN, Weizmann Institute, DAVID GOLDHABER-GORDON, Stanford University — A quantum dot consists of a confined droplet of electrons connected to electron reservoirs by tunnel barriers. When the dot has an odd number of electrons it has a net spin. The electrons in the reservoir can screen this spin via the Kondo effect, which corresponds to a many-body, highly correlated electron state. We study a lateral GaAs/AlGaAs double quantum dot, where one or both of the dots can be in the Kondo regime. The dots are also coupled to each other, and this inter-dot interaction can compete with the Kondo effect. We report transport measurements in this system at low electron temperatures and for a variety of inter-dot couplings.

12:03PM Z27.00005 Exhibition of tunnel coupling of negatively charged dangling bonds on Si Surface Using Scanning Tunneling Microscope

, M. BASEER HAIDER, Dept of Physics, King Fahad University of Petroleum & Minerals, Saudi Arabia, L. LIVADARU, Dept of Physics, University of Alberta, Canada, J. PITTERS, National Institute for Nanotechnology, National Research Council of Canada, Canada, R. WOLKOW, Dept of Physics, University of Alberta, Canada — We have performed Scanning tunneling microscopy study of hydrogen terminated Si (100). We will show that single Si atoms in a solid state environment can be served as quantum dots. These negatively charged quantum dots can be tunnel coupled to the nearby Si quantum dots. We will demonstrate that this tunnel coupling can be controlled by adjusting the separation between the two Si atomic quantum dots. Moreover electron occupation in the tunnel coupled Si quantum dots can be controlled. We have used this tunnel coupling effect of Si atomic quantum dots to fabricate Quantum Cellular Automata Cells. Quantum Cellular Automata are used to transmit binary information through electrostatic interaction between adjacent cells without the transfer of charge from one cell to the next. Devices based on Quantum Cellular Automata will consume much less power compared to the conventional transistor based devices. Moreover, since there is no transfer of charge so power dissipation during its operation is minimal compared to conventional semiconductor devices. This Si based Quantum Cellular Automat Cell works at room temperature.

12:15PM Z27.00006 The RKKY Interaction and the Nature of the Ground State of Double Dots in Parallel

, MANAS KULKARNI, Stony Brook University and Brookhaven National Laboratory, ROBERT KONIK, Brookhaven National Laboratory — We argue through a combination of slave boson mean field theory and the Bethe ansatz that the ground state of closely spaced double quantum dots in parallel are Fermi liquids. We do so by studying the dots conductance, impurity entropy, and spin correlation. In particularly we find that the zero temperature conductance is characterized by the Friedel sum rule, a hallmark of Fermi liquid physics, and the impurity entropy vanishes in the limit of zero temperature, indicating the ground state is a singlet. This conclusion is in contradistinction to a number of numerical renormalization group studies. We suggest a possible reason for the discrepancy. Our findings are also consistent with a 1/N diagrammatic approach to the same setup.

12:27PM Z27.00007 Frequency-dependent Fano factor of multilevel systems with inelastic decay processes[1]

, FARZAD QASSEMI, Institute for Quantum Computing and Department of Physics and Astronomy, University of Waterloo, Ontario, Canada, BILL COISH, Department of Physics and Astronomy, McGill University, Montreal, Canada, JOAKIM BERGLI, Department of Physics, University of Oslo, Norway, FRANK K. WILHELM, Institute for Quantum Computing and Department of Physics and Astronomy, University of Waterloo, Ontario, Canada — We study the frequency-dependent noise of electrons passing through a multilevel quantum dot or molecule accounting for "dark" states through which current is prohibited and inelastic transitions between the levels. Our theory results in simple closed-form expressions directly relating the frequency-dependent noise to inelastic decay rates in the limit where the rates are widely separated. To demonstrate the method, we apply it to evaluate the shot noise for electrons passing through single and double quantum dots in the presence of multiple spin decay mechanisms.

[1]Thanks to our sponsors Quantumworks, NSERC, CIFAR and Waterloo Inst for Nanotechnology.

12:39PM Z27.00008 Electron Localization in the Inhomogeneous Electron Gas: Quantum Point Contacts , ABHIJIT C. MEHTA, Duke University, CYRUS J. UMRIGAR, Cornell University, A. DEVRIM GUCLU, National Research Council of Canada, HAROLD U. BARANGER, Duke University — We use Quantum Monte Carlo (QMC) techniques to investigate the behavior of electrons in an inhomogeneous quasi-one-dimensional wire as a model of quantum point contact geometries. Previous QMC work by Guclu et al. demonstrated that electrons can be strongly localized in quantum point contacts, and this result was reproduced by Welander et al. using LSDA calculations. We model a quantum point contact as a constriction in a quantum ring, and we use variational and diffusion Monte Carlo to investigate the effects of different point contact lengths and geometries on the electronic properties of the QPC. A key issue is how robust the previous results are to the length of the constriction, the depth and steepness of the confining potential, and to increasing the density of the electrons in the high-density lead region.

12:51PM Z27.00009 Electron pair tunneling resonance in a double-dot interferometry , JINHONG PARK, H.-S. SIM, KAIST — It is difficult to experimentally detect an electron pair tunneling resonance in a quantum dot with repulsive Coulomb interactions, since it is usually masked by lower-order single-electron tunneling processes. We propose to use an Aharonov-Bohm interferometry consisting of two quantum dots for the detection. We find that in the second harmonics of the interference current, pair tunneling processes give a leading non-monotonous contribution around the bias voltages at which pair tunneling resonances appear. The second-harmonics differential conductance shows the signal of a pair tunneling resonance as well as the destructive interference of two pair tunneling resonances.

1:03PM Z27.00010 Giant current fluctuations in an overheated single-electron transistor , MATTI LAAKSO, TERO HEIKKILÄ, Low Temperature Laboratory, Aalto University, YULI NAZAROV, Kavli Institute of Nanoscience, Delft University of Technology — Interplay of cotunneling and single-electron tunneling in a thermally isolated single-electron transistor leads to peculiar overheating effects. In particular, there is an interesting crossover interval where the competition between cotunneling and single-electron tunneling changes to the dominance of the latter. In this interval, the current exhibits anomalous sensitivity to the effective electron temperature of the transistor island and its fluctuations. We present a new theoretical method for the study of the temperature fluctuations and induced fluctuations of other quantities, e.g., current, based on the Fokker–Planck equation. We apply this method to the study of the current and temperature fluctuations in an overheated SET around the crossover interval.

1:15PM Z27.00011 Electron exchange between quantum dot and ring by jumping in magnetic field , IGOR FILIKHIN, SERGEI MATINYAN, JAMES NIMMO, BRANISLAV VLAHOVIC, North Carolina Central University — Semiconductor heterostructures as quantum dots (QD) or quantum rings (QR) demonstrate discreet atom-like energy level configuration. In the presented work we show that in the weak coupled Double Concentric Quantum Ring (DCQR) electron position jumping can exist due to the energy level crossing. We study DCQR composed of GaAs in an $Al_{0.70}Ga_{0.30}As$ substrate under influence of magnetic field. In our model the DCQR is considered in three dimensional space within single sub-band effective mass approach [1]. Magnetic field is applied in z direction, perpendicular to the DCQR plane. The electron position in DCQR is defined by effective radius which is radius of most probable localization of a single electron. We study electron structure of QD located at the center of QR. The electron position jumping between QD and QR is considered. Discussed will be possibility of experimental implementations of the jumping effect for composite object of QD and QR.

[1] I. Filikhin, V. M. Suslov and B. Vlahovic, Phys. Rev. B 73, 205332 (2006).

1:27PM Z27.00012 Quantum phase transition of light as a control of the entanglement between interacting quantum dots , ANGELA BARRAGAN, Instituto de Fisica, Universidad de Antioquia, Medellin, Colombia; Instituto de Ciencias Nucleares, Universidad Nacional Autonoma de Mexico, Mexico, CARLOS VERA-CIRO, Instituto de Fisica, Universidad de Antioquia, Medellin, Colombia; Kapteyn Institute, University of Groningen, Groningen, The Netherlands, IAN MONDRAGON-SHEM, Instituto de Fisica, Universidad de Antioquia, Medellin, Colombia; Department of Physics, Cornell University, Ithaca, NY, USA — We study coupled quantum dots arranged in a photonic crystal, interacting with light which undergoes a quantum phase transition. At the mean-field level for the infinite lattice, we compute the concurrence of the quantum dots as a measure of their entanglement. We find that this quantity smoothly changes in the vicinity of the phase transition, and in a step-like fashion in the Mott-insulator phase. This behavior can be externally monitored through the second-order correlation function for the light in each lattice site. For the finite case, we discuss boundary induced effects using a mean-field ansatz, as well as the impact of having finite temperatures on the entanglement of the quantum dots.

1:39PM Z27.00013 First-principles study of the energy and spin structure of excited states of NV^-center in diamond and its corresponding Hubbard model parameters , SANGKOOK CHOI, MANISH JAIN, STEVEN G. LOUIE, University of California, Berkeley and Lawrence Berkeley National Laboratory — A negatively charged nitrogen-vacancy pair defect (NV) in diamond is one of the promising candidates to embody a qubit for quantum computation in solid states. It is an individually addressable quantum system that may be initialized, manipulated, and measured with high fidelity at room temperature due to a long coherence time of the spin in the ground states and long-life time of the excited states. The knowledge of the electronic and spin structures of the NV center in the ground as well as excited state is crucial in understanding them. Here, we evaluate the energies and spin structures of its excited states employing the first-principles GW-BSE methods. We further obtain the Hubbard model parameters for this defect system by comparing the excited-state energies from our ab-initio GW-BSE calculation with those from the model Hamiltonian. This work was supported by NSF Grant No. DMR10-1006184, the U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at LBNL's NERSC facility.

Friday, March 25, 2011 11:15AM - 12:39PM –

Session Z29 GQI: Focus Session: Superconducting Qubits - Coherence and Materials III C148

11:15AM Z29.00001 Improving the Quality Factor of Microwave Compact Resonators , K. GEERLINGS, S. SHANKAR, E. EDWARDS, L. FRUNZIO, R.J. SCHOELKOPF, M.H. DEVORET, Applied Physics Dept., Yale University — Superconducting microwave resonators are now widely used for coupling to superconducting qubit systems. Compact resonators [1] consisting of an interdigitated capacitance and a meander inductance take up much less space than a typical coplanar waveguide resonator. Since the design of compact resonators and qubits share common features, qubit decoherence mechanisms can be studied through the measurement of resonator loss. We measured of order 100 resonators and have achieved internal quality factors in excess of 300,000. Results indicate loss appears to be due to spurious two level systems. Loss increases when the participation of surfaces in the energy density is increased. Thus a large separation of electrodes is preferred, in agreement with the findings of other groups. Work in progress involves the combination of these resonators with transmon qubits. Work supported by IARPA, ARO and the NSF.

[1] M.S. Khalil, F.C. Wellstood, and K.D. Osborn, arXiv:1008.2929

11:27AM Z29.00002 Radiative Losses in Superconducting Coplanar Resonators , JAMES WENNER, R. BARENDS, R.C. BIALCZAK, Y. CHEN, J. KELLY, M. LENANDER, E. LUCERO, M. MARIANTONI, M. NEELEY, A.D. O'CONNELL, P. O'MALLEY, D. SANK, A. VAINSENCHER, H. WANG, M. WEIDES, T. WHITE, Y. YIN, J. ZHAO, A.N. CLELAND, JOHN M. MARTINIS, UC Santa Barbara — Radiation is a potential loss mechanism in superconducting qubits. Radiation loss was studied in superconducting coplanar resonators, which are important both in coupling superconducting qubits and because they provide a simple system to quantitatively measure the resulting effects. We fabricated 8 GHz resonators and measured the resulting reduction of the high-power Q. We found it was necessary to design the resonators carefully to reduce stray coupling between the resonators so that losses would be dominated by radiation. The radiation loss is measured to be 30 times greater than predicted by a simple theoretical model, but was predicted accurately by simulation data. We attribute this to the effects of the device mount and the finite substrate height on the radiation pattern. We conclude that radiation is an unlikely decoherence mechanism for the present generation of qubits and resonators.

11:39AM Z29.00003 Minimal resonator loss for circuit quantum electrodynamics , RAMI BARENDS, UC Santa Barbara, N. VERCRUYSSEN, A. ENDO, P.J. DE VISSER, T. ZIJLSTRA, T.M. KLAPWIJK, Delft University of Technology, P. DIENER, S.J.C. YATES, J.J.A. BASELMANS, SRON Netherlands Institute for Space Research, H. WANG, M. HOFHEINZ, J. WENNER, M. ANSMANN, R.C. BIALCZAK, M. LENANDER, E. LUCERO, M. NEELEY, A.D. O'CONNELL, D. SANK, M. WEIDES, A.N. CLELAND, J.M. MARTINIS, UC Santa Barbara — In Josephson quantum information processing superconducting coplanar waveguides are used as memory elements and coupling buses. Quality factors of these resonators reach up to a million at high excitation powers, but decrease down to below $100x10^3$ at the single photon level in the presently used materials, such as Al and Nb. We report quality factors of up to $500x10^3$ by using NbTiN or Re and removing the dielectric from regions with high electric fields. Using a model-analysis and by a comparison with Ta, the crucial sources of intensity-dependent loss are dielectrics on the surface of the metal and substrate. Our approach shows that using non-oxidizing superconductors such as Re and NbTiN and removing dielectrics is a straightforward route to high quality factors in the single photon regime.

11:51AM Z29.00004 Low-loss superconducting microwave resonators with NbN films[1] , C. SONG, B. XIAO, M. WARE, B.L.T. PLOURDE, Syracuse University — The native oxide that forms on the surface of most superconducting thin films contains a distribution of two-level system (TLS) defects that results in a significant microwave loss channel at low temperatures and powers. One of the key limitations in the quality factor of microwave devices in this regime for superconducting quantum information processing schemes is due to this surface loss mechanism. Thus, nitride superconducting materials are promising candidates due to their lack of a significant surface oxide. We have fabricated coplanar waveguide microwave resonators from reactively sputtered NbN films on sapphire and Si substrates. We characterize the resonators with measurements of the center frequency and quality factor as a function of temperature and power. In the low-temperature and low-power limit, we have observed quality factors for NbN resonators in excess of 200,000.

[1]Supported by IARPA

12:03PM Z29.00005 Low Loss Superconducting Titanium Nitride Coplanar Waveguide Resonators , MICHAEL VISSERS, DAVID WISBEY, JIANSONG GAO, JEFFREY KLINE, MARTIN WEIDES, DAVID PAPPAS, NIST-Boulder — The introduction of new, low loss superconducting materials will be necessary for the improvement of superconducting qubits. To fulfill this aim, thin films of titanium nitride (TiN) were sputter-deposited onto intrinsic Si and c-plane sapphire wafers with and without SiN buffer layers. The films were then fabricated into RF coplanar waveguide resonators, and internal quality factor measurements were taken at millikelvin temperatures in both the high and low power limits, i.e. many and single photon regimes, respectively. At high power, internal quality factors (Qi's) higher than 10^7 were measured for multiple TiN films with a predominantly (200) orientation. Films that showed significant (111) texture invariably had much lower Qi's in this regime, on the order of 10^5. Our studies show that the (200) TiN is favored for growth at high temperature on either bare Si or substrates with SiN buffer layers. However, growth on bare sapphire or Si (100) at low temperature resulted in primarily a (111) orientation. Ellipsometry and Auger measurements indicate that the (200) TiN growth on the bare Si substrates is correlated with the formation of a thin, $\sim$2nm, layer of SiN during the pre-deposition procedure. We found that TiN grown on these surfaces also showed significant increases of Qi in the low power limit, while thicker SiN buffer layers resulted in reduced Qi's.

12:15PM Z29.00006 Dielectric loss measurements using an embedded transmission line resonator[1] , BAHMAN SARABI, M.J.A. STOUTIMORE, MOE KHALIL, SERGIY GLADCHENKO, University of Maryland and Laboratory for Physical Sciences, ALEXANDER KOZEN, GARY RUBLOFF, F.C. WELLSTOOD, J.C. LOBB, University of Maryland, K.D. OSBORN, Laboratory for Physical Sciences — Lossy dielectrics are a major source of decoherence in superconducting qubits. Superconducting linear resonators have proven to be ideally suited for measuring loss in different dielectrics due to their versatility and relative simplicity in design, fabrication, and measurement. We will present data from samples where the low-loss coplanar resonators are fabricated on top of AlOx dielectric films grown using atomic layer deposition (ALD). Although the low-power loss can be extracted from this geometry, embedding the dielectric under study between metal films has advantages that we will discuss. In addition, ALD films can be grown conformally and without pinholes to small thicknesses in comparison to conventional PECVD films. This allows us to make lumped-element resonators with a relatively small footprint, which can easily be embedded within the transmission line.

[1]This research was supported by the Intelligence Advanced Research Projects Activity through the U.S. Army Research Office award No. W911NF-09-1-0351.

12:27PM Z29.00007 Design and Fabrication of High Q Titanium Nitride Resonators , DAVID WISBEY, JIANSONG GAO, MICHAEL VISSERS, JEFFREY KLINE, MARTIN WEIDES, DAVID PAPPAS, National Institute of Standards and Technology — Titanium nitride (TiN) is a new material that shows promise in quantum information circuits as a low loss material for resonators, and as a multiplexed kinetic inductance photon detector. We have measured lumped element LC resonators and coplanar waveguides resonators. For the lumped element resonator we report internal quality factor (Qi) of over 300,000 at low power, in the single photon regime, and 4 million at high power, and for a half wave coplanar waveguide we report low power Qi of 800,000 and high power Qi of 5 million. We found that overetch in single layer devices can shift the resonance frequency and affect the internal quality factor Qi, and that as the trench depth grew, both the resonance frequency and internal quality factor increased. When designing resonators it is important to know quantities such as the kinetic inductance, superconducting transition temperature (Tc), penetration depth, and amount of overetch so the resonator can be accurately simulated.

Friday, March 25, 2011 11:15AM - 2:03PM –

Session Z33 DCMP: Quantum Fluids and Solids II C143/149

11:15AM Z33.00001 Dissipation of compound torsional oscillator loaded with solid ^{4}He containing ^{3}He impurity level from 0.3 to 25 ppm[1] , PATRYK GUMANN[2], MICHAEL KEIDERLING, DAVID RUFFNER, Rutgers University, HARRY KOJIMA — High sensitivity of supersolid phenomenon in solid ^{4}He to low levels of ^{3}He impurity(x_3) is a puzzle not yet understood. We have analyzed the data taken using our compound torsional oscillator on the variation of dissipation as x_3 was varied between 0.3 and 25 ppm. The compound oscillator allows studies of the dissipation at two oscillator mode frequencies(0.5 and 1.2 kHz). Arrhenius plots of temperatures, where peaks in dissipation occur, vs. frequency allow extracting the activation energy and the characteristic time. The data are consistent with distributions of activation energy whose widths increase with x_3 but the mean value of $\sim$ 430 mK independent of x_3. The characteristic time varies approximately as $\propto x_3^{2/3}$. Temperature dependence of the dissipation is consistent with Debye model but frequency dependence is not. We give an interpretation of the characteristic time in terms of diffusion of ^{3}He along dislocation lines.

[1]Research supported in part by NSF.

[2]Present address: Institute for Quantum Computing, University of Waterloo, Waterloo, Canada

11:27AM Z33.00002 The rotation anomaly of high quality ^{4}He single crystals , XAVIER ROJAS, ARIEL HAZIOT, Ecole Normale supérieur, Paris, JOSHUA T. WEST, MOSES H.W. CHAN, The Pennsylvania State University, HUMPREY MARIS, Brown University, SÉBASTIEN BALIBAR, Ecole Normale supérieur, Paris — We have built a transparent torsional oscillator in order to monitor the growth of ^{4}He crystals near 20 mK. It allows us to measure the rotational inertia of high quality oriented single crystals and compare it with low quality crystals or polycrystals grown at constant volume. It is also possible to vary the ^{3}He concentration from 0 to 0.3 ppm (natural purity). Since the change in TO period associated with the change in shear modulus of the He sample could be calculated, we could see if supersolidity is really due to superflow along dislocation lines.

11:39AM Z33.00003 Shear Modulus of Solid Helium Confined in Aerogel[1] , ARIF RABBANI, JOHN BEAMISH, University of Alberta — Torsional oscillator experiments on ^{4}He show supersolid behavior which appears to be associated with disorder. However, confining helium in the pores of an aerogel does not enhance the supersolid decoupling, even though x-ray measurements confirm that the crystals are highly disordered. Solid helium's shear modulus also shows anomalous behavior below 150 mK, stiffening as mobile dislocations are pinned by ^{3}He impurities at low temperatures. A highly porous material such as aerogel should also provide effective pinning sites for dislocations. We have made shear modulus measurements on solid ^{4}He grown in a 95% porosity aerogel. We see large modulus decreases as the samples are warmed but these occur at much higher temperatures and over a broader range than in bulk ^{4}He. The frequency dependence of the modulus and dissipation are consistent with a thermally activated process. The activation energies are roughly 10 to 15 K and may be associated with vacancy motion.

[1]This work was supported by NSERC.

11:51AM Z33.00004 Possible glass anomalies in the shear modulus and dielectric function of solid helium , JUNG-JUNG SU, MATTHIAS J. GRAF, ALEXANDER V. BALATSKY, Los Alamos National Laboratory — The shear modulus of solid ^{4}He exhibits an anomalous change at low temperature that is qualitatively similar to a frequency change in torsional oscillator experiments. We propose that in solid ^{4}He the stiffening of the shear modulus with decreasing temperature can be described with a generalized susceptibility including a glassy backaction by assuming a distribution of temperature-dependent relaxation times $\tau(T)$. The glass susceptibility captures the freezing out of glassy degrees of freedom below a characteristic crossover temperature T_X, when the dynamic response of the solid satisfies $\omega\tau(T_X) \sim 1$, thus leading to a viscous response. We predict that the maximum change of the amplitude of the shear modulus and the height of the dissipation peak are independent of the applied frequency ω. Recent measurements of the dielectric function $\epsilon(\omega)$ by the UFL group show a similar amplitude increase. We propose that changes in $\epsilon(\omega)$ are due to the glassy dynamics of low-lying excitations and are related to the shear modulus through acousto-optical coupling. We predict a dissipation peak in the imaginary part of the dielectric function, where the change in the real part is largest.

12:03PM Z33.00005 Stress induced roughening of superclimbing dislocation in solid ^{4}He[1] , DARYA ALEINIKAVA, ANATOLY KUKLOV, CSI, CUNY — We investigate numerically superclimb [1] of dislocation in solid ^{4}He biased by externally imposed chemical potential μ. The effective action takes into account quantum phase slips in the core superfluid as well as the core displacement in Peierls potential within the Granato-Lücke string model. The bias produces stress on the core and this can result in dislocation roughening. Such roughening is characterized by hysteretic behavior at temperatures (T) below some threshold $T_{\rm hyst}$. At $T > T_{\rm hyst}$ strong resonant peaks develop in the dislocation differential response. These peaks exhibit periodic behavior vs μ, with the period determined by Peierls potential and dislocation length. We explain these effects by thermally assisted tunneling of jog-antijog pairs across the barrier created by Peierls potential and the bias. Since superclimbing is controlled by core superflow, speed of sound along the superfluid core exhibits dip-like features at the peak positions. We propose that this effect is seen in the mass transport experiment [2].

[1] S. G. Söyler, et al, Phys. Rev. Lett. **103**, 175301 (2009).
[2] M. W. Ray and R. B. Hallock, Phys. Rev. Lett. **105**, 145301 (2010).

[1]We acknowledge support by NSF, grants PHY1005527 and PHY0653135,and by CUNY, grant 63071-00 41.

12:15PM Z33.00006 Andreev-Lifshitz Theory Applied to Normal Solids under Pressure[1] , MATTHEW SEARS, WAYNE SASLOW, Texas A&M University — On letting the superfluid density go to zero, the Andreev-Lifshitz hydrodynamic theory of supersolids becomes applicable to an ordinary solid.[2] Under applied pressure P_a, needed to produce solid He^3 and He^4 or to be of geophysical relevance, the system has both an elastic stress λ_{ik} and an internal pressure P, with $P\delta_{ik} = P_a\delta_{ik} + \lambda_{ik}$ in equilibrium. P may be thought of as being due to a vacancy fluid. For P_a small compared to the bulk modulus, Maxwell relations give $P \sim P_a^2$. The dynamical equations lead to three sets of propagating elastic modes (longitudinal and transverse sound) and two diffusive modes (one largely of entropy density and one largely of vacancy density – or, more generally, defect density), all of which we study for non-zero P_a.[3] The vacancy diffusion mode has diffusion constant $D_L \sim P_a^2$, and is diffusive because its associated internal pressure fluctuation P' nearly cancels its lattice stress fluctuation λ'_{ik}. This mode permits the system to respond differently to transducers with different surface treatments. We specifically have in mind solid ^{4}He, which requires $P_a \sim 25$ bars to solidify; however, the results should apply to any solid under pressure.

[1]Supported by Department of Energy grant DE-FG02-06ER46278.

[2]A. F. Andreev and I. M. Lifshitz, Sov. Phys. JETP 29, 1107 (1969).
[3]M. R. Sears and W. M. Saslow, Phys. Rev. B 82, 134304 (2010).

12:27PM Z33.00007 Quantum phases of grain boundaries in solid ^{4}He[1] , DEBAJIT GOSWAMI, KINJAL DASBISWAS, ALAN DORSEY, Department of Physics, University of Florida — First-principles Monte Carlo simulations show that the core of a dislocation in solid ^{4}He is superfluid and has Luttinger-liquid like properties [Phys. Rev. Lett. **99**, 035301 (2008), Phys. Rev. Lett. **103**, 175301 (2009)]. Low angle grain boundaries in crystals can be thought of as a linear array of dislocations, suggesting that a grain boundary in solid ^{4}He can be modeled as an array of coupled Luttinger liquids. By exploiting this analogy, in this work we study the quantum phases of the grain boundary, as well as analogies with dipolar condensates in one dimensional optical lattices.

[1]This work is supported by the NSF

12:39PM Z33.00008 Supersolid ^{4}He monolayer , MASSIMO BONINSEGNI, University of Alberta — The conditions for the existence of a low temperature supersolid ^{4}He monolayer are investigated by Monte Carlo simulations. The crystalline film considered here is one that not registered with the underlying substrate crystal structure. Its superfluid response is underlain by large zero-point motion of atoms in the direction perpendicular to the substrate. It is proposed that the physics described here might be observable in a helium film adsorbed on a Ni substrate.

12:51PM Z33.00009 U(1) $\times$ U(1) Kosterlitz-Thouless transition of the Larkin-Ovchinnikov phase in an anisotropic two-dimensional system , CHUNGWEI LIN, XIAOPENG LI, W. VINCENT LIU, University of Pittsburgh — We study Kosterlitz-Thouless (KT) transitions of the Larkin-Ovchinnikov (LO) phase for a two-dimensional system composed of coupled one-dimensional tubes. The main character of LO phase is a stripe structure (periodic in only one direction) in the order parameter. The low energy excitations involve the deformation of the stripe configuration and the fluctuation of the phase which can be described by two anisotropic XY model. We compute from a microscopic model the coefficients of XY model from which the KT transition temperatures are determined. We found the $T^{KT} \propto t_\perp$ for small intertube tunneling $t_\perp$. As $t_\perp$ increases the system undergoes a first-order transition to normal phase at zero temperature. Our method can be used to determine the Goldstone excitations of any stripe order involving charge or spin degrees of freedom.

1:03PM Z33.00010 Small-angle Neutron Scattering Measurements of Liquid Helium Mixtures Confined in MCM-41[1] , HELMUT KAISER, Low Energy Neutron Source (LENS), Indiana University, TIMOTHY PRISK, PAUL SOKOL, IAN STEWARD, Indiana University Department of Physics, CLAUDIA PANTALEI, Ecole Normale Superieure — Small-angle neutron scattering (SANS) was used to study the isotopic distribution of liquid helium mixtures confined in MCM- 41, a silica glass with a 2D hexagonal net of monodisperse cylindrical pores, as a function of filling and He^3 concentration. The ordered pore array of MCM-41 gives rise to Bragg reflections with intensities determined by both how the liquid fills the pores and how the isotopes are distributed within the pores. The modulation in peak intensity can be modeled by writing down a form factors for cylindrical objects with varying scattering length density. Comparison will be made with small-angle X-ray (SAXS) scattering measurements performed with synchrotron light on liquid helium mixtures confined in aerogel.

[1]This work was supported by award 70NANB5H1163 from NIST, U.S. DOC. This Research at Oak Ridge National Laboratory's High Flux Isotope was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U. S. Department of Energy.

1:15PM Z33.00011 Deep Inelastic Neutron Scattering Study of Nanoconfined Liquid Helium Mixtures[1] , PAUL SOKOL, TIMOTHY PRISK, NARAYAN DAS, Indiana University Department of Physics — The single-particle momentum distribution $n(p)$ plays a central role in the contemporary understanding of quantum many- body systems, especially the helium liquids. The superfluid behavior of liquid He^4 below the famous lambda-point temperature is associated with the Bose condensation of a macroscopic fraction of the He^4 atoms to the zero momentum state. This manifests itself in $n(p)$ as a δ-function singularity at $p = 0$. Similarly, the Fermi liquid character of He^3 is associated with a sharp discontinuity in the Fermi surface at the Fermi momentum p_F. Using the Wide Angular Chopper Spectrometer at the Spallation Neutron Source, we recently carried out a deep inelastic neutrons scattering study of dilute He^3 + He^4 solutions confined in mesoporous MCM-41 in order to investigate the effects of confinement on the non-classical momentum distribution of an isotopic helium solution. The Bose condensate fraction, Fermi surface, average isotopic kinetic energies, and related work in the literature will be discussed.

[1]This work was supported by award 70NANB5H1163 from NIST, U.S. DOC. This research at ORNL's Spallation Neutron Source was sponsored by Scientific User Facilities Division, Office of Basic Science, U.S. DOE.

1:27PM Z33.00012 A Luttinger liquid core inside helium-4 filled nanopores , ADRIAN DEL MAESTRO, Johns Hopkins University — We study the effects of confining helium-4 at low temperatures inside long narrow pores with nanometer radii using worm algorithm path integral quantum Monte Carlo. The results show that even in the phase with a finite superfluid response, the interaction between helium atoms and the surface of the pore induces radial density oscillations which decay as the center of the pore is approached. For some special radii, an "inner tube" of helium atoms exists, and a careful scaling analysis confirms that it behaves like a one dimensional Luttinger liquid at low energies.

1:39PM Z33.00013 ^{4}He Adsorption on a Single Graphene Sheet: Path-integral Monte Carlo Study , YONGKYUNG KWON, School of Physics, Konkuk University, DAVID CEPERLEY, Dept. of Physics, U. of Illinois at Urbana-Champaign — We have performed path-integral Monte Carlo calculations to study ^{4}He adsorption on a single graphene sheet, where the ^{4}He-substrate interaction is described by the sum of the helium-carbon pair potentials. Among those proposed to account for helium scattering data on the graphite surface, we employ three different types of the inter-atomic pair potentials; a spherical 6-12 potential, an anisotropic 6-12 potential, and an anisotropic Yukawa-6 potential. Regardless of the choice of the pair potential, a first ^{4}He monolayer is found to show the $C_{1/3}$ commensurate structure at a surface density of 0.0636 Å^{-2} and to go through the domain wall phases for densities above the commensurate one before crystallizing into an incommensurate triangular solid. Below the commensurate density, however, the low-temperature phase of this helium adlayer varies depending on the choice of the ^{4}He-substrate interaction. The calculation based on the spherical pair potentials suggests a superfluid liquid phase at lower densities while incorporation of anisotropy into the helium-carbon pair potential results in a low-density state of a solid with clustered vacancies. Finally we observe van der Waals correlation between the upper monolayer and the one below the graphene sheet. The effects of this interlayer correlation on a possible formation of stable vacancies will be discussed.

1:51PM Z33.00014 Commensurate-Incommensurate Transition in ^{4}He Monolayer Adsorbed on a C_{60} Molecule , HYEONDEOK SHIN, YONGKYUNG KWON, School of Physics, Konkuk University — Path-integral Monte Carlo calculations have been performed to study adsorption of ^{4}He on a single C_{60} fullerene molecule. In order to account for helium corrugations on the molecular surface, the sum of all interatomic pair potentials between a carbon atom and a ^{4}He atom is used for the ^{4}He-C_{60} interaction. The radial density distributions reveal a layer-by-layer growth of ^{4}He with the first adlayer being located at a distance of $\sim$ 6.2 $\mathring{A}$ from the center of a C_{60} molecule. This first layer is found to exhibit various quantum states as the number of adsorbed ^{4}He atoms N varies. For N=32 the helium layer shows a commensurate solid structure with twenty helium atoms being localized on the tops of the hexagon centers of the C_{60} surface and the other twelve atoms above the pentagon centers. As more ^{4}He atoms are added, a commensurate-incommensurate transition is observed. After going through various domain wall states the first layer is crystallized into an incommensurate solid for $N \sim 52$. We find that solid states observed for N=32,44, and 48 do not show any superfluid response even below 0.2 K while domain-wall fluids formed with 45 to 47 ^{4}He atoms show significant superfluid fractions below 0.6 K. Finally different quantum states oberseved in the first ^{4}He layer around a C_{60} are compared with phase diagrams determined for the helium monolayer on a graphite surface.

Friday, March 25, 2011 11:15AM - 2:15PM –

Session Z35 DCMP: Insulators and Dielectrics II C140

11:15AM Z35.00001 Opacification of dielectrics oxides investigated by infrared emittance spectroscopy , MYRIAM ECKES, DOMINGOS DE SOUSA MENESES, MOHAMMED MALKI, PATRICK ECHEGUT, CEMHTI-CNRS, Universite d Orleans, Orleans, France — With increasing temperature, some compounds that are transparent in the near infrared range at room temperature become progressively opaque towards the liquid phase. Such a behavior deeply impacts their thermal radiative properties which knowledge is of main importance in crystal growth processes for example. To understand this phenomena, infrared emittance spectra were acquired from room temperature up to the liquid state on crystalline $LaAlO_3$ and $LiAlO_2$. The samples are heated with a CO_2 laser that allows a direct measurement of emittance up to their melting point and in a wide spectral range, i.e. between 50 and 10000 cm^{-1}. In the transparency region, we observed an increase of emittance up to 1000 K for $LaAlO_3$ (more than 1000 K before the solid to liquid transition) and no significant increase of emittance for $LiAlO_2$ before the solid to liquid phase transition. The experimental data have been fitted with a dielectric function model including a Debye relaxation term. The absorption mechanism at the origin of the opacification is thermally activated and has a relaxation time compatible with a motion due to electrons. Electrical conductivity measurements of these compounds were also made up to 800K.

11:27AM Z35.00002 Non-equilibrium ballistic phonon transport in microstructures , JARED HERTZBERG, OBAFEMI OTELAJA, RICHARD ROBINSON[1], Cornell University — We demonstrate a method to locally excite and detect phonon modes in silicon microstructures. Decay of quasiparticles injected into an adjacent superconducting film excites phonons in a non-thermal spectral distribution [1]. Phonons of frequency of order 100 GHz are detected by the excitations they cause in a second superconducting film, after ballistically traversing microstructures of 10 to 50 micron dimension. Measurements are made at temperatures of 0.3 to 1.2 K. Such a device advances the goal of building a nanoscale phonon spectrometer to study acoustic confinement and surface scattering effects. This work is supported by KAUST (KUS-C1-018-02), NSF (DMR 0520404), and DOE (DE-SC0001086).

[1] W. Eisenmenger, A. H. Dayem, Phys. Rev. Lett. 18, 125 (1967).

[1](corresponding author)

11:39AM Z35.00003 Dielectric measurements above 100 GHz using a high-Q open hemispherical resonator , REZWANUR RAHMAN, JOHN SCALES, Department of Physics, Colorado School of Mines — High-Q cavities can be used to study materials (or perturbations to materials) whose effects are too small to be seen by other methods. We have developed a millimeter wave cavity operating above 100 GHz in order to measure the dielectric properties of thin films and ultra low loss materials. The cavity is a open hemispherical resonator. Millimeter waves are introduced and measured via 2 closely spaced sub-wavelength holes in the center of a 15cm spherical, copper mirror. Cavity perturbation techniques are applied to extract the complex permittivity of a sample. This is a paraxial system and axissymmetric modes are of primary interest but nonaxisymmetric modes area also generated and need to be dealt with. Applications to thin films and other materials will be shown. This was was partially supported by US Department of Energy under grant DE-FG02-09ER16018

11:51AM Z35.00004 ABSTRACT WITHDRAWN –

12:03PM Z35.00005 Comparison between Resonant Inelastic X-Ray Scattering and the Dynamical Structure Factor , CHUNJING JIA, CHENG-CHIEN CHEN, BRIAN MORITZ, ADAM SORINI, THOMAS DEVEREAUX, Stanford/SLAC — Momentum dependent resonant inelastic X-ray scattering (RIXS) is an effective probe of many-body excitations. Theoretical and experimental work has shown that under certain circumstances RIXS can be viewed as an approximate probe of the dynamical structure factor $S(q,\omega)$. We perform cluster diagonalization combined with the bi-conjugate gradient stabilized method to model the RIXS spectra and $S(q,\omega)$ for the single-band and multi-orbital Hubbard models. While these two cross sections share some similar features, there are significant quantitative differences, which highlight the qualitative distinction between these two probes.

12:15PM Z35.00006 Observations of ferroelastic switching by Raman spectroscopy in 18-percent ceria-stabilized zirconia , AMY BOLON, Texas A&M University, JUAN MUNOZ SALDANA, Cinvestav-Quetetaro, MOLLY GENTLEMAN, Texas A&M University — Ferroelastic switching has been shown to be responsible for significant increases in the toughness of tetragonal zirconia ceramics. Observations of switching and measurements of coercive stress have generally been limited to TEM studies on large single crystals. In this study we show that it is possible to observe ferroelastic switching in 18 mole-percent ceria stabilized zirconia using polarized confocal Raman spectroscopy. Observations were made on bulk polycrystalline samples indented with a standard Vicker's indent and exhibited reorientation of crystal domains along the crack as well as near the crack tip. Coercive stress measurements were made by loading the samples uniaxially while making measurements of domain orientation.

12:27PM Z35.00007 Impact of Bond Coordination and Percolation on Mechanical Properties of a-SiC:H Thin Films

, SEAN KING, JEFF BIELEFELD, Intel Corporation, BRIAN DALY, Vassar College — Plasma Enhanced Chemically Vapor Deposited a-SiC:H thin films are compelling materials for both semiconductor nano-electronic and MEMS/NEMS technologies due to the extreme chemical inertness of this material and the ability to tune a variety of material properties across an extreme range of values. As one example of the latter, we demonstrate that using PECVD the Young's modulus of a-SiC:H thin films can be varied from $<$ 10 GPa to $>$ 200 GPa and the Hardness can be varied over an equally impressive range of $<$ 0.5 to $>$ 30 GPa. Utilizing Fourier Infrared-Transform Spectroscopy, we show that this remarkable range in materials properties is achieved primarily via the incorporation of terminal hydrogen groups which lowers the overall connectivity of the Si-C network bonding. We find that once the average network coordination number for Si and C falls below 2.6, the Si-C network becomes under constrained and there is a loss of rigidity percolating through the system. There results are compared and found to be in agreement with constraint theory for amorphous materials.

12:39PM Z35.00008 First Principles Investigation of Structure and Electronic Properties of $a-$ Si_3N_4

, RAVI PRAMOD VEDULA, NATHAN L. ANDERSON, ALEJANDRO STRACHAN, Purdue University — We use a combination of molecular dynamics with empirical inter-atomic potentials and density functional theory (DFT) calculations to generate an ensemble of statistically independent, well relaxed a-Si_3N_4 structures. Variations in the annealing conditions used to generate the structures lead to zero-stress structures spanning a wide range of densities (2.6g/cm^3 to 3.1g/cm^3) but exhibiting very similar cohesive energies. The bulk modulus was found to be varying between 110-180 GPa depending on the density. The predicted density variation agrees well with the range in experimentally observed density, resulting from different fabrication conditions. The radial distribution functions and angle distributions for different densities are in good agreement with diffraction experiments; further validating our models. The slow annealing procedure used to generate the structures leads to well equilibrated structures with relatively small density of coordination defects and several defect free structures. We also compute the formation energy and charge transition levels for the defects found.

12:51PM Z35.00009 Thermal transport and surface sensitivity in suspended amorphous silicon nitride thin films[1]

, R. SULTAN, A.D. AVERY, D. BASSETT, B.L. ZINK, University of Denver, Physics and Astronomy — Thermal transport in disordered materials continues to provide surprising new results, which often have direct consequences for applications ranging from quantum computation to cutting-edge cosmology. For example, some of the most sensitive detectors of radiation currently in use are thermal detectors that use highly sensitive micromachined thermometers to register the temperature rise caused by absorption of incident light or particles. To achieve this sensitivity, the thermometer is commonly thermally isolated using free-standing amorphous silicon-nitride membranes. As a result, the heat flow through this material is often a critical design parameter. In this talk we present recent measurements of thermal conductivity of a large number of suspended silicon-nitride structures. The results show not only deviation from previously reported measurements, but also very clear but somewhat puzzling dependence on the surface preparation of the structures. Such surface-sensitivity is expected at very low temperatures, but is seen in our experiments even near 300 Kelvin, where one normally expects heat flow to be dominated by carriers with very short mean-free-paths. We discuss possible interpretation of our results and compare to other recent surprises in the thermal properties of disordered materials.

[1]We acknowledge support of the NSF CAREER program and DOE-NNSA.

1:03PM Z35.00010 Accessing short and intermediate range orders of silicate glasses by infrared spectroscopy

, DOMINGOS DE SOUSA MENESES, Université d'Orléans, Polytech'Orléans, Avenue du Parc Floral, BP 6749, 45067 Orléans Cedex 2, France, CRISTIANE N. SANTOS, MYRIAM ECKES, CNRS, UPR3079 CEMHTI, 1D Avenue de la Recherche Scientifique, 45071 Orléans Cedex 2, France 2, YANN VAILLS, Université d'Orléans, Polytech'Orléans, Avenue du Parc Floral, BP 6749, 45067 Orléans Cedex 2, France, PATRICK ECHEGUT, CNRS, UPR3079 CEMHTI, 1D Avenue de la Recherche Scientifique, 45071 Orléans Cedex 2, France 2 — The characterization of short and intermediate range orders in glasses is a very active field since this knowledge is of main importance for understanding how order impacts their properties. The chemical simplicity of binary silicate glasses makes them model systems that are suitable to show how their dielectric functions include such kind of information. We show that it is possible to extract from infrared reflectivity measurements no solely quantitative information on short range order, i.e. populations of Q^n tetrahedral units (n : number of bridging oxygens) but also intermediate range information like the presence and evolution of 3D network silicate clusters and silicate sheet clusters. Examples will be given for alkaline silicates glasses and discussed in the light of predictions obtained from structural glass models and literature results.

1:15PM Z35.00011 In situ high-temperature infrared emissivity spectroscopy of silicate glasses and glass-ceramics[1]

, CRISTIANE N. SANTOS, DOMINGOS DE SOUSA MENESES, VALERIE MONTOUILLOUT, PATRICK ECHEGUT, CEMHTI - CNRS, Universite d Orleans, Orleans, France — Glasses and glass-ceramics are materials of widespread application in industry, building, photonics, microelectronics and medicine. Glass-ceramics are obtained by controlled glass crystallization, and many efforts have been done in the last years to better understand the structural changes occurring in this process. Here we show that in situ infrared emissivity spectroscopy is also a suitable technique for this purpose and a wide spectral and temperature range could be accessed (25-16000 cm^{-1} and 400-1700 K, respectively). We use a home-made instrument composed of two spectrometers, and a CO_2 laser for locally heat the glass samples up to the melt. A dielectric function model was applied to fit the experimental data and compute the materials optical properties. We show that using new decomposition procedure quantitative information on the distribution of the Q^n tetrahedral units (n being the number of bridging oxygen) can be obtained. The results at room temperature are in good agreement with recent molecular dynamics simulations. The major changes occur during quartz crystallization, with a remarkable increase of Q^4 units.

[1]Supported by ANR Postre

1:27PM Z35.00012 CrN electronic structure and vibrational modes: an optical analysis[1]

, XUNYUAN ZHANG, DANIEL GALL, Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, 110 8th ST, Troy, NY 12180 — The electronic structure of the paramagnetic insulating phase of CrN is investigated using optical spectra from epitaxial CrN(001) layers. The imaginary part of the dielectric function indicates direct interband transitions at $\hbar\omega$ = 0.64, 1.5 and 2.9 eV, and suggests a depletion in the density of states at the Fermi level. This is attributed to local magnetic moments that cause splitting of the t_{2g} bands and the formation of an indirect band gap of 0.19$\pm$0.46 eV, as estimated by comparing the optical transition energies with reported direct gap energies from calculations with different magnetic ordering and Coulomb interaction terms. The dielectric function shows a strong resonance at $\hbar\omega_0$ = 48.7$\pm$0.2 meV, and values of dielectric constants ε_{dc} = 53$\pm$5 and ε_∞ = 22$\pm$2, respectively, providing values for transverse and longitudinal optical phonon frequencies at the zone center of 11.7 and 18.2 THz, respectively. The vibrational frequencies are confirmed by Raman spectroscopy peaks at 800, 1170, and 1330 cm^{-1} which are attributed to 2TO(X), 2LO(X), and 2LO(L) modes.

X.Y. Zhang and D. Gall, *Phys. Rev. B* **82**, 045116 (2010).

[1]This research was supported by the National Science Foundation, under grant No. 0645312.

1:39PM Z35.00013 Surface states control and thermoelectric properties of CrN films , ANTIA S. BOTANA, ALBERTO PIÑEIRO, University Santiago de Compostela, VICTOR PARDO, University of California Davis, DANIEL BALDOMIR, University Santiago de Compostela — The manipulation of the electronic structure of a material by quantum confinement has attracted much attention recently, e.g. the appearance of conducting surface states or the novel phenomena at the interface between oxides being the most notorious. CrN is a degenerate semiconductor with large thermoelectric power in the bulk[1]. We have performed electronic structure calculations in thin CrN films and studied the evolution of the electronic structure and conduction properties (calculated using Boltzmann formalism) with thickness, focussing on the evolution of the Seebeck coefficient and electrical conductivity. We have utilized a density functional theory (LDA+U) formalism for our calculations with the U value (4 eV) that reproduces the experimental gap for the material as a bulk. When nanostructured, (almost conducting) surface states arise due to the dangling bonds at the surface that reduce the symmetry of the octahedral crystal field around Cr. When the film is relaxed, a gap opens and the material remains semiconducting. In addition, we have analyzed the role of these surface states in a possible improvement of the CrN thermoelectric properties by studying the figure of merit dependence with thickness.
[1] C. X. Quintela et al., Appl. Phys. Lett. 94, 152103 (2009).

1:51PM Z35.00014 Temperature Dependence of Internal Deformation Field in Zeolites[1] , WONSUK CHA, SANGHOON SONG, NAK CHEON JEONG, TUNG PHAM, Sogang University, Korea, ROSS HARDER, Advanced Photon Source, ANL, GANG XIONG, University College London, UK, KYUNG BYUNG YOON, Sogang University, Korea, IAN K. ROBINSON, University College London, UK, HYUNJUNG KIM, Sogang University, Korea — We studied temperature dependent internal deformation field distributions in zeolite microcrystals using coherent x-ray diffraction. We measured the coherent x-ray diffraction patterns around (200) and (020) Bragg peaks of the crystals. The three-dimensional real space images were obtained by phasing and inverting the oversampled diffraction patterns using the phase retrieval algorithm combined with error reduction and hybrid input-output method. The internal deformation fields show unusual temperature dependent behaviors which might be originated from the synthesis and calcination process.

[1]This work was supported by National Research Foundation of Korea (Nos. 2010-0000112 and R15-2008-006-01001-0), Seoul Research and Business Development Program (10816), and Sogang University Research Grant (2010).

2:03PM Z35.00015 Tension in the Initial Growth Stages of Sputter Deposited WSi_2 on Si in Multilayers[1] , ALBERT MACRANDER, Argonne, KIMBERLEY MACARTHUR, Argonne/NIU, BING SHI, Argonne, RAY CONLEY, ANL/BNL — We concentrate on the initial stages of growth of sputtered amorphous multilayers with equal WSi_2 and Si layer thicknesses of 5.5 nm, and we report observations of tension in the first 1.1 nm of WSi_2 grown on Si layers. Measurements of wafer curvature were made *in-situ* in the sputtering chamber. Stresses in the conjugate interface of Si on WSi_2 were observed to be significantly smaller. A clear asymmetry in the stress of these conjugate interfaces rules out an explanation based solely on lattice misfit. We find a value of 1.3×10^{10} dynes/cm^2 for the biaxial film stress at the WSi_2 on Si interface grown at 2.3 mTorr of Ar pressure, a value comparable to values calculated for hybridization of Si(111) facets by various adatoms [1]. Our observations thereby support a model for chemically induced changes in packing density during sputtering of the interfaces. As an example of a particular application, WSi_2/Si multilayers consisting of many hundreds periods have been used to make lenses for nanofocusing of hard x-rays [2-3].
[1] D. Vanderbilt, PRL 59, 1456 (1987). [2] H.C. Kang et al. PRL 96, 127401 (2006); APL 92, 221114 (2008). [4] L. Zhou et al. PRB 82, 075408 (2010).

[1]Supported DOE Office of Science, BES, No. DE-AC02-06CH11357.

Friday, March 25, 2011 11:15AM - 2:15PM –
Session Z39 DCP: Surfaces, Interfaces and Colloids A124/127

11:15AM Z39.00001 Two-dimensional soft solids: a rheological study[1] , GABRIEL ESPINOSA, Department of Physics, Simon Fraser University, Burnaby, BC, DUYANG ZANG, Laboratory of Materials Science in Space, Northwestern Polytechnical University, Xi-an, China, DOMINIQUE LANGEVIN, Laboratoire de Physique des Solides, Université Paris Sud, Orsay, France, BERNARD BINKS, Department of Chemistry, University of Hull, Hull, UK — Many soft solids, such as concentrated suspensions, emulsions, foams, behave in a similar way under an applied shear: they exhibit a Maxwell-type relaxation with a characteristic relaxation time that varies inversely with the applied shear rate. When the storage and loss moduli are measured at different frequencies and constant shear rate, the curves obtained can be rescaled [1]. We will show here that the behavior in two dimensions can be strikingly similar. We will present data on monolayers of nanoparticles and on mixed layers made with DNA and surfactant. The physical origin of the relaxation time will be discussed. The nonlinear behavior will be also discussed. Depending on the compaction degree, the layers can behave as brittle or plastic solids. This has been confirmed by images of the layers after a shear deformation made using Brewster angle microscopy.

[1] H. M. Wyss, K. Miyazaki, J. Mattsson, Z. Hu, D. R. Reichman, and D. A. Weitz, Phys. Rev. Lett. **98**, 238303 (2007).

[1]G.E. Acknowledge to Conacy for a doctoral fellowship.

11:27AM Z39.00002 ABSTRACT WITHDRAWN –

11:39AM Z39.00003 Direct measurement of short range colloidal interactions using digital holographic microscopy[1] , REBECCA W. PERRY, Harvard University, Sch. of Engineering and Applied Sciences, JEROME FUNG, DAVID M. KAZ, GUANGNAN MENG, Harvard University, Dept. of Physics, VINOTHAN N. MANOHARAN, Harvard University, Dept. of Physics and Sch. of Engineering and Applied Sciences — Using digital holographic microscopy, we record the 3D positions of micron-sized polystyrene particles as they approach and retreat from each other. Analysis of the holograms using an exact solution for the scattering from pairs of spheres allows us to separate vibrational, translational, and rotational motion. The vibrational mode supplies the information needed to characterize the inter-particle interactions down to separation distances on the order of 10 nm. In particular, we study an aqueous system of one micron diameter sulfate-coated polystyrene beads suspended in a solution of 95 nm hydrogel particles. The attractive depletion interaction we measure deviates from the Asakura-Oosawa model, likely because of electrostatic interactions at these short distances.

[1]We acknowledge support from NSF through grant no. CBET-0747625 and the NSF graduate research fellowship program.

11:51AM Z39.00004 Fabrication of Monolayer of Polymer/Colloids Hybrid at a Water-Air Interface , CHI-CHIH HO, TING-HUI CHEN, PO-YUAN CHEN, KENG-HUI LIN, WEN-TAU JUAN, WEI-LI LEE, Institute of Physics, Academia Sinica, INSTITUTE OF PHYSICS, ACADEMIA SINICA TEAM — Polymer-assisted assembly of polystyrene (PS) colloids with diameter ranging from 100 nm to 1 μm at water-air interface is demonstrated. Initially, PS colloids were slowly spread onto water surface and crystallized into triangular lattice with finite separation between colloids due to the coulomb repulsive force. By adding merely 1-3 ppm water-soluble polyethylene oxide (PEO) in water, the colloids gradually moved closer. Eventually, the separation between colloids was equal to or less than 60 nm determined from its diffraction pattern by a laser beam. In addition, the Brownian motion of colloids was suppressed by the PEO adsorption effect which was demonstrated from the analysis of colloids trajectory recorded by ultra high speed camera. We showed that the resulting monolayer of colloids /PEO hybrid can be deposited on various substrates, including a plastics sheet, curved surface and even across 10 μm-diameter hole. Our method may further extend the scope of nanosphere lithography technique for large area nanostructure fabrication.

12:03PM Z39.00005 Heterogeneous crystallization of hard-sphere colloids near a wall[1] , KYRIL SANDOMIRSKI, Heinrich-Heine-Universitaet Duesseldorf, IPkM, Universitaetstraße 1, D-40225 Duesseldorf, Germany, ELSHAD ALLAHYAROV[2], Physics Department, CWRU, Cleveland OH, USA, HARTMUT LÖWEN, Heinrich-Heine Universitaet Duesseldorf, Institut fuer Theoretische Physik II, Universitaetstraße 1, D-40225 Duesseldorf, Germany, STEFAN EGELHAAF, Heinrich-Heine-Universitaet Duesseldorf, IPkM, Universitaetstraße 1, D-40225 Duesseldorf, Germany — Confocal microscopy experiments and equilibrium Brownian Dynamics computer simulations were combined to investigate heterogeneous crystallization near a hard wall in a suspension of hard-sphere colloids. Particles near the wall initially rearrange, before an extended regime of steady-state crystal growth is observed. Finally, a depletion zone develops which slows down the progressing crystal-fluid interface. In good agreement between experiment and simulation, the steady-state growth velocity shows a maximum in its dependence on the bulk volume fraction. Beyond this, these techniques allow us to obtain local microscopic information on the level of individual particles, namely the temporal evolution of the density profiles in the fluid and crystal phase as well as the width of the interface.

[1]This work was supported by the DFG (SPP 1296). E.A. gratefully acknowledges support from a US DoE Grant (DE-FG02-05ER46244).
[2]also at OIVTRAN Moscow, Russia, and HHU Düsseldorf, Germany

12:15PM Z39.00006 ^{19}F NMR Study of Molecular Aggregation of Lithium Perfluorooctylsulfonate in Water at Temperatures from 30 to 250 $^\circ$C , DOBRIN BOSSEV, Indiana University, MUTSUO MATSUMOTO, MASARU NAKAHARA, Kyoto University — ^{19}F NMR chemical shifts have been measured to determine the critical micelle concentration (cmc) and aggregation number (m) of lithium perfluorooctylsulfonate (LiFOS) in water at temperatures ranging from 30 to 250 $^\circ$C under the saturation pressure. The cmc slightly increases in the temperature range from 30 to 100 $^\circ$C, whereas above 125 $^\circ$C the increase is much steeper; cmc is 6.5, 13.2, and 161 mmol kg^{-1} at 30, 100, and 250 $^\circ$C, respectively. The aggregation number, estimated on the basis of a mass action model exhibits a rapid decrease in the temperature range of 30 - 125 $^\circ$C and becomes almost constant at higher temperatures; m is 36, 6.8, and 2.4 at 30, 100, and 250 $^\circ$C, respectively. Thermodynamic parameters indicate similar values for the free energy at all temperatures, and constant values for the enthalpy and entropy of aggregation at high temperatures.

12:27PM Z39.00007 Dielectric dispersion of clustered living cells via the boundary integral equation method , SAI KIT YUNG, KIN LOK CHAN, KIN WAH YU, The Chinese University of Hong Kong — We have developed a boundary integral equation (BIE) method for computing the dielectric response of clusters of biological particles like living cells. In the BIE, we formulate a surface integral equation for the scalar potential for an arbitrary number of particles of various shapes [1]. BIE method avoids matching the complicated boundary conditions on the surfaces of the particles. Numerical solutions of the eigenvalue equation yield a dielectric dispersion spectrum through the spectral representation [2]. While BIE method is valid for arbitrary surfaces, we confirm it for two approaching cylinders and a concentric cylinder. In many typical cases, the numerical results are in excellent agreement with the exact analytic results. Moreover, BIE method offers a convenient way to compute the alternating current responses, and hence the dielectric dispersion of clustered cell suspensions.

[1] Yu KW, Wan JTK, Computer Physics Communications 142, 368 (2001).
[2] Huang JP, Yu KW, Phys. Rep. 431, 87 (2006).

12:39PM Z39.00008 Multi scale computer simulations of the self-assembly of block copolymeric beta-peptides , JAGANNATH MONDAL, ARUN YETHIRAJ, University of Wisconsin Madison — There is considerable interest in a class of molecules made from β-amino acids (which contain an additional backbone carbon atom when compared with natural amino acids). Block copolymers of β-peptides, where one block is hydrophobic and the other is hydrophilic, self-assemble into micelles. In this work we use computer simulations to provide insight into the self-assembly of these molecules. All-atom simulation results for the free energy of association of a pair of these block co polymeric β- peptides show that a $homochiral$ hydrophobic block promotes self assembly compared to a $heterochiral$ hydrophobic block, consistent with experiment. We have also developed a coarse-grained model for these block co-polymers and simulations using this model show that these molecules spontaneously forms micelles, and the morphology of these micelles is concentration dependent, with spherical micelles at low concentrations and worm-like micelles at high concentrations.

12:51PM Z39.00009 Ab initio Study of Structure and Hydrogen Bonding of Cellulose Crystals and Surfaces[1] , JAMES DAVENPORT, YAN LI, Brookhaven National Laboratory — We have studied the equilibrium structure and hydrogen bonding of cellulose crystals and surfaces using semi-empirical dispersion corrections to density functional theory (DFT+D)[1], which has been shown to be an efficient alternative to more advanced methods for weakly bound aromatic assemblies[2]. The predicted crystal structures for both I_α and I_β phases agree well with experiments. The cohesive energy was decomposed into interchain and intersheet interactions and analyzed in terms of hydrogen bonding and van der Waals dispersion forces. Both interactions were found to be responsible for holding cellulose sheets together. In particular, the dispersion corrections to DFT proved to be indispensable in reproducing the equilibrium intersheet distance and binding strength. Adsorption energy and configuration of water molecules on cellulose surfaces were found to depend sensitively on the surface orientation, adsorption site and contribution from vdW interactions.

[1] S. Grimme, J. Comput. Chem. 27, 1787 (2006).
[2] Y. Li, D. Lu, H-V. Nguyen and G. Galli, J. Phys. Chem. A 114, 1944 (2010).

[1]This work was funded by US Department of Energy under Contract No. DE-AC02-98CH10886.

1:03PM Z39.00010 Interfacial free energy and stiffness of the solid-melt interface of NaCl , TATYANA ZYKOVA-TIMAN, Chemistry Department, Cambridge Uni, ERIO TOSATTI, SISSA-ISAS, International School for Advanced Studies, DAAN FRENKEL, Chemistry Department, Cambridge Uni — The importance of the interfacial free energy for the equilibrium morphology of crystals is well understood. In contrast, much less is known about to the so-called "interfacial stiffness" that governs fluctuations of, e.g., solid-liquid interfaces. We carried out molecular dynamics simulations of capillary wave fluctuations on various faces of NaCl crystals in contact with its melt, that provides new information on the behaviour of this interface at the atomistic level. The capillary fluctuations connect directly with the interfacial stiffness, and indirectly also to the interface free energy. In our simulations we studied the (100)-liquid interface and adjacent vicinals. From the angular dependence of the surface stiffness, we deduce an estimate of NaCl(100)-melt interfacial free energy and discuss limitations of the fluctuation approach. Finally we compare this estimate of the surface free energy with values obtained through other methods [1,2,3] and discuss the differences [4].

[1] T. Zykova-Timan, D. Ceresoli, U. Tartaglino, and E. Tosatti, Phys. Rev. Lett. 94, 176105 (2005). [2] C.Valeriani, E. Sanz and D. Frenkel, J. Phys. Chem. ,122, 194501 (2005). [3] T. Zykova-Timan, C. Valeriani, E. Sanz, E. Tosatti and D. Frenkel, Phys. Rev. Lett., 100, 036103 (2008).

1:15PM Z39.00011 Utilization of Metal Oxides and Chalcogenides Stabilized in Organic Solvents , LESTER LAMPERT, ROBBY FLAIG, JORGE CAMACHO, JAMES HAMILTON, University of Wisconsin-Platteville — Metal oxides and metal chalcogenides are important materials for a variety of applications including photocatalysis for decomposition of water, conductive and optical coatings, catalysts, photovoltaics, pryoelectrics, self-cleaning surfaces, pigments, and high efficiency Li-insertion materials in batteries among many other applications. Fundamental discoveries of surprising solubility of insoluble materials such as single and multi-walled carbon nanotubes and graphene has lead us to discover that certain metal oxides and metal chalcogenides such as TiO2 are soluble in certain solvents. Due to the industrial importance of TiO2, discovering stable pure solvent systems demonstrates a possibility to avoid surface modification of TiO2 nanoparticles by use materials such as of (3-methacryloxypropyl)-trimethoxysilane and various other methods of artificial stabilization. We have created thin films of TiO2, transparent ultraviolet (UV) –absorptive polymers, and Li-ion battery anodes with graphene-TiO2 hybrid materials.

1:27PM Z39.00012 EPR, Endor and DFT Studies on X-Irradiated Single Crystals of L-Lysine HCl $2H_2O$ and L-Arginine HCl H_2O , YIYING ZHOU, WILLIAM H. NELSON — When proteins and DNA interact, arginine and lysine are the two amino acids most often in close contact with the DNA. In order to understand the radiation damage to DNA in vivo, which is always associated with protein, it is important to learn the radiation chemistry of arginine and lysine independently, and then complexed to DNA. This work studied X-irradiated single crystals of L-lysine·HCl·$2H_2O$ and L-arginine·HCl·H_2O with EPR, ENDOR techniques and DFT calculations. In both crystal types irradiated at 66K, the carboxyl anion radical and the decarboxylation radical were identified. Specifically, the calculations performed on the cluster models for the carboxyl anion radicals reproduced the proton transfers to the carboxyl group from the neighboring molecules through the hydrogen bonds. Moreover, computations supported the identification of one radical type within irradiated arginine as the guanidyl radical anion with an electron trapped by the guanidyl group. Based on the radicals detected in the crystal irradiated at 66K and at 298K, and the annealing experiments from the irradiation at 66K, the mechanisms of the irradiation damage on lysine and arginine were proposed, and the possible effects of irradiated arginine and lysine to the DNA within chromatin were analyzed.

1:39PM Z39.00013 Detection of Nitro aromatics via fluorescence quenching of pegylated and siloxanated 4, 8-dimethylcoumarins[1] , ABHISHEK KUMAR, MUKESH PANDEY, JAYANT KUMAR, University of Massachusetts Lowell — There is considerable interest in developing chemical sensors for detection of trace explosives. Optical sensors, which rely on the change in optical properties of the material, proved to be very effective. Therefore, there is a need to develop materials for optical sensors which can interact specifically with analytes and detect them sensitively. Here, we report the synthesis of co-polymers of 4, 8-dimethylcoumarins with poly (ethylene glycol) (PEG) and polydimethylsiloxane (PDMS) using *Candida Antarctica lipase* as a catalyst under solvent-less condition. The low T_g of PEG and PDMS may facilitate porous structure in solid films which allows quencher molecules to easily diffuse in and out of these films. In addition, the co-polymers prevent aggregation and lend themselves easily for thin film fabrication which otherwise is difficult because of low molecular weight of coumarin. Fluorescence quenching of these co-polymer in presence of nitro aromatics, 2,4-dinitrotoulne and 2,4,6-trinitrotoluene, in solution and in vapor phase will be reported.

[1]National Science Foundation

1:51PM Z39.00014 Correlated electrolyte solutions and ion-induced attractions between nanoparticles , JOS ZWANIKKEN, MONICA OLVERA DE LA CRUZ — Information about the degree of association can be obtained from a nonlinear Debye-Hueckel theory [1], in agreement with simulation and experimental results [2], in strong contrast with the widely applied (linear) Debye-Hueckel limiting law. The radial distribution functions calculated within this nonlinear theory are indistinguishable from molecular dynamics simulations of the restricted primitive model for divalent salts up to 0.1 molar concentrations. We apply the method to study the cohesive effects of strong couplings between ions on the effective interactions between nanoparticles, and the screening cloud around functionalized nanoparticles.

[1] J. W. Zwanikken, and M. Olvera de la Cruz, Phys. Rev. E 82, 050401(R) (2010).
[2] C. Valeriani, P. Camp, J. Zwanikken, R. van Roij, and M. Dijkstra, J. Phys.: Condens. Matter 22, 104122 (2010); Soft Matter 6, 2793 - 2800 (2010).

2:03PM Z39.00015 ABSTRACT WITHDRAWN –

Friday, March 25, 2011 11:15AM - 2:15PM –

Session Z40 DPOLY: Semi Crystalline Polymers: Morphology and Electronics A122/123

11:15AM Z40.00001 Structure Evolution of Propylene-1-Butylene Random Copolymer under Uniaxial Stretching: from Unit Cells to Lamellae[1] , YIMIN MAO, Chemistry Department, Stony Brook University, Stony Brook, NY 11794-3400, CHRISTIAN BURGER, XIAOWEI LI, BENJAMIN HSIAO — Crystallization changes of propylene-1-butylene (P-H) random copolymer with low butylene content (5.7 mol%) under uniaxial tensile deformation at high temperature (100 °C) was investigated using time-resolved wide- and small-angle X-ray scattering (WAXS/SAXS) techniques. Structure and preferred orientation at length scales of crystal unit cell and lamellae were investigated explicitly using 2D whole pattern analysis. γ-phase was found to be the dominant initial modification which was transformed into α-phase during stretching, forming more stable parallel packed polymer chains in the unit cell. 2D WAXS analysis enabled us to identify three orientation modes from different crystal forms, i.e., γ-phase with tilted cross-β configuration, α-phase with parallel chain packing and *a*-axis orientation of α-form crystals in daughter lamellae. 2D SAXS analysis based on stacking model enabled us to understand the development of the four-point pattern under deformation.

[1]We thank National Science Foundation for financial support and Derek W. Thurman and Andy H. Tsou from ExxonMobil company for providing copolymer samples.

11:27AM Z40.00002 An In-Situ X-ray Scattering Study during Uniaxial Stretching of Ionic liquid/Ultra-High Molecular Weight Polyethylene Blend

, XIAOWEI LI, YIMIN MAO, HONGYANG MA, BENJAMIN S. HSIAO, Stony Brook University — The 1-docosanyl-3-methylimidazolium bromide ionic liquid (IL) was incorporated into ultra-high molecular weight polyethylene (UHMWPE) to form IL/UHWMPE blend by solution mixing. The structure evolution of this blend system during uniaxial stretching was followed by in-situ synchrotron wide-angle X-ray diffraction (WAXD) and small-angle X-ray scattering (SAXS) techniques. During deformation at room temperature, the elongation-to-break ratio of the IL/UHMWPE blend increased by 2 - 3 times compared with pure UHMWPE sample, where the blend did not lose the tensile strength. Deformation-induced phase transformation from orthorhombic to monoclinic phase was observed in both blend and neat UHMWPE. During deformation at high temperature (120 °C), no phase transformation was observed in both samples. However, the blend showed better toughness, higher crystal orientation, and tilted lamellar structure at high strains.

11:39AM Z40.00003 Microscopic kinetic model for polymer crystal growth[1]

, WENBING HU, Department of Polymer Science and Engineering,Stat Key Lab of Coordination Chemistry, School of Chemistry and Chemical Enginnering, Nanjing University — Linear crystal growth rates characterize the net result of competition between growth and melting at the liquid-solid interfaces. The rate equation for polymer crystal growth can be derived with a barrier term for crystal growth and with a driving force term of excess lamellar thickness, provided that growth and melting share the same rate-determining steps at the growth front. Such an ansatz can be verified by the kinetic symmetry between growth and melting around the melting point of lamellar crystals, as made in our recent dynamic Monte Carlo simulations. The profile of the growth/melting front appears as wedge-shaped, with the free energy barrier for intramolecular secondary crystal nucleation at its top, and with the driving force gained via instant thickening at its bottom. Such a scenario explains unique phenomena on polymer crystal growth, such as chain folding, regime transitions, molecular segregation of polydisperse polymers, self-poisoning with integer-number chain-folding of short chains, and colligative growth rates of binary mixtures of two chain lengths.

[1]Financial support from NNSFC No. 20825415 and NBRPC No. 2011CB606100 is acknowledged.

11:51AM Z40.00004 Polyethylene crystallization in compatibilized polyethylene/polyamide 6 blends

, SIMONA CECCIA, CNRS/Rhodia UMR5268, St.Fons (France), KATERINA HYNSTOVA[1], Institute of Materials Science, Faculty of Chemistry, Brno University of Technology (Czech Republic), ALEXANDRA FABRE, LISE TROUILLET-FONTI, DIDIER LONG, PAUL SOTTA, 1CNRS/Rhodia UMR5268, St.Fons (France) — Blends of semicrystalline polymers can exhibit much better properties than each of the pure polymers regarding e.g. impact/modulus compromise. Controlling the crystallization mechanisms (nucleation, kinetics) is a key factor to obtain the desired morphologies which lead to these unique properties. We have studied the crystallization of polyethylene (PE) in blends of PE and polyamide 6 (PA) compatibilized by PE functionalized with maleic anhydride (PE-g-MA, 1 wt% MA) obtained by reactive blending. Samples with different amounts of PA6 (0-60 %vol) have been investigated by polarized optical microscopy and Differential Scanning Calorimetry. The samples were heated at a temperature above the melting temperature of PE and below the melting temperature of PA, and then cooled at the selected crystallization temperature. We describe how the crystallization kinetics is modified by the presence of PA and MA.

[1]2nd affiliation: CNRS/Rhodia UMR5268, St.Fons (France)

12:03PM Z40.00005 Kinetic Partitioning of 1-Butene Defect in Random Propylene 1-Butene Copolymers by Time-Resolved FTIR

, CAROLINA RUIZ-ORTA, RUFINA G. ALAMO[1], FAMU-FSU College of Engineering Chemical and Biomedical Engineering Department, 2525 Pottsdamer St., Tallahassee, FL 32310 — Two different types of regularity bands are identified in a time-resolved FTIR crystallization of a series of random isotactic propylene 1-butene copolymers with a concentration of 1-butene from 2 to 19 mol%. The first type are bands associated with 31 helices of isotactic sequences of different n length (n, number of monomer units). The second are regularity bands at 830, 920, 1010 and 1240 cm-1 associated with continuous sequences of the chain that include the 1-butene comonomer. Conformational changes during the isothermal crystallization process were monitored with these regularity bands. The variation of the intensity of regularity band at 920 cm-1 with crystallinity content and a shift of the 841 cm-1 ($n = 12$) at lower frequencies correlate with the content of comonomer included in the crystal. Changes in frequency of the $n = 12$ band with varying crystallization temperature (Tc), and with crystallization time at a fixed Tc are associated with the kinetic partitioning of the comonomer units, that was quantified with data obtained from 13C NMR. The frequency shift is absent in copolymers with co-units that are excluded from the crystalline regions, such as the 1-octene comonomer.

[1]corresponding author

12:15PM Z40.00006 Homogeneous bulk, surface, and edge nucleation in crystalline nanodroplets

, JESSICA L. CARVALHO, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, L8S 4M1 — We present a study on the homogeneous nucleation of dewetted poly(ethylene oxide) droplets on a substrate that is itself crystallisable. While the chemical properties of the substrate prepared in either the amorphous or crystalline state are identical, the surface landscape varies widely. We observe a large difference in the substrate's nucleating ability depending on how it is prepared. Furthermore, the scaling dependence of the nucleation rate on the size of the droplets depends on the substrate surface properties. The birth of the crystalline state can be directed to originate predominantly within the bulk, at the substrate surface or at the droplet's edge depending on how we tune the substrate.

J.L. Carvalho and K. Dalnoki-Veress, Phys. Rev. Lett in press, 2010.

12:27PM Z40.00007 Molecular simulation of homogeneous crystal nucleation of n-alkane melts

, PENG YI, GREGORY RUTLEDGE, Massachusetts Institute of Technology — One of the most important phenomena in molecular systems is homogeneous nucleation of the crystal phase from a melt. This phenomenon is particularly interesting for chain molecules due to their strong anisotropy and their conformational flexibility. In this work we report the results of molecular simulations of homogeneous crystal nucleation of n-eicosane (C20) from the melt. A realistic united atom force field was employed. The crystal phase and melting behavior were first determined by ramping temperature in a set of MD simulations. The nucleation trajectory was then sampled using MD simulations at about 20% supercooling; and the nucleation free energy was sampled using Monte Carlo umbrella sampling method for three temperatures, ranging from 10% to 20% supercooling. A first-passage time technique was used to determine the critical nucleus and the nucleation rate. Detailed examination of the simulations reveals the critical nucleus to be a bundle of stretched segments about 8 CH2 groups long, organized into a cylindrical shape. The remaining CH2 groups form a disordered interfacial layer. By fitting the nucleation free energy curve to the cylindrical nucleus model, the crystal-melt interfacial free energies are calculated to be about 10 mJ/m2 for the side surface and 4 mJ/m2 for the end surface. We also discussed the effect of using different nucleus definitions

12:39PM Z40.00008 Hierarchal Ordered Structures in Hybrid Functional Supramolecules and Macromolecules[1] , STEPHEN CHENG, WEN-BIN ZHANG, CHIEN-LUNG WANG, XINFEI YU, YIWEN LI, XUEHUI DONG, RYAN VAN HORN — To create new functional materials for advanced technologies, control over their hierarchical structure and order is vital for obtaining the desired properties. We utilized and functionalized fullerene (C_{60}) and polyhedral oligomeric silsesquioxane (POSS), and assembled both of these particles with polymers to form those hierarchical structures. In order to do so, we have developed a novel way of attaching C_{60} and POSS onto other organic materials in a highly efficient and controlled manner via "click" chemistry. The structure of this assembly along with the resulting ordered structures were analyzed to determine their structure-property relationships. Examples are materials of POSS-[60]Fullerenoacetate conjugate crystals, giant surfactant of polystyrene-(carboxylic acid-functionalized polyhedral oligomeric silsesquioxane) amphiphile and porphyrin-C_{60} hybrids for intra- and inter-columnar in supramolecular double cable structures.

[1]This work was supported by NSF (DMR-0516602 and DMR-0906898).

12:51PM Z40.00009 Nanoconfined Ferroelectricity in Polymers[1] , LEI ZHU, Department of Macromolecular Science and Engineering, Case Western Reserve University, FANGXIAO GUAN, JING WANG, Polymer Program, Institute of Materials Science and Department of Chemical, Materials and Biomolecular Engineering, University of Connecticut, QING WANG, Department of Materials Science and Engineering, Pennsylvania State University — In this presentation, a low loss polystyrene (PS) was grafted as side chains onto the P(VDF-CTFE) main chain. After PVDF crystallization, dielectric PS side chains were segregated to the crystalline-amorphous interface, forming a finite confinement layer for ferroelectric PVDF crystals. We speculated that less space charge was induced during electric poling because of the nanoscale confinement effect. Consequently, a fast discharge speed, relatively high energy density, and low losses were achieved.

[1]This work is supported by ONR (N00014-05-1-0338) and NSF (DMR-0907580).

1:03PM Z40.00010 Quantifying the rapid dynamics of polyelectrochromic switching in polymer acid-doped polyaniline , JACOB TARVER, YUEH-LIN LOO, Department of Chemical and Biological Engineering, Princeton University — Films cast from particles comprising polyaniline template synthesized on poly(2-acrylamido-2-methyl-1-propanesulfonic acid) exhibit polyelectrochromism and possess superior switching times ($<$10 s) and enhanced stability relative to other polymer acid-doped polyaniline systems. Solvent annealing in dichloroacetic acid induces polymer chain relaxation and further improves the speed ($\sim$1 s) and stability of electrochromic cycling. Electrochromic responses before and after solvent annealing can be described by Avrami kinetics that capture the influence of the film's mesoscale structural development and reveal variations in the dimensionality of reaction fronts when switching between the insulating and conducting states. Transitions from the conductive state are best fit by an Avrami exponent of 1.5 and are consistent with a reaction homogenously initiated throughout the film. Transitions to the conductive state require fits with exponents $\geq$2, suggesting nucleation and auto-accelerated propagation of conductive pathways away from the film/electrode interface in a manner analogous to polymer crystallization.

1:15PM Z40.00011 Enhanced RF Heating of Poly(N-Isopropylacrylamide) Gels by Utilization of Multiferroic Nanoparticles , EZEKIEL WALKER, University of North Texas, YUKIKUNI AKISHIGE, Shimane University, JAMES ROBERST, TONG CAI, ZHIBING HU, ARUP NEOGI, University of North Texas — Poly(N-Isoproylacrylamide) polymer hydrogels possess the special property of a discontinuous volumetric phase transition. This phase transition can be induced by external stimuli such as temperature, light, electric or magnetic fields, PH, and others. Of great interest is the functionalization of the gels to external stimuli for faster and more uniform spatial response. An efficient route to functionalization, specifically for termperature and light, is to utilize nanoparticles with EM resonances in the polymer network. The nanoparticles would be distributed throughout the gels, and an EM source resonant with the nanoparticle-gel structure would be used to induce a hysteresis-like effect to heat the gels, thereby, electromagnetically controlling the phase of the gel. KF-$BaTiO_3$ and $BiFeO_3$ are two sets of promising multiferroic nanoparticles that have exhibited resonances in the GHz region. Here, we present our findings for the functionalization and enhancement of the gels for radio-frequency light using KF-$BaTiO_3$ and $BiFeO_3$.

1:27PM Z40.00012 Manipulating functional properties at the interface of composite organic semiconductors , PANAGIOTIS MANIADIS, TURAB LOOKMAN, AVADH SAXENA, DARYL SMITH, Los Alamos National Laboratory — The formation of interfaces between different conjugated polymers is very important for the function of organic solar cells and other organic semiconductor devices. We propose a mechanism to control the properties of these interfaces with the addition of specially designed macro-molecules, with functional units. We develop the framework, using self consistent field theory (SCF), to study the concentration and the correlation function related to these functional units. When the functional units include a dipole moment, the average dipole moment and the standard deviation is expressed as a function of the SCF propagators. For electrostatic dipoles we also calculate the electric field difference created by the dipoles, as well as the charge distribution.

1:39PM Z40.00013 The Role of Exciton Dynamics in Photorefractivity in Organic Semiconductors , MOHAMMAD SAMIULLAH, Truman State University — A theory of the photorefractive effect in organic photorefractive materials based on formation, diffusion and dissociation of excitons in organic polymer semiconductors will be presented. A comparison with experimental results shows that the exciton dynamics plays an important role in the creation of the space charge field, and should be considered when selecting candidates for photorefractivity in organic systems.

1:51PM Z40.00014 Smart lens made of dielectric elastomer: simulation study , HONG TANG, Temple University — Electroactive Polymers (EAPs) are polymers that exhibit a change in size or shape when stimulated by an electric field. The common applications of this type of material are in actuators and sensors. A typical characteristic property of an EAP is that they will undergo a large amount of deformation while sustaining large forces. It has been demonstrated that EAPs can exhibit a strain from 10% to 300%. A dielectric elastomer (DEA) is a compliant capacitor, where a passive elastomer film is sandwiched between two compliant electrodes. When a voltage is applied, the electrostatic pressure arising from the Coulomb forces acting between the electrodes, therefore the electrodes squeeze the elastomer film. Based on the finite element analysis, we simulated the deformation of a polymer lens made of transparent dielectric elastomer materials under an application of electric field, which is provided by the transparent thin metal layers coated on the upper and lower surfaces of the lens. The focus of the lens can be adjusted by the applied electric field strength. By designing the electrode configuration on the lens surfaces, one can achieve both the positive and negative adjustment for the focus length.

2:03PM Z40.00015 ABSTRACT WITHDRAWN –

Friday, March 25, 2011 11:15AM - 2:15PM –

Session Z42 DPOLY: Biopolymers: Molecules, Solutions, Networks, and Gels A302/303

11:15AM Z42.00001 How do polymers degrade? , SUPING LYU — Materials derived from agricultural products such as cellulose, starch, polylactide, etc. are more sustainable and environmentally benign than those derived from petroleum. However, applications of these polymers are limited by their processing properties, chemical and thermal stabilities. For example, polyethylene terephthalate fabrics last for many years under normal use conditions, but polylactide fabrics cannot due to chemical degradation. There are two primary mechanisms through which these polymers degrade: via hydrolysis and via oxidation. Both of these two mechanisms are related to combined factors such as monomer chemistry, chain configuration, chain mobility, crystallinity, and permeation to water and oxygen, and product geometry. In this talk, we will discuss how these materials degrade and how the degradation depends on these factors under application conditions. Both experimental studies and mathematical modeling will be presented.

11:51AM Z42.00002 Stretching semiflexible filaments with quenched disorder[1] , PANAYOTIS BENETATOS, EUGENE M. TERENTJEV, Cavendish Laboratory, University of Cambridge, UK — Many biopolymers, such as DNA, are characterized by sequence heterogeneity. At large scales, this heterogeneity may behave as a quenched random variable. We consider a wormlike chain with uncorrelated quenched disorder in its arc-length dependent spontaneous curvature. In the weakly bending approximation, we obtain analytic results for the elastic response to a stretching force applied at its end-points. We show that the effect of quenched disorder does not always reduce to a simple renormalization of the bending stiffness of the pure system. We also discuss a formally similar disordered system where a stretched wormlike chain is subject to random uncorrelated transverse forces.

[1] This work was supported by EPSRC via the TCM Programme Grant.

12:03PM Z42.00003 Chains Are More Flexible Under Tension[1] , ANDREY DOBRYNIN, JAN-MICHAEL CARRILLO, University of Connecticut, MICHAEL RUBINSTEIN, University of North Carolina — The mechanical response of networks, gels, and brush layers is a manifestation of the elastic properties of the individual macromolecules. The two main classes of models describing chain elasticity include the worm-like and freely jointed chain models. The selection between these two classes of models is based on the assumptions about chain flexibility. We are proposing a unified chain deformation model that describes the force deformation curve in terms of the chain bending constant, K, and bond length, b. This model demonstrates that the worm-like and freely jointed chain models correspond to two different regimes of polymer deformation, and the crossover between these two regimes depends on the chain bending rigidity and the magnitude of the applied force. Polymer chains with bending constant $K > 1$ behave as a worm-like chain under tension in the interval of the applied forces $f \leq KkT/b$ and as a freely jointed chain for $f \geq KkT/b$. (k is the Boltzmann constant and T is the absolute temperature.) The proposed crossover expression for chain deformation is in excellent agreement with the results of the molecular dynamics simulations of chain deformation and single molecule deformation experiments of biological and synthetic macromolecules.

[1]NSF: DMR-1004576, CHE-0911588, DMR-0907515, CBET-0609087

12:15PM Z42.00004 Statistical Mechanics of Helical Wormlike Model[1] , YA LIU, TONI PEREZ, WEI LI, JAMES GUNTON, Lehigh University, AMANDA GREEN, Bucknell University — The bending and torsional elasticities are crucial in determining the static and dynamic properties of biopolymers such as dsDNA and sickle hemoglobin. We investigate the statistical mechanics of stiff polymers described by the helical wormlike model. We provide a numerical method to solve the model using a transfer matrix formulation. The correlation functions have been calculated and display rich profiles which are sensitive to the combination of the temperature and the equilibrium torsion. The asymptotic behavior at low temperature has been investigated theoretically and the predictions fit the numerical results very well. Our analysis could be used to understand the statics of dsDNA and other chiral polymers.

[1]This work is supported by grants from the NSF and Mathers Foundation.

12:27PM Z42.00005 DNA walks one step at a time in electrophoresis , JUAN GUAN, BO WANG, STEVE GRANICK, U of Illinois-Urbana Champaign — Testing the classical view that in DNA gel electrophoresis, long polymer chains navigate through their gel environment via reptation, we reach a different conclusion: this driven motion proceeds by stick-slip. Our single-molecule experiments visualize fluorescent-labeled lambda-DNA, whose intramolecular conformations are resolved with 30 ms resolution using home-written software. Combining hundreds to thousands of trajectories under amplitudes of electric field ranging from zero to large, we quantify the full statistical distribution of motion with unprecedented statistics. Pauses are seen between steps of driven motion, probably reflecting that the chain is trapped inside the gel matrix. The pausing time is exponentially distributed and decreases with increasing electric field strength, suggesting that the jerky behavior is an activated process, facilitated by electric field. We propose a stretch-assisted mechanism: that the energy barrier to move through the gel environment is first overcome by a leading segment, the ensuing intramolecular stress from stretching causing lagging segments to recoil and follow along.

12:39PM Z42.00006 The effects of end-interactions on semiflexible polymers looping , JAEOH SHIN, WOKYUNG SUNG, Pohang University of Science and Technology — Biopolymer looping is a ubiquitous dynamic process that occurs in cell, such as gene regulation and protein folding. We study the dynamics of looping for a variety of chain contour and persistence lengths via simulation and analytical theory. To speed up the looping time in simulation, which is very long for the short, rigid chains, we use the path integral hyperdynamics method. We analyze the effects of static and hydrodynamic interactions between the end beads on the looping time.

12:51PM Z42.00007 Modeling of biomimetic peptoid polymers , DINA MIRIJANIAN, STEVE WHITELAM, Lawrence Berkeley National Laboratory — Peptoids are sequence-specific, oligo-N-substituted glycine polymers that can mimic the structural motifs and functionalities of proteins. Recently, novel sheet-like nanostructured materials have been self-assembled from peptoids under physiological conditions. These structures are biocompatible and may be selectively functionalized. We have constructed atomistic models of peptoids using high level ab initio calculations to guide the parameterization of a classical force field based on the CHARMM22 peptide force field. Atomistic molecular dynamics simulations show the accessible configurations of peptoids in water to be markedly different from those of peptides. We have also used our parameterized force field to study the molecular structure of peptoid sheet-like nanostructures.

1:03PM Z42.00008 Periciliary Layer as a Protective Barrier of Human Airways[1] , LIHENG CAI, BRIAN BUTTON, RICHARD BOUCHER, MICHAEL RUBINSTEIN, University of North Carolina at Chapel Hill — The human airway surface layer consists of an overlaying gel-like mucus layer and a lower periciliary layer (PCL) protecting epithelial surface from mucus and the pathogens it contains. We investigated the permeability of the PCL using polymers that can readily penetrate through mucus. We found that in dilute solutions dextran larger than ~30 nm are excluded from the PCL, whereas dextran smaller than that can penetrate the PCL. The penetration depth increases (distance of dextran from epithelial surface decreases) as the dextran size decreases. We also found that the PCL can be compressed by semidilute solutions of dextran larger than 50 nm with concentration above a certain value, at which the solution correlation length (osmotic pressure) is about 30 nm (300 Pa). Above this concentration the height of the PCL decreases with the increasing concentration (osmotic pressure). The dependence of the PCL height on correlation length for semidilute solutions that compresses it is similar to the dependence of distance from cell surface on dextran size for the case of the PCL penetration by smaller polymers from dilute solutions. Our results suggest that the PCL protects the airways by limiting the penetration of inhaled infectious particles.

[1]Supported by NSF CHE-0911588 and NIH 1-R01-HL077546-03A2.

1:15PM Z42.00009 Cellulose aerogel from ionic liquid solution dried by silylation , DMITRY REIN, YACHIN COHEN, Technion — Aerogels are a class of materials characterised by a highly porous structure with low solids content. There is much interest in cellulose aerogel (aerocellulose) as a biodegradable and sustainable material. Cellulose lyogel can be fabricated from its solution in ionic liquids (IL) by coagulation with a nonsolvent such as water. However, subsequent drying capillary forces in the gel pores that result in severe shrinkage and pore closure. The use of supercritical fluids for drying or freeze-drying entails high equipment and energy requirements. We describe the fabrication and structure of aerocellulose fabricated from IL solution with a simple novel drying process: Addition of a compatible reactive agent (trimethylchlorosilane) and its diffusion into the water-swollen cellulose hydrogel pores results in a reaction with water as well as the pore surface hydroxyl groups. The remaining hydrophobic compound (hexamethyldisiloxane-HMDS), which fills the initially hydrophilic cellulose hydrogel pores, has a low intrinsic surface tension in the pores allowing easy drying with minimal shrinkage. Furthermore it allows modification of the pore surface and even fabrication of cellulose-polysiloxane composites. Relations between aerocellolose processing conditions and the resulting structural features will be discussed.

1:27PM Z42.00010 Macroscopic structure and properties of aqueous methylcellulose gels , TIRTHA CHATTERJEE, ROLAND ADDEN, MEINOLF BRACKHAGEN, ALAN I. NAKATANI, DAVID REDWINE, ROBERT L. SAMMLER, The Dow Chemical Company, DPCE TEAM — Cold semi-dilute aqueous methylcellulose (MC) solutions are known to undergo thermoreversible gelation when warmed. Here, studies on two MC materials, which contrast in thermal gelation performance (gel temperature, hot gel modulus etc.) even though they were prepared with similar methyl ether substitution levels and molecular weight distributions are presented. Small-angle neutron scattering (SANS)* measurements reveal differences in their gel structures which presumably are relevant to their thermal gelation performances. MC gel with higher gel temperature and lower hot gel modulus contains a single temperature invariant characteristic length ($\sim$ 1000 Å). However, besides this length scale, an additional and distinct smaller structure is also observed for the material with the lower gel temperature and the higher hot gel modulus. Further, in this case, the characteristic length scale decreases as temperature rises where as, the other length scale (smaller in size) remain almost temperature-invariant. The smaller domain size of the gel structure leads to the higher hot gel modulus for these methylcellulose materials. *Performed at NG3 beamline, NCNR, NIST.

1:39PM Z42.00011 Responsive Gelation in Physical Double Network Hydrogels from Artificial Protein Polymers , B.D. OLSEN, M.J. GLASSMAN, MIT — Artificial protein polymers with responsively associating groups on two different length scales are engineered in order to form physical double networks with potential application as shear-thinning hydrogels that may be toughened after injection. Gel-forming molecules are prepared by conjugating poly(N-isopropylacrylamide) (PNIPAM) at both ends of an artificial protein polymer to form PNIPAM-protein-PNIPAM triblock copolymers. Aggregation of the polymer endblocks forms a longer length scale network, while associating coiled-coil groups within the protein midblock form a shorter length scale network. At low temperatures where the coiled-coil domains are physically crosslinked but the copolymer endblocks are soluble, the materials form soft shear-thinning hydrogels. Elevating the temperature results in self-assembly of the second network, as manifest by stiffening of the gels. The structure of the materials is characterized using light scattering, X-ray scattering, and microscopy. Kinetics of the second network formation are characterized by linear oscillatory shear rheology, and nonlinear rheology is used to characterize the effect of the second network on the yield stress in these gels.

1:51PM Z42.00012 Universality in Nonlinear Elasticity of Biological and Polymeric Networks and Gels[1] , JAN-MICHAEL CARRILLO, ANDREY DOBRYNIN, Department of Physics, University of Connecticut — Networks and gels are part of our everyday experience starting from automotive tires and rubber bands to biological tissues and cells. Biological and polymeric networks show remarkably high deformability at relatively small stresses and can sustain reversible deformations up to ten times of their initial size. A distinctive feature of these materials is highly nonlinear stress-strain curves leading to material hardening with increasing deformation. This differentiates networks and gels from conventional materials, such as metals and glasses, showing linear stress-strain relationship in the reversible deformation regime. Using theoretical analysis and molecular dynamics simulations we propose and test a model that describes nonlinear mechanical properties of a broad variety of biological and polymeric networks and gels by relating their macroscopic strain hardening behavior with molecular parameters of the network strands. This model provides a universal relationship between the strain-dependent network modulus and the network deformation and explains strain-hardening of natural rubber, synthetic polymeric networks, and biopolymer networks of actin, collagen, fibrin, vimentin and neurofilaments.

[1]NSF: DMR-1004576

2:03PM Z42.00013 Criticality and isostaticity in fiber networks[1] , XIAOMING MAO, OLAF STENULL, TOM C. LUBENSKY, University of Pennsylvania, CHASE P. BROEDERSZ, FRED C. MACKINTOSH, Vrije Universiteit — We investigated the elastic response of model semiflexible networks based on diluted periodic lattices, using a new effective medium theory and numerical simulations. In this model, central forces link nearest neighbor sites and bending forces link second neighbor sites along fibers. We found that by turning on fiber bending rigidity, the central force rigidity critical point became unstable, and the lattices lose rigidity at a lower threshold that is independent of fiber bending rigidity. We calculated scaling relations and exponents at both critical points. In addition to the bending and stretching dominated regimes, we identified a novel bend-stretch coupled regime in the vicinity of the central force critical point, in which the shear modulus exhibits a fractional power-law dependence on both the fiber bending and stretching rigidities.

[1]This work has been supported in part by NSF-DMR-0804900 and FOM/NWO.

Friday, March 25, 2011 11:15AM - 2:15PM –

Session Z43 DPOLY: Liquid Crystalline Order in Polymer and Complex Fluids A306/307

11:15AM Z43.00001 Nonlinear Dielectric Response of the Liquid Crystal 8CB near the phase transitions , HANNAH BUCHANAN, University of West Florida — The nonlinear dielectric response of the liquid crystal (LC) 8CB (4'-octyl-4-cyanobiphenyl) was measured near the smectic-nematic and nematic-isotropic phase transitions. The sample was filled in a commercially available LC capacitor cell of dimensions (1 cm $\times$ 1 cm $\times$ 9 μm). The cell was mounted in a temperature-controlled environment with a stability and resolution of 1 mK. The capacitance of the cell was measured at different temperatures in the range 25 – 45 $^\circ$C covering both phase transitions, and over a range of frequencies up to 100 kHz, and a signal level in the range of 0 – 5V, using a lock-in amplifier (SRS830) and LCR meter (Fluke PM6304). Nonlinear effects were observed in the capacitance even at a 200 mV signal level, and very large changes in the capacitance, both linear and nonlinear, were observed in the nematic phase, near each phase transition. *Undergraduate physics students **Recent physics graduates

11:27AM Z43.00002 A Novel Liquid Crystal Elastomer with Large Spontaneous Length Changes , PATRICIA CLADIS, ALCT, Inc., SIMON KRAUSE, YUSRIL YUSUF[1], Gadjah Mada University, Yogyakarta, 55281, Indonesia , SHOHEI HASHIMOTO[2], Kyushu University, Fukuoka 819-0395, Japan, LEONID FEL[3], Technion-IIT, 32000 Haifa, Israel, SHOICHI KAI[4], Kyushu University, Fukuoka 819-0395, Japan, HEINO FINKELMANN, Makromolekulare Chemie, Freiburg University, 79104 Freiburg, Germany — An order parameter describes an elastomer where a liquid crystal is cross linked at a temperature T_L far from its clearing temperature. At T_L, there is a first order constant density phase transition where the order parameter vanishes and the elastomer has cubic symmetry. Below T_L it is an icosahedral nematic and above a biaxial nematic. This theory quantitatively accounts for spontaneous shape change, nonlinear elasticity and gelation dynamics in a novel liquid crystal elastomer.

[1]Kyushu University, Fukuoka 819-0395, Japan
[2]Department of Applied Quantum Physics and Nuclear Engineering
[3]Department of Civil Engineering
[4]Graduate School of Systems Life Sciences

11:39AM Z43.00003 Magnetic field directed self-assembly of liquid crystalline block copolymers for membrane applications[1] , MANESH GOPINADHAN, PAWEL W. MAJEWSKI, CHINEDUM O. OSUJI, Yale University — The use of magnetic fields is presented as a facile approach to the control of long range order and alignment of block copolymers. Using SAXS we demonstrate the alignment of lamellar and hexagonally packed cylinder morphologies of a poly(ethylene oxide)-based LC diblock copolymer by slow cooling in the presence of the field through the order-disorder transition. Non-degenerate alignment of the lamellar system is enabled by sample rotation and alignment in the system is shown to be driven by the diamagnetic anisotropy of the LC mesogen, and not anisotropy resulting from crystallization of the PEO block. We consider the effects of lithium doping and field strength on the order-disorder transition of the system, and the effect of lithium content on the critical field required for attaining well aligned films. The controlled alignment of PEO channels over large areas offers a route to selective ion transport in solid state batteries.

[1]This work is funded by the NSF under DMR-0847534.

11:51AM Z43.00004 Temperature Dependent Self-Assembly of Side-Group Liquid Crystalline Block Copolymers in LC Solvent , PAUL PIROGOVSKY, ZULEIKHA KURJI, ROHAN HULE, JULIA KORNFIELD, California Institute of Technology — Side Group Liquid Crystalline Polymers (SGLCPs) take on anisotropic conformations in a small molecule LC solvent. This conformation is affected by both the temperature and the sense of attachment of the mesogenic side group (either parallel or perpendicular to the backbone). Covalently linking the SGLCP with a random coil (PS) block leads to a block copolymer that self assembles into anisotropic micelles. Transmission Electron Microscopy was used to view these micelles in real space and determine their size and structure. Small Angle Neutron Scattering (SANS) was performed on dilute (1 wt%) solutions of a series of SGLCPs (homopolymers and block copolymers with a range of polystyrene block lengths) dissolved in deuterated 5CB. A rubbed alignment layer and a magnetic field were used to break symmetry and allow the ordered structure to be seen. PS-b-SGLCP block copolymers were seen to form self-assembled structures that changed qualitatively with the changing PS block length and the temperature. Most intriguingly, several polymers exhibit mutually orthogonal anisotropies at different length scales.

12:03PM Z43.00005 In-Situ X-Ray Diffraction Study of the Elongation Behavior of a Main Chain Liquid Crystal Elastomer[1] , SONAL DEY, D.M. AGRA-KOOIJMAN, LEELA JOSHI, SATYENDRA KUMAR, Kent State University, WANTING REN, WHITNEY M. KLINE, ANSELM C. GRRIFIN, Georgia Institute of Technology — We studied the structural evolution of a main chain smectic elastomer under uniaxial stress and during strain recovery. At low strains, both the alkyl chains and the smectic layers are oriented on average parallel to the strain direction. At higher strains, the development of layer undulations is observed at ∼50% which gradually evolve into chevron-like smectic structures as revealed by the four diffuse spots in small angle x-ray diffraction patterns. This is accompanied with an enhancement of the smectic order as inferred from higher intensity of small angle peaks and larger orientational order parameter, S [for example, $S(20\%) = 0.33$; $S(110\%) = 0.86$]. During strain recovery, two relaxation rates of 6.5 min and 38.5 min are observed which are associated with relaxations of the mesogenic part and the elastomer network, respectively.

[1]Supported by the Office of Basic Energy Sciences, DOE grant DE-SC0001412 and by National Textile Center Award M04-GT21.

12:15PM Z43.00006 Evaporative Self-Assembly and Formation of the Lyotropic Liquid Crystalline Phase of Poly(3-hexyl thiophene)[1] , MIN SANG PARK, AVISHEK AIYAR, JUNG OK PARK, ELSA REICHMANIS, MOHAN SRINIVASARAO, Georgia Institute of Technology — In this study, we electrically and optically interrogated the evolution of the thin film structure in conjugated systems using poly(3-hexylthiphene) (P3HT) as a model semiconducting polymer. In an effort to understand the electrical properties of the conducting channel in terms of polymer chain orientation and relaxation in solution, we performed in-situ micro-Raman measurements using polarized incident light. We measured the extent of molecular chain alignment during the process of film formation and showed the existence of a lyotropic liquid crystal phase at the three-phase contact line. The variation of frequency dispersion and the shift of position for Raman active mode, combined with the structural anisotropy of P3HT films, suggest a phase transition to the lyotropic liquid crystalline phase. The orientational order of P3HT chains in the liquid crystalline phase was quantified as a function of evaporation time using solidified solvent, 1,3,5-triclorobenzene (1,3,5-TCB).

[1]This work was supported, in part, by the Office of Basic Energy Science, Department of Energy, Grant No. DESC0001412 and by an NSF, Grant No. DMR0706235.

12:27PM Z43.00007 Lyotropic nematic droplets of single-walled carbon nanotubes in super acids: equilibrium shape and dynamics , NATNAEL BEHABTU, BUDHADIPTA DAN, Rice University, LEE TAEWOO, IVAN SMALYUKH, University of Colorado , MATTEO PASQUALI, Rice University — The balance between surface tension, elastic energy and surface anchoring creates nematic droplets with elongated shape, called tactoids. Here we report equilibrium shape and coalescence dynamics of single-walled carbon nanotube (SWNT) nematic droplets in superacids. Surprisingly, we observe bipolar tactoids with uniform aspect ratio. The uniform aspect ratio is not expected based on theoretical arguments that indicated that aspect ratio should drop with domain volume. Bipolar order contrasts recent findings of uniform order in liquid crystalline tactoid droplets of aqueous SWNTs stabilized with bile salts. The coalescence dynamics is highly influenced by the drop elasticity. Coalescence pathways that lead to defect creation are not observed, unlike spherical nematic droplets. Instead coalescence proceeds by tangentially matching the nematic director of two drops.

12:39PM Z43.00008 The unique behavior of chiral templated polymers swollen with liquid crystals , MICHAEL MCCONNEY, JENNIFER HURTUBISE, VINCENT TONDIGLIA, TIMOTHY WHITE, TIMOTHY BUNNING, Materials and Manufacturing Directorate, Air Force Research Laboratory — Liquid crystals (LC) have the capability of impart a degree of order onto the molecular structure of polymers, essentially acting as "smart solvents." Furthermore, structured materials have the ability to force liquid crystals into structures that are far from the bulk LC structure. Our studies are aimed at exploring the interplay between LC templated polymers and polymer templated LCs. Specifically we investigated a unique swelling-deswelling phase transition involving an ordered liquid crystal solvent and a structured polymer. The polymer is formed through anisotropic photopolymerization of LC monomers in a chiral LC fluid, is only attached from one surface of a single cell, and only spans a fraction of the cell thickness. The details of the transition were studied with various techniques including DSC, confocal microscopy, polarized microscopy, and visible/near-IR spectrometry. The unusual thermally induced structural changes result in large changes to the reflection wavelength of the cholesteric LC cells.

12:51PM Z43.00009 The Shape of Structured Polymer Vesicles[1] , MARK BOWICK, Syracuse University, MIN-HUI LI, Institut Curie (Paris), HOMIN SHIN, UMass Amherst, XIANGJUN XING, Shanghai Jiao Tong University, ZHENWEI YAO, Syracuse University — Polymer vesicles are stable robust vesicles made from block copolymer amphiphiles. Recent progress in the chemical design of block copolymers has lead to the creation of a variety of polymer vesicles with varying internal structure, functionality and shape. By choosing suitable liquid-crystalline polymers for one of the copolymer components one can create vesicles with internal nematic or smectic order. This talk will address the possible shapes of these *structured* vesicles as well as their inherent topological defects.

[1]Supported by NSF grant DMR 0808812

1:03PM Z43.00010 Curvature-induced transitions in two-dimensional nematics , BADEL L. MBANGA, Department of Polymer Science and Engineering, University of Massachusetts, Amherst, Massachusetts 01003, USA, C.D. SANTANGELO, Department of Physics, University of Massachusetts, Amherst MA, 01003, G.M. GRASON, Department of Polymer Science and Engineering, University of Massachusetts, Amherst, Massachusetts 01003, USA — Anisotropic particles absorbed to a fluid interface are known to significantly alter the structure and mechanics of these surfaces, possibly even stabilizing surfaces of complex, bicontinuous topology, as in "bijels" formed from arrested spinodally- decomposing fluid mixtures. We study the intricate interplay between the morphology of these interfaces and the alignment of anisotropic elongated particles with nematic order. Here we present results from computer simulation of nematic order on hyperbolic surfaces using a model that accounts for the contribution of both the intrinsic and extrinsic curvatures to the energetics of topological defects defects.

1:15PM Z43.00011 Effect of chain stiffness on structural and thermodynamic properties of polymers , KIRAN KHANAL, JUTTA LUETTMER-STRATHMANN, Departments of Chemistry and Physics, The University of Akron — The stiffness of the chains affects many properties of polymers. We investigate structural and thermodynamic properties of a bond- fluctuation lattice model for semiflexible polymer chains. Monte Carlo simulations for polymer melts for a range of values of the bending penalty, density, and temperature show elongation of the polymer conformations with increasing chain stiffness but no transition to a nematic phase. Results for average bead-bead interaction energy and bending energy were studied separately and showed that the bending energy is almost independent of the filling fraction, suggesting that the stiffness of the chains can be treated as a single chain property. We calculated the bending energy from the partition function of a pair of neighboring bonds and find excellent agreement between theory and simulation. Equation of state properties of the lattice model were determined from insertion methods and thermodynamic integration. We develop a theoretical description of these properties and use it to determine model parameters for real polymer melts from a comparison with experimental data.

1:27PM Z43.00012 Symmetric reflection band broadening of weakly polymer stabilized cholesteric thin films using low DC electric fields , MADELINE DUNNING, CHRISTOPHER BAILEY, ANASTASIA VOEVODIN, VINCENT TONDIGLIA, LALGUDI NATARAJAN, TIMOTHY WHITE, TIMOTHY BUNNING — We report on a new, low field electro-optical effect in weakly polymer stabilized cholesteric liquid crystals with negative dielectric anisotropy. By applying low DC electric fields ($<3V/\mu m$), a symmetric broadening of the cholesteric reflection band can be seen, resulting in band width increases by factors of two or more. An intensive study of the various experimental parameters combined with numerical calculations of the transmission spectra, indicate that the polymer interacts with the electric fields resulting in an approximately constant pitch gradient across the cell thickness. Our results show that the maximum pitch distortions reach values of approximately 15% the zero voltage value for notches in the visible range (pitches of 300-400nm), but increase along with the pitch. Possible physical mechanisms will be explored and discussed that might explain this interesting electro-optical effect.

1:39PM Z43.00013 Structure of Rigid Hard-Ring Fluids , MARIAM NOURI, MARC ROBERT, Department of Chemical and Biomolecular Engineering, Rice University — Structure of fluids of molecules consisting of rigid rings of hard spheres is studied in two, quasi two, and three dimensions, using Monte Carlo computer simulations in the canonical ensemble. For rings of various size and for a wide range of densities, results are reported for the pair distribution function of the ring centers and for the pair distribution of the ring orientations. For dense fluids in two dimensions, a shoulder, precursor of the freezing transition, is observed in the second peak of the pair distribution function of the ring centers, as previously seen in the simple hard-sphere fluid. In quasi two dimensions, where the centers of the rings are confined to a plane but the rings themselves can wobble out of plane, a liquid crystalline nematic phase is observed at sufficiently high densities. Results are also presented for three dimensions.

1:51PM Z43.00014 Fast Off-Lattice Monte Carlo Simulations with a Novel Soft-Core Spherocylinder Model , JING ZONG, XINGHUA ZHANG, QIANG (DAVID) WANG, Colorado State University — Fast off-lattice Monte Carlo simulations with soft-core repulsive potentials that allow particle overlapping give orders of magnitude faster/better sampling of the configurational space than conventional molecular simulations with hard-core repulsions (such as in the Lennard-Jones potential).[1] Here we present our fast off-lattice Monte Carlo simulations on the structures and phase transitions of liquid crystals and rod-coil diblock copolymers based on a novel and computationally efficient anisotropic soft-core potential that gives exact treatment of the excluded-volume interactions between two spherocylinders (thus the orientational interaction between them favoring their parallel alignment). Our model further takes into account the degree of overlap of two spherocylinders, thus superior to other soft-core models that depend only on their shortest distance. It has great potential applications in the study of liquid crystals, block copolymers containing rod blocks, and liquid crystalline polymers.

[1] *Q. Wang and Y. Yin*, **J. Chem. Phys., 130**, 104903 (2009).

2:03PM Z43.00015 Solvent involved self-crystallization of C_{70} molecules into high definition cube microstructure[1] , CHIBEOM PARK, HEE CHEUL CHOI, Department of Chemistry and Division of Advanced Materials Science, Pohang University of Science and Technology (POSTECH) — C_{70} molecules dissolved in mesitylene (good solvent) are self-crystallized into cube shape microstructure by the addition of isopropyl alcohol (poor solvent). Through control experiments attempted with different types of alcohols as well as in the replacement of mesitylene with other similar solvents, such as toluene, m-xylene, and m-dichlorobenzene, it is confirmed that mesitylene plays a critical role to guide C_{70} molecules to form cube microcrystal with high definition edges and surfaces. Thermal gravimetric and crystallographic analyses show that the crystal structure is simple cubic whose unit cell is composed of one C_{70} and two mesitylene molecules. The photoluminescence intensity from C_{70} cube crystals are enormously increased compared to C_{70} powder. Such abnormal photoluminescence increase is mainly attributed to the high crystallinity of C_{70} cubes as confirmed by time-resolved photoluminescence lifetime measurements.

[1]C. Park, E. Yoon, M. Kawano, T. Joo, and H. C. Choi, Angew. Chem. Int. Ed. (to be published)

Friday, March 25, 2011 11:15AM - 1:51PM –

Session Z44 DMP DPOLY: Focus Session: Organic Electronics and Photonics – New Materials and Applications A309

11:15AM Z44.00001 Ambipolar Electric Double Layer Transistors Using Organic Single Crystals , TAISHI TAKENOBU, Waseda University, PRESTO, DI WEN, Waseda University, HIDEKAZU SHIMOTANI, The University of Tokyo, SHIMPEI ONO, CRIEPI, YOSHIHIRO IWASA, The University of Tokyo, CREST — Among organic devices, ambipolar transistors are very unique device, in which both electrons and holes are equally mobile and we are able to observe light emission through the recombination of them. Progress in the applications of such light-emitting transistors (LETs) based on organic single crystals has provided possibilities in developing organic laser. However, in these LETs, the current density is still low for lasing, and, therefore, a different device structure is necessary to overcome this issue. Here we show the first demonstration of organic ambipolar electric double layer transistors (EDLTs), in which the gate dielectric is not a conventional insulator but an electrolyte. The peculiar merit of EDLT is extremely high conductivity due to the huge capacitance of the EDL formed at the organic/electrolyte interfaces. Consequently, we can increase current density. In this study, we used rubrene single crystal and ion-gel as the active material and electrolyte, respectively. These present results will provide a prospect for further development in LET operation.

11:27AM Z44.00002 Refractive Indices of Specific Nonconjugated Conductive Polymers: Organic Nanometallic Systems , PRASHANT DUBEY, SAPANA SHRIVASTAVA, MRINAL THAKUR, Photonic Materials Research Laboratory, Auburn University, AL 36849 — Exceptionally large quadratic electro-optic effect and two-photon absorption coefficients have been recently reported for nonconjugated conductive polymers after doping. These polymers include: cis- and trans- polyisoprene, poly(β-pinene) and others. The large optical nonlinearities observed in these materials have been attributed to the nanometallic state with subnanometer dimensions that is formed upon doping and charge-transfer. Measurement and calculation of linear refractive indices of these novel nonlinear optical systems before and after doping are important. Linear absorption coefficients (UV-Visible) of trans-1,4-polyisoprene have been measured for different doping levels of iodine. Refractive indices have been calculated using Kramers-Kronig transformation of absorption data for different doping levels. Numerical integration using MATLAB software was used for these calculations. Refractive indices at specific wavelengths have been determined by measuring reflectivity at normal incidence. The calculated and measured values of refractive indices have been compared. Results on calculations and measurements on these novel systems will be discussed.

11:39AM Z44.00003 ABSTRACT WITHDRAWN –

11:51AM Z44.00004 Sub-diffraction limited features in three-dimensional photopatterned, two-photon excimer-forming fluorescent dye-doped films , CHRISTOPHER RYAN, BRENT VALLE, JOSEPH LOTT, JACK R. JOHNSON, JIE SHAN, KENNETH D. SINGER, Case Western Reserve University, CHRISTOPH WEDER, University of Fribourg, DAVID A. SCHIRALDI, Case Western Reserve University — 3D Photopatterning is a key process in optical data storage, photolithography and other applications. Two photon active systems are a popular choice to pattern in 3D. The main challenges pertain to the contrast and density of the patterned features. By making use of a thermal threshold process which induces dye deaggregation, high contrast features are written with diameters smaller than the system's diffraction limit. A polymer film was doped with a two photon active dye that possesses two distinct fluorescence states in its monomer and excimer phases. The film's phases are stable at room temperature, and have a threshold response to heating. By selective exposure to a pulsed 675 nm source, the film is photopatterned in 3D as the focused pulses are absorbed and thus anneal the sample. Because the change is physical rather than chemical, the mechanism is shown to be a threshold process. As a result, sub diffraction limit photopatterns are demonstrated in the medium.

12:03PM Z44.00005 Low threshold conjugated polymer lasers by intrinsically directed resonator design , ALEXANDER KUEHNE, DAVID WEITZ, Harvard University — Creation of laser cavities requires external imposition of an optical feedback system onto the gain medium. By contrast, we use functional conjugated polymers that can be chemically or physically patterned from within to form diffractive laser resonators. One realization is based on a chemically-modified polyfluorene, which can be patterned into distributed feedback (DFB) resonators of any desired grating period. A different route is by physically pattering conjugated polymers into sub-micrometer colloids via microfluidics. These systems can be tuned with respect to particle size and their arrangement in the resulting laser structure. We show random lasing for a photonic-glass, self-assembled from monodisperse conjugated polymer particles.

12:15PM Z44.00006 Effects of polar analytes on the transport properties of organic semiconductor field-effect chemical sensors , DAVIANNE DUARTE, Univeristy of Texas at Austin, BRIAN COBB, ANANTH DODABALAPUR, University of Texas at Austin — Chemical recognition or sensing in organic thin film transistors (TFTs) can be achieved by direct analyte interaction or the inclusion of specific receptor molecules added to the semiconducting surface. Overall, sensing is dependent on the interactions occurring between the molecule and the OTFT active region, which includes the semiconductor and semiconductor-insulator interface. The magnitude of the interaction will depend on the molecules polarizability and the partition function of the analyte vapor. We employ a range of analytes (cyclohexane, ethanol, and styrene) with different solvations parameters (polarizability/dipolarity levels) to gain more clarity on their effects of the charge transport properties in OTFTs. Receptors are used to understand in more detail the physical and chemical interactions, which contribute to the sensor response. The receptors themselves have diverse polarizability/dipolarity parameters, which produce varying sensing behaviors dependent on the solvation parameters of the analytes.

12:27PM Z44.00007 Chemical vapor sensors using a poly(triarylamine) semiconductor modified through incorporation of organic receptors[1] , BRIAN COBB, DAVIANNE DUARTE, ANANTH DODABALAPUR, University of Texas at Austin — A poly(triarylamine) (PTAA) semiconducting active layer has been employed in order to produce OFET chemical sensors displaying excellent stability in air, with minimal bias stress effects. We propose a "chemical fingerprint" sensing array comprised of a single base polymer (PTAA), with the selectivity of individual devices modified through the incorporation of a variety of small molecule receptors. This allows for consistent device operation and optimization of the array. The effect of various receptors will be discussed, and reported while sensing alcohol vapors. Different methodologies will be proposed for incorporation of receptors into the device, including incorporation into the PTAA film and separate deposition on top of the PTAA film. The relative merits of each approach will be discussed, including the effect on both threshold voltage and carrier mobility.

[1]PTAA material supplied by Merck.

12:39PM Z44.00008 Nonadiabatic exciton dynamics in conjugated polymers , ADAM WILLARD, University of Texas, Austin, PETER ROSSKY — The results of mixed quantum/classical simulations of the nonadiabatic excited state dynamics of sexithiophene and the C60-sexithiophene interface are presented. The model is capable of describing the photogeneration and subsequent time-evolution of excitons in conjugated polymers at model bulk heterojunction interfaces. The effect of chain length and electric field on exciton mobility is discussed for both single-chain and π-stacked sexithiophene oligomer. In addition the dynamics of exciton dissociation at the C60-sexithiophene interface are described.

12:51PM Z44.00009 ABSTRACT WITHDRAWN –

1:03PM Z44.00010 Solution Processable Organic Solar Cell Microarrays for Use in MEMS[1] , JENNIFER TRINH, Swarthmore College, JASON LEWIS, PATRICK TOGLIA, XIAOMEI JIANG, University of South Florida — We have developed an innovative way to fabricate organic solar arrays for application as DC power supplies in electrostatic MEMS devices. The generation 1 microarray consists of 20 small (1 mm^2) solar cells connected in series (total device area of 2.2 cm^2). The device uses an active layer of poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl-C61-butyric acid methyl ester ($PC_{61}BM$), which are mixed together (1:1 mass ratio) in appropriate solvent. We manipulated active layer nanomorphology by choice of solvents and annealing conditions. The optimized generation 1 device has an open-circuit voltage of 11.5V, short-circuit current density of 1 mA/cm^2, and a power conversion efficiency of 2% under simulated solar AM1.5 illumination. The generation 2 microarray has a new design with reduced series resistance and improved cell occupancy. The generation 2 arrays have demonstrated improved device efficiency and power output density. Detailed analysis of device physics in both generation microarrays will be presented. The procedure described has potential for producing microarrays as small as 0.01 mm^2.

[1]This work was supported by the NSF REU program (award No DMR-1004873). Authors at USF would like to thank New Energy Technology Inc. and Florida High Tech Corridor Matching Fund (FHT 09-18).

1:15PM Z44.00011 Synthesis and characterization of a new TPA-Thiophene based molecule for potential Organic PV applications , PRASHANT SARSWAT, University of Utah, Salt Lake City, Utah 84112, AMARCHAND SATHYAPALAN, MICHAEL FREE, University of Utah, Salt Lake City, Utah 84112 — Triphenylamine (TPA) containing molecules possess unique optical and photovoltaic properties. These molecules show very strong visible absorption due to unique electronic structure. Another class of molecules, thiophene derivatives and resulting polymers have higher hole mobility amongst other conjugate co-polymers. In view of these aspects, we have designed a new conjugated thiophene containing molecule with TPA. A solution processable technique is reported to synthesize this newly designed star shaped molecule with TPA derivative as its core and thiophene derivative as branches. The synthesized molecule is systematically characterized by studying Mass spectroscopy, Raman spectroscopy, UV-Vis spectroscopy, and cyclic voltammetry. This molecule shows solubility in various common organic solvents, broad absorption in spectral range of 300-650 nm, and good thermal stability. An atomistic simulations based on density functional theory was carried out to validate HOMO and LUMO levels. The cyclic voltammetry analysis is consistent with atomistic simulation results. A 3D simulated orbital image reveals that the HOMO level corresponds to oxygen as well as carbon in a benzene ring.

1:27PM Z44.00012 Quadratic Electro-optic Effect in the Nonconjugated Conductive Polymer Trans-1,4-polyisoprene Measured at 1.55 μm , SAPANA SHRIVASTAVA, MRINAL THAKUR, Photonic Mat. Res. Lab, Auburn University, AL 36849 — Quadratic electro-optic effect in the nonconjugated conductive polymer, iodine-doped trans-1,4-polyisoprene has been measured at a longer wavelength (1.55 μm) and x-ray diffraction of the polymer film has been studied. Optical absorption spectra of trans-1,4-polyisoprene (TPI) show two peaks after doping, one at 4.2eV (295 nm) due to radical cation and the other at 3.2eV (388 nm) due to charge-transfer from double to dopant. X-ray diffractometer scans show that the trans-1,4-polyisoprene film has γ-phase crystal structure. Upon doping intensities of two peaks were observed increase without significant changes in overall peak positions. Field induced birefringence technique has been used to measure quadratic electro optic effect at 1.55 μm (which is away from resonance) and an exceptionally large Kerr coefficient ($2.5x10^{-10}$ m/V^2) has been obtained. This large nonlinearity has been attributed to the subnanometer-size metallic quantum dot structure produced upon doping of this polymer.

1:39PM Z44.00013 Photo-active Silicon Containing Polymer Films; An Approach Towards All-Solution Processable Devices[1] , SCOTT LEFEVRE, XINXING LIU, LEONARD INTERRANTE, CHANG RYU, Rensselaer Polytechnic Institute — The continuous drive for smaller, cheaper electronic devices elucidates the necessity for the design and incorporation of materials with improved properties along with a greater ease of processability. Polycarbosilanes (PCSs) are a class of organic-inorganic hybrid materials which exhibit increased chemical and thermal stability, appreciable hydrophobicity, and significant mechanical robustness. Recently, we have developed UV-crosslinkable cyclolinear PCSs by the incorporation of aryl substituted disilacyclobutane (DSCB) rings into the backbone. This novel material exhibits a low dielectric constant (k), making it an attractive new material in the development of interlayer dielectrics. Preliminary data shows that there is a maximum UV-crosslinking depth of approximately 30 microns. Additionally we have successfully demonstrated the resist capabilities of this material by patterning micro-scale (about 10 microns) features with a surface roughness variation of approx. 1 percent. Finally, new approaches towards taking advantage of the reactivity of polysilanes and the effect of molecular weight and polydispersity will be discussed.

[1]NSF - CHE 0412198, DMR 0722563, MRI 0722563

Friday, March 25, 2011 11:15AM - 2:15PM –

Session Z45 DAMOP: Bose-Einstein Condensates, Matter Optics, and Atomic Interferometry

11:15AM Z45.00001 New Facility to Probe Physics With Degenerate Bose and Fermi Gas , SUBHADEEP DE, Joint Quantum Institute, National Institute of Standard and Technology and University of Maryland, MD, USA, DANIEL L. CAMPBELL TEAM, ABIGAIL R. PERRY TEAM, RYAN PRICE TEAM, IAN B. SPIELMAN TEAM — A new facility to produce dual species degenerate Bose and Fermi gas is under construction at JQI. This apparatus is designed to create degnerate mixtures of bosonic rubidium (^{87}Rb) and fermionic lithium (^{6}Li). A degenerate Bose-Fermi mixture supports many quantum phase transitions, giving an experimental platform to study many-body statics, dynamics, and perhaps precision measurements. High T_c superconductivity could be probed, where fermions are bound into Cooper pairs by boson mediated interactions. Dual species heteronuclear molecules with large permanent electric dipole moment may lead to a system for implementing quantum bits. A spin-polarized, non-interacting, degenerate ^{6}Li gas coupled to ^{87}Rb atoms in an optical lattice will give rise to a long range, spin-dependent interactions to realize quantum magnetism and potentially supersolidity. Far red-detuned lattices are far weaker, in recoil units, for Li as compared to Rb. So, in the Mott phase of Rb - one atom per lattice site - the three body recombination of Li-Li-Rb is greatly suppressed. Thus the wide ^{87}Rb-^{6}Li Fesbach resonance at 1.1 kG is expected to effectively control fermion mediated interactions.

11:27AM Z45.00002 Solitons and Breathers in Strongly Repulsive Bose-Einstein Condensates , WILLIAM REINHARDT, University of Washington, Seattle, INDUBALA SATIJA, George Mason University, BRYCE ROBBINS, Colorado School of Mines, CHARLES CLARK, Joint Quantum Insititue, National Insitute of Standard and Technology — Collisional dynamics of solitary matter waves of hard core bosons, consisting of dark and bright waves as well as supersonic periodic trains, reveals remarkable richness and coherence, with the phase of the condensate playing a key role. Depending upon the condensate density, we see two distinctive effects in the collision of these waves: intuitively expected repulsive collision due to hard core boson constraint and also collisions in which they "pass through" each other without distortion. In addition to confirming the soliton status of the solitary waves, our studies reveal a variety of multi-solitons including a family of breathers, that can be demonstrated in an optical lattice with appropriate phase imprinting.

11:39AM Z45.00003 Macroscopic two-state systems in trapped atomic condensates , DMITRY MOZYRSKY, DMITRY SOLENOV, Los Alamos National Laboratory — We consider a macroscopic two-sate system based on persistent current states of a Bose-Einstein condensate (BEC) of interacting neutral atoms confined in a ring with a weak Josephson link [1]. We demonstrate that macroscopic superpositions of different BEC flows are energetically favorable in this system. Moreover, a macroscopic two-state dynamics emerges in the low energy limit. We also investigate fundamental limitations due to the noise inherent to the interacting BEC of Josephson-ring geometry. We show that the coherent macroscopic dynamics is readily measurable for an experimentally accessible range of parameters.

[1] D. Solenov and D. Mozyrsky, arXiv:1009.1901 [cond-mat.quant-gas].

11:51AM Z45.00004 Analysis of a free oscillation atom interferometer , RUDRA KAFLE, Worcester Polytechnic Institute, DANA ANDERSON, JILA, NIST, and University of Colorado, Boulder, ALEX ZOZULYA, Worcester Polytechnic Institute — We analyze a Bose-Einstein condensate (BEC) - based free oscillation atom Michelson interferometer in a weakly confining harmonic magnetic trap. A BEC at the center of the trap is split into two harmonics by a laser standing wave. The harmonics move in opposite directions with equal speeds and return under the influence of the trapping potential at their classical turning points. The harmonics are allowed to pass through each other and a recombination pulse is applied when they overlap at the end of a cycle after their return at the second time. We derive an expression for the contrast of the interferometric fringes and obtain the fundamental limit of performance of the interferometer in the parameter space. The results are also compared and contrasted with the results of our previous work on a single- and double reflection atom Michelson interferometers.

12:03PM Z45.00005 Atomic population distribution in the output ports of a waveguide interferometer with optical splitting and recombination , EBUBECHUKWU ILO-OKEKE, ALEX ZOZULYA, Worcester Polytechnic Institute — Manipulation of atomic Bose-Einstein condensates (BECs) in an atom waveguide interferometer relies on the use of off-resonant laser pulses to split a cloud of BEC into two clouds that travel along different paths and are then recombined using the same laser pulses. During the evolution of the condensates, residual spatial-dependent phase is accumulated due to the confining potential and the inter-atomic interactions within the condensates. Additional phase is accumulated due to the mode-entangled state of the clouds after splitting that causes each atom in the condensate to evolve at a different rate. The recombination laser pulses are sensitive to these phases and the population of atoms in the atomic samples that emerge after recombination depends on them. We derive an expression for the probability density distribution of observing any number of atoms in the clouds after recombination and give a parameter space for optimum operation of the interferometer in the presence of phase due to mode-entangled state of BEC clouds and the residual spatial-dependent phase.

12:15PM Z45.00006 Momentum-space engineering of gaseous Bose-Einstein condensates[1] , BRANDON BENTON, JEFFREY HEWARD, Georgia Southern University, MARK EDWARDS, Georgia Southern University and NIST, CHARLES CLARK, NIST — We show how the momentum distribution of gaseous Bose–Einstein condensates can be shaped by applying a sequence of standing–wave laser pulses. We present a theory, whose validity was demonstrated in an earlier experiment,[2] of the effect of a two–pulse sequence on the condensate wavefunction in momentum space. We generalize the previous result to the case of N pulses having arbitrary pulse areas and separated by arbitrary time intervals and show how these parameters can be engineered to produce a desired final momentum distribution. We find that several momentum distributions, such as single–state distributions or a range of momentum states which are important in initial state selection in atom–interferometry applications, can be engineered with high fidelity with two or three pulses. We present several examples of such distributions and show how the fidelity improves as more pulses are added. We also give some ideas of how these momentum distributions can be applied to atom interferometry.

[1]Support provided by NSF grant number PHY-0758111.

[2]L. Deng, et al., PRL **83**, 5407 (1999)

12:27PM Z45.00007 Enhanced atom interferometry through quantum information science[1] , MARK EDWARDS, Georgia Southern University and NIST, BRANDON BENTON, MICHAEL KRYGIER, Georgia Southern University, CHARLES W. CLARK, Joint Quantum Institute — New designs for atom interferometers can be inspired by quantum information science (QIS). QIS–inspired atom interferometer (AI) designs have the potential for producing AIs with enhanced sensitivity and robustness. We compare the sensitivity of a standard Mach–Zehnder (M–Z) Bragg AI with an AI whose design is based on the idea of decoherence–free subspaces (DFS).[2] We studied the performance of both atom interferometers using an enhanced version of a previously developed Bragg interferometer prototyping model.[3] This model approximates the effect on the condensate of multiple Bragg pulses separated by time delays using two elements: the effect of a single pulse and condensate evolution between pulses. The overall effect is rapidly approximated by following the steps of the interferometric process. We describe this model and then present the comparison of the performance of the M–Z interferometer with that of the DFS–inspired interferometer.

[1]Support provided by NSF grant number PHY-0758111.

[2]D.A. Pushin, M. Arif, and D.G. Cory, Phys.Rev. A **79**, 053635 (2009)

[3]S.E. Simsarian et al., Phys. Rev.Lett. **85**, 2040 (2000).

12:39PM Z45.00008 Eigenvalues of the linearized collision operator for a Bose-condensed gas , ERICH GUST, L.E. REICHL, University of Texas at Austin — Beginning from a Hamiltonian description, we have derived the kinetic equation for the elementary excitations of an interacting gas of bosons with and without a condensate. This kinetic equation is the quantum analog of the Boltzmann equation for a classical gas. Linearizing the kinetic equation about the equilibrium state allows us to treat it as a linear integral operator equation and find its eigenvalues. These eigenvalues give the rates at which different eigenmodes relax to equilibrium. They also provide a relationship between the microscopic properties of the interacting particles and the macroscopic properties of the gas.

12:51PM Z45.00009 Single-Particle Spectral Density of a Bose-Condensed Gas in the Two-Fluid Hydrodynamic Regime , EMIKO ARAHATA, NIKUNI TETSURO, Tokyo University of Science, ALLAN GRIFFIN, University of Toronto — In Bose supefluids, the single-particle Green's function can be directly related to the superfluid velocity-velocity correlation function in the hydrodynamic regime. An explicit expression for the single-particle spectral density was originally written down by Hohenberg and Martin in 1965, starting from the two-fluid equations for a superfluid. We give a new simple derivation of their results. Using these results, we calculate the relative weights of first and second sound modes in the single-particle spectral density as a function of temperature in a uniform Bose gas. We show that the second sound mode makes a dominant contribution to the single-particle spectrum in relatively high temperature region. We also discuss the possibility of experimental observation of the second sound mode In a Bose gas by photoemission spectroscopy.

1:03PM Z45.00010 A new self-consistent perturbation expansion for Bose-Einstein condensates satisfying conservation laws and Goldstone's theorem[1] , TAKAFUMI KITA, Department of Physics, Hokkaido University, Sapporo, Japan — Quantum-field-theoretic descriptions of Bose-Einstein condensates (BEC) have suffered from the lack of self-consistent approximation schemes satisfying Goldstone's theorem and dynamical conservation laws simultaneously. I will report on a new perturbation expansion of the kind developed recently and its predictions on the single-particle and two-particle excitations of BEC. It is shown that the single-particle Bogoliubov excitations are generally different from the two-particle density fluctuations in contradiction to the conclusion of previous studies. I will elucidate some properties of the two distinct modes in connection with Goldstone's theorem on spontaneously broken symmetries. References: T. Kita, Phys. Rev. B80, 214502 (2009); Phys. Rev. B81, 214513 (2010).

[1]Supported by Grant in a Grant-in-Aid for Scientific Research from the Ministry of Education, Culture, Sports, Science and Technology of Japan.

1:15PM Z45.00011 Hamiltonian monodromy in the spectrum and dynamics of a spin-1 Bose condensate , AUSTEN LAMACRAFT, University of Virginia — A spin-1 Bose condensate in a magnetic field in the single mode approximation – valid for sufficiently small condensates – represents a rather simple dynamical system. In this talk I will show that there is nevertheless scope for some rather unusual behavior. In particular, this system displays the phenomenon of *Hamiltonian monodromy*, a topological obstruction to the existence of global action-angle variables. I will discuss the signatures of this phenomenon in the classical dynamics and quantum spectrum

1:27PM Z45.00012 Ground States of a Mixture of Two Species of Spinor Bose Gases with Interspecies Spin Exchange , YU SHI, Fudan University — We consider a mixture of two species of spin-1 atoms with both interspecies and intraspecies spin exchanges, and find out the exact ground states in various parameter regimes. We describe the quantum phase diagrams in the space of parameters, including intraspecies and interspecies spin coupling strengths as well as the magnetic field. The boundaries where the ground states are either continuous or discontinuous are determined, with the latter identified as where quantum phase transitions take place. Interspecies spin exchange leads to features beyond the usual ones of a single species of spinor atoms.

1:39PM Z45.00013 Bound states of a localized magnetic impurity in a superfluid of paired ultracold fermions , DAVID PEKKER, Physics Department, Harvard University, Cambridge, Massachusetts 02138, USA, ERIC VERNIER, Departement de Physique, Ecole Normale Supe'rieure, Paris, France, MARTIN ZWIERLEIN, MIT-Harvard Center for Ultracold Atoms, Research Laboratory of Electronics, and Department of Physics, Cambridge, MA 02139, USA, EUGENE DEMLER, Physics Department, Harvard University, Cambridge, Massachusetts 02138, USA — The nature of states formed around localized impurities can be a valuable probe of the properties of a quantum many body system. We propose using a deep optical lattice to localize an impurity atoms. We show that such and impurity atom acts like a magnetic impurity and leads to the formation of a pair of Shiba bound states inside the superconducting gap as well as possible bound states below the Fermi. The properties of these localized bound states can be read out using RF spectroscopy.

1:51PM Z45.00014 Spectroscopy for cold atom gases in periodically modulated optical lattice potential[1] , AKIYUKI TOKUNO, THIERRY GIAMARCHI, DPMC-MaNEP, University of Geneva — Cold atoms in optical lattices are vigorously studied experimentally and theoretically as one of the candidates for a quantum simulator. At the same time, further development of probes to microscopic structure of systems is needed. We propose a novel spectroscopy in cold atom experiments by use of periodic phase-modulation of optical lattice potentials. Corresponding to the statistics of atoms, we formulate the different observables: The energy absorption rate for bosonic atom gases, and the doublon production rate for fermionic atom gases. These observables are formulated within the linear response theory. Interestingly they are given by the imaginary part of the retarded current-current correlation function which is familiar as a quantity corresponding to an optical conductivity. As an example, we discuss one-dimensional Mott insulating state, and also compare our spectroscopy with another known spectroscopy by amplitude-modulation of an optical lattice.

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2:03PM Z45.00015 Subwavelength localization of a single atom via resonance fluorescence photon statistics , M. AL-AMRI, The National Center for Mathematics and Physics, KACST, P.O. Box 6086, Riyadh 11442, Saudi Arabia, SHUAI YANG, M. SUHAIL ZUBAIRY, Institute for Quantum Studies and Department of Physics, Texas A&M University, College Station, Texas 77843, USA — A subwavelength localization scheme of a single atom is investigated. The localization is based on the interaction of the two-level atom with a standing wave laser field. The photon statistics of resonant fluorescence depends on the Rabi frequency of the driving laser field and thus the position of the atom inside the standing wave. We show that this dependence can be used to localize the atom to a subwavelength accuracy.